Call:
pca.xyz(xyz = xyz96, rm.gaps = TRUE)

Class:
pca

Number of eigenvalues:
1089

|    | Eigenvalue | Variance | Cumulative |
|----|------------|----------|------------|
| PC 1 | 1451.111  | 72.530 | 72.530     |
| PC 2 | 128.498   | 6.423  | 78.952     |
| PC 3 | 99.560    | 4.976  | 83.929     |
| PC 4 | 67.942    | 3.396  | 87.324     |
| PC 5 | 46.299    | 2.314  | 89.639     |
| PC 6 | 44.221    | 2.210  | 91.849     |

(Obtained from 96 conformers with 1089 xyz input values).

+ attr: L, U, z, au, sdev, mean, call

[,1] [,2] [,3] [,4] [,5] [,6]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
  -26.174766 -49.19484841 -13.655031  -8.4493930  1.6 48399e+00  -4.410633
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
  -7.137154 -43.56926318 -12.301589  15.2993715  1.29 1078e+01  10.959699
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
  -9.109342 -41.94685048   1.522348 -34.4764359 -1.99 3688e+01  11.397632
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-19.659492 -40.28741188 -26.246999  12.7487217  9.8 12384e+00 -12.332311
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
  52.364186 -7.89376335  10.282222   2.053072e+00 -9.113038
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-24.106361  0.62970302 -15.802666   7.3011151  1.205262e+01 -2.752951
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59f3306825e8.final.pdb
  51.814984  6.72738105 -4.898246  -3.8622086  1.459474e+00  3.485695
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0f06f3e342df706.final.pdb
-24.134824  1.31358996 -17.286999  12.7487217  9.8 12384e+00 -12.332311
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-40.739549  8.82544584 -2.865992  -4.7338000  1.223670e+00 -2.362576
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-32.050664 -9.71362521  13.466948  -5.339163  -5.491641e+00 -9.002533
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-40.739549  8.82544584 -2.865992  -4.7338000  1.223670e+00 -2.362576
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  52.299583  2.79894692 -4.531414  -3.1529005  4.29366e+00 -4.249328
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\14f35328d47579a.final.pdb
  52.342705 -0.62283021 -5.059441  -3.231690  -7.361823e+00 -8.448938
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\15f027089e2f4c42.final.pdb
Supplementary Text 10

52.532401  4.27560457  -4.147460  -2.9836572 -4.73 4571e+00  -5.132649
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb

-28.902894  -6.40891637  13.458951  -1.0404743  3.6 28293e+00   3.215256
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb

-28.505208  -3.41648142  13.458951  -1.0404743  3.6 28293e+00   3.215256
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-32.505208  -3.41648142  13.458951  -1.0404743  3.6 28293e+00   3.215256
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4fcb3b46e33793b0.final.pdb

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Supplementary Text 10

-38.545747 8.28082718 -3.047010 -4.7473510 4.85690e-01 -1.313072
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-31.978950 -9.55981126 13.234022 -0.4563775 -5.2 94403e+00 -8.794916
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51.814984 6.72738105 -4.898246 -3.8622086 1.459474e+00 3.485965
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Page 3
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-4.24262393 -0.6334991 -1.2152996 2.02246774 -0.18597880 -2.55500038
 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431 cf2dcb.final.pdb
-2.79492795 1.8929649 1.0360744 -1.41074777 -0.62236801 -2.16266062
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-0.53023594 -1.4549806 2.6204689 -0.03383169 -1.62484768 1.59986497
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0.76069826 -1.1874767 3.2907087 -1.6924185 -7.35444915
 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
|    | [13] | [14] | [15] | [16] | [17] | [18] |
|----|------|------|------|------|------|------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | 2.86301556 | -0.1152982 | 4.0142605 | -1.10186286 | 2.05229672 | 3.19795907 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 11.39867438 | -0.5557751 | -6.6070054 | -0.30822971 | 0.53455022 | -3.34364361 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dfd6a42fc83b81e5d.final.pdb | 0.48171388 | 0.5745522 | 3.3279979 | -2.73958005 | -1.14381389 | 2.12598443 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | -12.57544097 | 3.5180732 | -3.0000051 | 2.14175007 | 5.17018932 | -0.19038377 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ff3584e22003fb92.final.pdb | 5.90438095 | -0.8914895 | 2.4181353 | 0.20996334 | -0.93579462 | 0.46350045 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ff8e2bf87e52caa29.final.pdb | -3.64246511 | 0.7569109 | -0.6655648 | -1.08306161 | 0.47400424 | 0.63188736 |

Supplementary Text 10
Supplementary Text 10

-0.0538718 0.59886337 1.75160181 -0.291728471 -1.51760899 -1.43438685
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0.4425926 -0.71789746 1.360764591 -1.433499856 -0.3551152 -0.14573774
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9bbee0d5986c138f.final.pdb
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-2.0448768 -3.74324546 0.66987993 -0.8600025 -1.96871687
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d8ed0d81fb3ef.final.pdb
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1.8917372 0.57254799 0.39349573 0.235028651 -0.83870835 -0.14695232
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Supplementary Text 10

2.6584788 -1.37690172 -0.850635548 0.905999631 0.51461139 -0.19327067 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0089ef10197e2.final.pdb
-1.1211910 -2.07969992 0.97239744 -1.12836573 -0.84974698 -1.11357735 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
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-1.1211910 -2.07969992 0.97239744 -1.12836573 -0.84974698 -1.11357735 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
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0.4425926 -0.7189746 1.360764591 -1.433499856 -0.35551152 0.14573774 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
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-0.58333227 -0.503918047 0.12981843 0.7153943 0.55739007 0.8779495 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e87e52e5ca29.final.pdb
-0.45857575 0.13212917 0.76244480 -0.96786909 -0.32630889 -1.0676521 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e87e52e5ca29.final.pdb
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| 0.2656218  | -0.04369875 | 1.25306725  | 0.18226422  | 0.59200913 |
| 1.27618713  | -1.39479006 | -0.56114201 | 1.74926814  | -1.63033525 |
| -0.26952708 | -0.12941955 | -0.84304595 | 0.27823393  | -0.19175687 |
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| -0.53845283 | 0.45912899 | 1.29450413  | 0.55999388  | -0.18555675 |
| 1.02237924  | -0.69007963 | 0.19667356  | 1.00416199  | -0.11894334 |
| -2.8320636  | -0.30864934 | 0.88248263  | -2.23735474 | 0.46375092 |
| 1.57161979  | -1.17561603 | -1.60580142 | -0.76697249 | 0.60828768 |
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| 0.49933552  | -0.50080956 | -0.65639268 | -2.34158965 | 0.67063515 |
| 0.89754771  | -0.04888646 | -0.5058208 | 1.66707110 | 0.50545166 |
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| 0.03153472  | 2.73282968 | 1.61787709  | -0.14693852 | 0.24279792 |
| 0.12652708  | -0.12941558 | -0.84304595 | 0.27823393  | -0.19175687 |
| 0.53845283  | 0.45912899 | 1.29450413  | 0.55999388  | -0.18555675 |
| -0.0499054  | -0.01544457 | 1.14608230  | -0.57045518 | -0.35809338 |
| 0.89754771  | -0.04888646 | -0.5058208 | 1.66707110 | 0.50545166 |
| -1.34508556 | 1.71876044 | 0.09916984  | 0.25083801  | -0.41906234 |
| -3.40788283 | -0.98525429 | -1.58733255 | -1.01960593 | 0.81095448 |
Supplementary Text 10

0.09546248 -0.217308714 -0.43966791 0.72492675 0.02042816 0.46649639
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### Supplementary Text 10

-0.0420658372  1.29880465  0.9289769013 -1.93795818  38 -0.3531834654
-0.0590305111

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-0.1551056616

-0.2229452700

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3.056070e-02  -0.0107851303  -0.021762472  -0.00435167  22  -0.0149708196

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| Filename | Coordinates | E-value |
|----------|-------------------------------------------------|---------|
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | -3.596739e-01 0.2380306139 -0.256905209 -0.0631080 773 0.0231669889 | -0.2261852614 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -4.32551e-01 0.2989878653 -0.085435587 -0.081188132 -0.4501844166 | 0.1739432325 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 1.120095e-02 -0.0045575621 0.002264678 0.00058933 78 0.0012649480 | -0.0009000797 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -4.891594e-02 0.0016807755 -0.098870765 -0.1844624296 -0.1110341283 | 0.1951618187 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 4.814485e-03 0.0059751644 0.073232390 -0.0892305923 -0.4195897121 | 0.2252196079 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 1.785559e-01 -0.1323680454 0.011637613 0.0471524315 0.3591539005 | -0.0395904229 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 7.528551e-01 -0.1510428549 -0.34818892 0.7308065654 0.1291457432 | -0.0632712074 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7cf6f.final.pdb | 4.44949e-01 -0.0853088981 -0.39639547 -0.318865727 -0.4196857682 | 0.1701517329 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8c6dfb.final.pdb | -1.364778e-01 0.0529804545 0.011637613 0.0471524315 0.3591539005 | -0.0189304229 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 1.716963e-01 -0.1423533127 0.04639842 0.1012552430 0.1408583742 | -0.0911145381 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -1.666599e-01 0.1490016192 0.064800598 -0.0479441841 0.3177195100 | 0.4225144482 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 2.136364e-01 -0.2319125719 0.056312081 0.0950392225 0.0119706188 | 0.1045795936 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 2.592581e-01 -0.1932705827 -0.064109958 -0.1303596181 -0.3293296546 | 0.1229777036 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f404822d30a.final.pdb | 3.433465e-02 -0.1626528834 0.23006804 -0.0586260915 -0.0788512547 | 0.524444882 |

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Supplementary Text 10

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| ee6862cbcad52078.final.pdb           | 1.578975e-02           |
| ef6a42fc83b81e5d.final.pdb           | -1.590648e-01          |
| ef8e88d4ad93a0ad.final.pdb           | -0.0005236504          |
| f14fca8deec4fa3.final.pdb            | 0.0008844115           |
| f83584e22003fb92.final.pdb           | -0.0026782897          |
| f8e2bf87e52caa29.final.pdb           | 0.0008844115           |
| 013d855ad26c877d.final.pdb           | -0.0940224196          |
| 0a2a705342ca0d54.final.pdb           | 0.0008844115           |
| 0a59fcedb4194d9.final.pdb            | 0.0008844115           |
| 0bda59f3306825e8.final.pdb           | -0.0023513075          |
| 0c6f26a78b57339c.final.pdb           | 0.1309313075           |
| 0d0f6f3e342df7e0.final.pdb           | 0.0471226534           |

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Supplementary Text 10

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Supplementary Text 10

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-1.018847e-14
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-3.074082e-14 -2.623631e-15 -2.623083e-17 -1.517406e-14 -1.964551e-14
-1.592391e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
-1.577107e-16  2.920932e-14  6.426787e-15 -1.197798e-14  1.488272e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
2.624486e-14  2.229334e-15  2.581785e-14 -7.741597e-15  1.308639e-14
1.471926e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
9.352726e-14  4.084586e-14 -2.945205e-14 -5.940097e-15  5.824937e-15
-1.770135e-13
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
7.762034e-15 -3.856939e-15  3.242394e-15 -2.813179e-16  1.746115e-15
3.044764e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fff4c.final.pdb
-3.074082e-14 -2.623631e-15 -2.623083e-17 -1.517406e-14 -1.964551e-14
-1.592391e-14
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-1.535093e-13  1.523443e-13  4.210175e-14  7.193408e-14  1.319873e-14
6.149613e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\66b9f10ffbf22872.final.pdb
-5.482566e-15 -1.931166e-13 -5.615668e-14  1.685899e-13 -1.522146e-13
3.939441e-13
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
9.138930e-14  1.233965e-13  4.128711e-14 -9.403103e-15 -1.068486e-14
-2.046094e-13
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-1.592391e-14
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-1.577107e-16  2.920932e-14  6.426787e-15 -1.197798e-14  1.488272e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fbd98e66a3f099.final.pdb
2.211832e-13 -1.231311e-13  3.270179e-14  1.519072e-13 -1.071978e-14
-2.131536e-13
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
-3.201416e-14 -9.805824e-15 -1.989747e-14 -3.438780e-15  1.561131e-14
-4.005168e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feca.final.pdb
| File Name                                      | Value         |
|-----------------------------------------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfe12d3f9.final.pdb | -3.201416e-14 -9.805824e-15 -1.989747e-14 -3.438780e-15 1.561131e-14 -4.005168e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -4.005168e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -3.074082e-14 -2.623631e-15 -2.623083e-17 -1.517406e-14 -3.137236e-14 -1.964551e-14 -1.592391e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -2.028111e-14 5.153400e-14 4.178973e-14 -6.898969e-15 -3.606480e-14 -2.865364e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -1.775165e-14 -1.180981e-14 -5.583617e-14 1.406991e-13 -1.454527e-13 -7.121626e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b8be0d5986c138f.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.785746e-14 -1.197798e-14 1.488272e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | -6.801229e-16 4.274583e-14 8.664453e-15 -4.657916e-14 2.648846e-14 -1.892834e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | 1.348875e-15 -5.054396e-14 -1.196149e-15 1.746700e-14 -6.459876e-15 -2.735628e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | -8.862383e-14 -3.220920e-14 3.951244e-15 3.302737e-14 -2.620916e-14 6.805999e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 2.624486e-14 2.229334e-15 2.581785e-14 -7.741597e-14 1.308639e-14 1.471926e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -1.476225e-13 -6.626498e-14 -1.676172e-14 2.326750e-14 -1.976720e-14 1.728077e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 5.658107e-14 2.397982e-15 -4.962489e-15 -4.429458e-14 2.458678e-16 -2.391727e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | -3.201416e-14 -9.805824e-15 -1.989747e-14 -3.438780e-15 1.561131e-14 -4.005168e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a8234e4b4c668e.final.pdb | -2.047043e-14 -3.218896e-14 -6.420380e-15 1.433466e-15 -1.313140e-14 5.939357e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | -6.801229e-16 4.274583e-14 8.664453e-15 -4.657916e-14 2.648846e-14 -1.892834e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 6.365762e-14 3.898767e-14 5.941835e-15 1.211323e-14 -1.035216e-14 -3.193949e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.785746e-14 -1.197798e-14 1.488272e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | Page 32
| Path                              | Values                  |
|----------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 1.497118e-14 1.041455e-14 -6.073787e-15 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | -1.917175e-14          |
|                                 | 1.497118e-14 1.041455e-14 -6.073787e-15 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 |
|                                 | 1.488272e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 |
|                                 | 1.488272e-14           |
Supplementary Text 10

-1.335155e-13 -5.104514e-14 -3.112507e-15 6.767784e-14 -7.261192e-14 2.525500e-13

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb 2.624486e-14 2.29334e-15 2.581785e-14 -7.41597e-15 1.308639e-14 1.471926e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb -2.01416e-14 -9.805824e-15 -1.989747e-14 -3.438780e-15 1.561131e-14 -4.005168e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb -1.577107e-16 2.920932e-14 6.426787e-15 -1.787546e-14 -1.197798e-14 1.488272e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb 7.669735e-14 -2.324602e-14 -4.415705e-14 -2.923247e-14 9.061931e-16 -4.197870e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682cbbcad52078.final.pdb 2.185115e-14 -1.423683e-14 -6.453643e-15 3.351051e-15 -1.200010e-14 -3.143223e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb -4.195704e-14 -2.205107e-15 1.296331e-14 4.544109e-14 7.154524e-15 -5.530855e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb 7.532164e-15 7.826037e-15 -3.278179e-14 -6.133335e-15 3.853632e-15 -6.473998e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb -8.862383e-14 -3.220920e-14 3.951244e-15 3.302737e-14 -2.628961e-14 6.805999e-14

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb -2.431776e-14 4.475164e-14 6.436609e-14 9.099464e-15 6.858779e-15 -2.460359e-14

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb -2.770907e-15 -5.880075e-16 1.745740e-14 -3.184710e-15 6.415690e-15 -5.087488e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb -1.329317e-15 2.257375e-15 1.224097e-14 -1.003331e-14 -1.132679e-15 1.525927e-16

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb -1.494349e-14 5.227116e-15 3.760672e-15 5.183850e-15 2.950899e-15 1.779989e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb 7.532164e-15 7.826037e-15 -3.278179e-14 -6.133335e-15 3.853632e-15 -6.473998e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb -3.243025e-15 2.602751e-14 6.256328e-14 3.038498e-14 3.906482e-14 5.405070e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb -1.013345e-14 -3.171548e-15 1.991855e-14 -1.78422e-14 1.263159e-14 -4.407448e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb 1.057847e-14 -1.017091e-14 1.050171e-14 -2.504137e-14 1.300640e-14
Supplementary Text 10

5.609272e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
4.464782e-14 -1.956165e-14 7.292530e-14 4.366196e-14 -3.899787e-15 -9.880935e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
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-9.352133e-15 -3.371810e-14 7.259466e-14 4.653460e-14 -2.738922e-14 -1.416495e-14
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-4.423259e-14 3.234497e-14 1.422936e-13 8.055188e-14 2.185603e-14 7.603450e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8cdefb.final.pdb
1.111594e-14 -2.499143e-14 -3.827101e-14 -3.921149e-14 -1.785807e-14 -4.757381e-14
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-9.254342e-16 -6.703257e-15 -6.046808e-14 -4.399996e-14 -1.441844e-14
Supplementary Text 10

9.609178e-14
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7.764450e-15 -1.067649e-14 -2.968543e-14 -9.470528e-15 -6.807880e-15
-9.297136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298f3e8.final.pdb
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-9.297136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eeefcfe12d3f9.final.pdb
1.802859e-14 1.499915e-14 7.608084e-15 -3.751741e-15 -4.236152e-15
-2.215127e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
-9.254342e-16 -6.703257e-15 -6.046808e-14 -4.399996e-14 -1.441844e-14
-2.545167e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
-1.826378e-14 6.410856e-15 -1.015893e-14 -2.418682e-14 6.879509e-15
1.133485e-14
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1.510580e-14 -1.129405e-14 7.046536e-14 1.864500e-14 5.153000e-14
4.196221e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\966ef9ac3fe7439f.final.pdb
-9.432072e-14 -3.043460e-16 1.677766e-13 1.543381e-14 4.900237e-14
4.150354e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\988be0d5986c138f.final.pdb
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5.609272e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\99c22fe4909d67e2fa.final.pdb
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-1.879518e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b34852716dadc62.final.pdb
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-1.352363e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c8f752b3616ee6833b.final.pdb
-2.010086e-14 -1.052585e-14 1.247396e-14 -3.416156e-14 -2.057465e-15
-2.059825e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d3a02c70083816d6a.final.pdb
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2.977142e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9e0c997db891e4082.final.pdb
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-2.115188e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f8a039a2d823c616.final.pdb
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-8.241805e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd474b9c71d42c.final.pdb
7.764450e-15 -1.067649e-14 -2.968543e-14 -9.470528e-15 -6.807880e-15
-9.297136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad48a823e4b4c668.final.pdb
6.456849e-15 4.889943e-15 3.194193e-15 -5.433404e-16 7.199383e-15
-3.566112e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\be16aba0d3b7b857.final.pdb
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-1.879518e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
-1.400804e-14 -3.767634e-15 -5.042295e-14 2.257124e-14 -4.052457e-16
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Supplementary Text 10

5.405070e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
5.764450e-14 -1.067649e-14 -2.968543e-14 -9.470528e-15 -6.807880e-15
-9.297136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
-2.112505e-14 -3.741017e-14 1.374997e-13 3.489597e-16 -2.311816e-14
-1.550385e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
1.153147e-14 8.313919e-15 1.593666e-14 2.311949e-14 1.999381e-14
2.977142e-14
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-9.297136e-15
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5.609272e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
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-3.599047e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
5.899700e-16 -6.172836e-15 1.616736e-16 -6.768521e-15 -4.587383e-15
4.262259e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-8.353261e-15 3.920274e-15 1.08937e-14 -1.144196e-14 2.705221e-15
-5.192418e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
3.116457e-15 -4.155256e-15 2.831961e-14 -3.958941e-15 2.931640e-15
-5.469283e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-2.010086e-14 -1.052585e-14 1.247396e-14 -3.416156e-14 -2.055746e-15
-2.059825e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
5.007080e-15 -3.065867e-14 1.946134e-14 -3.008755e-16 7.900675e-15
7.708287e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-3.243025e-15 2.602751e-14 6.256328e-14 3.038498e-14 3.906482e-14
5.405070e-14

[,55] [,56] [,57] [,58] [,59] [,60]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
5.711352e-15 4.140069e-15 3.926359e-15 -2.440733e-14 1.148276e-15
-3.095543e-17
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-4.293719e-15 -1.525319e-15 -9.027550e-14 2.756040e-14 -9.371331e-16
1.927776e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
2.437993e-14 1.045955e-15 1.375426e-15 -1.083461e-14
-3.095543e-17
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-3.243025e-15 2.602751e-14 6.256328e-14 3.038498e-14 3.906482e-14
5.405070e-14

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c0db.final.pdb
-4.292752e-14 2.785336e-15 1.847277e-14 7.086328e-14 -4.543704e-14
-1.224975e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb
-3.083613e-14 -1.728950e-14 4.727718e-15 5.063435e-14 -4.734983e-14
-3.202103e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
3.659442e-14 2.589823e-15 -8.223716e-15 -1.099400e-14 8.523480e-15
3.474900e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
-3.472744e-14 -2.965801e-14 3.189826e-14 5.557571e-14 5.343806e-15
1.113057e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ea456b26cb6a25f.final.pdb
-3.421557e-14 1.00087e-14 9.347539e-15 4.782763e-14 4.288101e-15
-1.378972e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
1.521346e-15 -2.045775e-16 4.163499e-15 3.764726e-15 3.79143e-15
1.294509e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
-1.907459e-14 2.112056e-16 8.565219e-15 5.504885e-14 -2.127674e-14
-1.132130e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091fe385efc95e.final.pdb
-1.436763e-14 9.562599e-16 -3.457347e-15 3.255239e-15 3.825799e-15
1.008582e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
-3.421557e-14 1.00087e-14 9.347539e-15 4.782763e-14 4.288101e-15
-1.378972e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
-6.089966e-14 2.781306e-16 -9.624228e-16 9.438078e-14 -3.759841e-14
-6.191373e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
-3.083613e-14 -1.728950e-14 4.727718e-15 5.063435e-14 -4.734983e-14
-3.202103e-14  

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-1.321303e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-6.199794e-14 -4.916267e-15 -4.190174e-14 2.172322e-13 6.913603e-14
-6.318084e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
1.357334e-14 6.832328e-15 2.057545e-15 7.507507e-15 4.792272e-15
4.838731e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
2.482117e-13 3.297788e-14 -5.173581e-14 -4.156296e-13 -1.990104e-14
-6.628858e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
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-1.321303e-14  

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2.595630e-14 -2.342737e-14 3.760608e-15 -2.163627e-13 -5.766795e-15
-2.003264e-14  

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-7.701131e-15  5.048490e-15  3.296685e-15  8.024277e-16 -4.574498e-15
 2.958279e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb

-6.427032e-15  2.839955e-14  4.515434e-15  5.322048e-16 -5.066744e-14
 9.427599e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb

-3.762464e-15  1.796162e-15 -1.532208e-15  7.982925e-15  2.732218e-14
 6.882928e-15

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-4.337579e-15  5.338666e-15  3.351783e-15  5.953267e-15  3.014653e-15
-8.695682e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb

-3.931110e-14 -1.783083e-14  2.620230e-14 -4.718803e-15  4.928841e-14
-2.715598e-14

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-1.898353e-14

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-1.646924e-14

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-1.157708e-14  6.311882e-15  2.375540e-14 -1.222380e-14  5.369500e-15
-1.061376e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
Supplementary Text 10
-1.002466e-14 -4.751689e-15 1.866112e-14 3.766703e-15 2.077368e-14
-1.099392e-14
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-4.006818e-14 4.423304e-15 1.022322e-15 4.978813e-15 2.983520e-14
3.771615e-14
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-4.337579e-14 5.338666e-15 3.351783e-15 5.953267e-15 3.014653e-15
-8.695682e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
4.310837e-14 5.950347e-14 -5.498989e-14 -2.630965e-14 -1.147134e-13
8.941137e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
6.551002e-15 -4.352331e-15 2.508944e-15 3.308046e-15 1.773428e-14
3.002570e-16
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-1.157708e-14 6.311882e-15 2.375540e-14 -1.222380e-14 5.369500e-15
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-3.93110e-14 -1.783083e-14 2.620230e-14 -4.718803e-14 4.928841e-14
-2.715598e-14
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1.055979e-13 2.121516e-14 -1.028893e-13 3.985812e-14 -2.169405e-14
9.065320e-15
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3.891158e-15 1.838959e-15 1.584722e-15 6.723323e-15 8.774813e-15
1.988957e-15
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-1.727354e-14 -1.615089e-14 1.296924e-14 6.562648e-15 1.715204e-14
-3.856668e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\95a2b70083816d6ba.final.pdb
-8.514097e-15 1.586069e-14 1.815100e-15 3.478571e-15 -1.280503e-15
1.599517e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
7.993531e-15 9.154677e-16 3.852478e-15 -9.369210e-16 -2.103608e-15
-1.704257e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac4f474b9c71d4dc.final.pdb
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb      | -8.860636e-15 -5.615253e-15 2.467642e-15 -3.293960e-14 3.169112e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb      | 1.916594e-14 -4.121028e-14 4.425473e-15 3.308465e-14 3.002570e-16    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb       | -6.427032e-15 2.839555e-14 4.515434e-14 5.322048e-16 -5.066744e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb       | 6.551002e-15 -4.352331e-15 2.508944e-15 3.308046e-15 1.77328e-14      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb       | 1.108713e-14 -4.189292e-14 -1.324305e-14 4.005829e-14 -4.490879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb       | 8.514097e-15 1.586069e-14 1.815100e-14 3.478571e-15 1.28053e-15        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb       | 6.551002e-15 -4.352331e-15 2.508944e-15 3.308046e-15 1.77328e-14      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb       | -6.95682e-15 -1.559643e-14 7.641560e-15 7.810729e-15 1.600610e-14     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | 5.459920e-15 -9.497893e-15 1.099733e-14 -4.286750e-15 -3.481716e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | -1.727354e-14 -1.615089e-14 1.296924e-14 6.562648e-15 1.715204e-14     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb       | 9.378663e-15 9.744863e-15 -9.796553e-15 1.573364e-14 1.110252e-14     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb       | -6.427032e-15 2.839555e-14 4.515434e-15 5.322048e-16 -5.066744e-14   |

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| File Path                          | Statistics                  |
|-----------------------------------|-----------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 1.015996e-14 -1.561563e-14 -1.705258e-14 4.649545e-15 3.276301e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | -1.154449e-14 3.385419e-14 -3.260354e-15 -6.205506e-15 2.090531e-15 7.679902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 1.854222e-15 1.015996e-14 -1.561563e-14 -1.705258e-14 4.649545e-15 3.276301e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 1.978223e-14 3.353066e-14 -8.588557e-15 4.493272e-16 1.632741e-14 9.615854e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 1.056299e-15 8.569803e-15 3.961161e-15 -2.692841e-15 1.649409e-14 -8.891952e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 1.177826e-15 -2.021332e-15 -8.125806e-15 3.706923e-15 8.043401e-15 -5.388677e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 8.577410e-15 -6.069163e-14 2.216882e-14 1.785279e-14 8.210350e-15 -6.751304e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 1.177826e-15 -2.021332e-15 -8.125806e-15 3.706923e-15 8.043401e-15 -5.388677e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 5.232021e-15 -1.001411e-13 2.576594e-14 8.855364e-15 -2.208114e-15 -1.342821e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 1.177826e-15 -2.021332e-15 -8.125806e-15 3.706923e-15 8.043401e-15 -5.388677e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 1.177826e-15 -2.021332e-15 -8.125806e-15 3.706923e-15 8.043401e-15 -5.388677e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 2.640849e-15 1.196406e-14 -3.098523e-15 1.324714e-15 -1.743042e-15 -4.958896e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 2.893614e-15 4.697824e-14 2.655261e-16 1.779656e-14 3.456192e-15 6.539322e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 5.232021e-15 -1.001411e-13 2.576594e-14 8.855364e-15 -2.208114e-15 -1.342821e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 5.026166e-15 -5.679872e-14 4.843694e-14 1.481221e-14 1.323353e-15 1.053126e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249a61.final.pdb | 5.103723e-15 3.825548e-14 -4.473345e-15 -6.701852e-15 1.474870e-15 1.667748e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245015047.final.pdb | 9.756861e-16 7.714666e-15 -1.090472e-14 2.299428e-15 -6.223045e-15 8.030705e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -1.112458e-14 2.286573e-14 -2.010996e-14 1.586057e-14 3.559807e-15 |
| File Path                                                                 | Values                          |
|--------------------------------------------------------------------------|---------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb      | -5.174177e-15                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0807eff10197e2.final.pdb      | 4.018363e-14                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb      | 2.577416e-14                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb      | 1.893073e-14                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb      | 1.115698e-16                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e502082718ec3a1.final.pdb       | -1.154449e-14                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5899d996d0a960.final.pdb       | -2.606708e-14                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb       | 7.049290e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | 3.517438e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb       | 9.756861e-16                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | -5.137130e-15                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584ee2203fb92.final.pdb       | -2.068685e-14                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52ca29.final.pdb        | 1.115698e-16                    |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
6.552014e-15 9.250064e-15 -5.073467e-16 1.037037e-15 1.052272e-14
6.553488e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-4.20354e-14 2.139071e-16 -5.468337e-15 9.599140e-15 6.723179e-16
2.198499e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab80392a8236c616.final.pdb
1.124777e-14 1.178413e-15 4.413570e-15 -9.559637e-15 9.672317e-16
1.648917e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
1.24863e-14 8.50958e-15 -1.029904e-16 9.31159e-15 3.690585e-15
5.269998e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
-4.921148e-16 2.713316e-15 1.876570e-15 8.495666e-15 1.355241e-15
-4.433468e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
1.598131e-16 9.625512e-15 -5.167626e-16 3.596865e-14 8.705823e-15
1.077781e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
1.568283e-14 9.007263e-16 -5.639073e-15 8.739094e-15 -1.083091e-14
1.129826e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
2.114877e-15 3.677278e-15 6.102134e-15 5.860816e-15 -3.249562e-15
-2.833522e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
3.050247e-14 -6.065923e-15 9.875332e-15 -7.070309e-15 -3.132769e-15
8.130654e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
2.114877e-15 3.677278e-15 6.102134e-15 5.860816e-15 -3.249562e-15
-2.833522e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
2.129904e-14 6.682673e-16 2.006433e-15 9.545347e-15 7.486160e-15
3.367161e-15

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-2.833522e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb
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-2.833522e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
8.654966e-16 5.784100e-15 2.296110e-15 -2.107636e-15 -6.768109e-16
1.152132e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
3.296302e-15 -7.024364e-15 1.220040e-14 1.412963e-15 -6.118815e-15
1.021901e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f855ff9d0681.final.pdb
2.129904e-14 6.682673e-16 2.006433e-15 9.545347e-15 7.486160e-15
3.367161e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
7.896366e-14 4.707579e-15 1.335268e-14 -1.696943e-14 6.178915e-16
1.810452e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-2.107494e-15 4.027692e-15 -3.797012e-15 3.603508e-15 1.151279e-15
1.662966e-14
Supplementary Text 10

-3.405353e-15 -4.885512e-15  2.054220e-15 -3.614815 e-15  4.380647e-16
-4.522840e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-1.541249e-14 -6.513208e-15 -1.755826e-14 -9.993966 e-15  1.364334e-14
-1.193901e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
-4.522840e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb
4.776692e-15 -5.323912e-15 -1.987145e-15 -9.838039e -16 -3.478360e-15
-1.184350e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-5.806513e-15 -3.258759e-15 -2.863137e-14  4.072143e-14  3.247350e-16
-7.675930e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7bb3547ea982ffc4.final.pdb
2.471472e-14 -4.666496e-15  5.565781e-14  7.037930e -15 -2.870939e-15
-3.949483e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
3.743609e-15 -5.083362e-15  7.368939e-16 -4.698983e -15 -3.210105e-15
-1.836938e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
7.713418e-15 -4.953917e-15 -2.915616e-17  4.000930e -16 -8.864234e-16
-2.030386e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
2.095939e-14  4.656210e-15 -1.903832e-14  2.164915e-15  6.955403e-15
1.149215e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
9.265464e-15 -3.127350e-15  5.267892e-15 -4.292924e-15 -5.153701e-15
-3.130082e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
9.265464e-15 -3.127350e-15  5.267892e-15 -4.292924e-15 -5.153701e-15
-3.130082e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8300c6e666a3f6099.final.pdb
7.393697e-15 -6.327589e-15  1.081462e-15  8.769858e-16 -1.420576e-15
-2.119822e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
4.729855e-15 -4.773679e-15  2.311029e-14 -6.284685e-15  1.776118e-15
-8.745359e-15

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9.405353e-15 -4.885512e-15  2.054220e-15 -3.614815 e-15  4.380647e-16
-4.522840e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
1.282267e-15 -1.002721e-14 -1.367355e-14  2.246984e-15 -2.603657e-15
7.730463e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
1.282267e-15 -1.002721e-14 -1.367355e-14  2.246984e-15 -2.603657e-15
7.730463e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8d6ef9ac3fe74395.final.pdb
2.915253e-14 -5.145933e-15  2.953836e-14  1.205167e-14  2.663438e-15
-6.262158e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b6be0d5986c138f.final.pdb
7.713418e-15 -4.953917e-15 -2.915616e-17  4.000930e -16 -8.864234e-16
-2.030386e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
-1.135433e-14 -6.577498e-15 -5.230871e-15 -2.624120e-15 -8.771900e-15
2.996420e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dd8ed0d81fb3ef.final.pdb
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb       | 8.326906e-15 -4.809014e-15 -2.660347e-14 4.762006e-15 -5.323154e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb     | 4.510477e-15 -3.321334e-15 7.525002e-15 7.112230e-16 -1.589400e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb     | 2.967792e-15 -2.046914e-15 5.324249e-14 1.602338e-14 8.409176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb     | -3.150485e-14 -1.577973e-14 -2.509634e-15 -1.037475e-14 -6.720895e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb      | 3.852155e-15 2.167662e-16 7.044260e-15 -8.595260e-15 -5.334035e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb     | 1.511412e-14 4.875993e-15 4.496065e-14 5.163103e-15 1.851431e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb     | 3.063734e-15 -3.139136e-14 -7.009297e-15 -4.371554e-15 -3.220514e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2.final.pdb      | -1.813374e-15 -3.148146e-14 3.807936e-15 -6.222692e-15 6.678067e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb     | 9.265464e-15 -3.127350e-15 5.267892e-15 -4.292924e-15 -5.153701e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a960.final.pdb       | 1.289142e-14 -3.582418e-15 1.113551e-14 7.310638e-15 -3.348522e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb      | 3.169070e-15 -6.815559e-15 -2.537720e-15 1.638490e-15 -2.50226e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea04b9545899c29d.final.pdb      | 2.147497e-15 -6.242934e-15 3.074238e-15 3.230073e-16 2.668825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862c6cad52078.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb      | 3.226227e-15 -5.653869e-15 2.566810e-16 -9.587024e-16 -2.513180e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb      | 4.510477e-15 -3.321334e-15 7.525002e-15 7.112230e-16 -1.589400e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcaec8deec43fa.final.pdb     | 9.908159e-15 -3.62213e-15 6.815559e-15 -2.537720e-15 1.638490e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f210fa706824ef88.final.pdb      | 1.511412e-14 4.875993e-15 4.496065e-14 5.163103e-15 1.851431e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f589d996d0a960.final.pdb        | 7.713418e-15 -4.953917e-15 -2.915616e-17 4.000930e-16 -8.864234e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f5d589d996d0a960.final.pdb      | 1.289142e-14 -3.582418e-15 1.113551e-14 7.310638e-15 -3.348522e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9d9e72307a2fbd.final.pdb       | 2.147497e-15 -6.242934e-15 3.074238e-15 3.230073e-16 2.668825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f9df9e72307a2fbd.final.pdb      | 3.331507e-15 -4.595263e-15 3.619835e-15 1.111330e-15 -2.979367e-15 |
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7.012994e-15 -1.837210e-15 1.310514e-14 1.757242e-16 -5.677499e-15
4.514904e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
7.560329e-15 -1.245404e-15 -1.773854e-15 -1.416813e-15 6.676971e-15
-4.249694e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
8.015421e-15 -1.813374e-15 -3.148146e-14 3.807936e-15 -6.222692e-15
6.678067e-15

[.85] [.86] [.87] [.88] [.89] [.90]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
2.891103e-15 4.378681e-15 1.676542e-15 1.312444e-15 3.425034e-15
1.992909e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
1.443981e-15 3.612021e-15 1.859945e-15 -1.294646e-15 4.626648e-15
3.335652e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
5.416414e-15 7.051135e-15 5.668438e-15 2.467777e-16 3.234264e-15
-1.032879e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-2.073185e-16 5.118219e-15 4.203942e-15 6.420404e-17 5.685833e-15
-2.234870e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-3.028361e-15 1.626444e-15 4.997963e-15 4.561950e-16 -1.518366e-16
5.153908e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
9.236635e-16 2.986249e-16 7.221863e-16 1.578924e-15 6.136201e-15
-4.931556e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
1.125166e-15 7.154897e-15 5.634003e-15 1.570263e-15 4.923059e-15
-4.713177e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
3.993799e-16 1.409016e-14 1.462596e-15 4.154625e-15 5.461729e-15
-2.943648e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-2.263026e-16 3.998751e-16 4.765847e-16 1.491020e-15 1.112383e-14
6.241926e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
1.685250e-15 6.294386e-15 1.318543e-16 1.517920e-15 5.790520e-15
-2.053376e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
-2.630262e-16 3.998751e-16 4.765847e-16 1.491020e-15 1.112383e-14
6.241926e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f945328d475799a.final.pdb
1.347211e-15 4.321226e-15 1.675364e-15 -2.750933e-15 1.013590e-14
-1.367987e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd391e54336d.final.pdb
-1.794374e-15 1.011730e-14 4.082122e-17 2.219483e-15 9.766407e-15
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| Path                                      | Values               |
|-------------------------------------------|----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 3.993799e-15 1.489094e-14 1.462596e-15 4.154625e-15 5.461729e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d573f3c8f7ef.final.pdb | -6.015478e-16 4.743119e-15 2.121147e-15 5.248281e-15 6.271844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6760178986bef01.final.pdb | -3.256581e-15 -2.366574e-15 -1.491010e-15 -6.893642e-15 -2.583302e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -2.943648e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -9.709793e-16 5.094756e-15 3.724242e-15 1.807111e-15 4.250892e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fca4.final.pdb | -2.105614e-14 1.062806e-14 7.467225e-15 1.415797e-14 1.412917e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716926411d4c2.final.pdb | 3.477353e-16 7.162596e-15 8.918755e-15 -1.108163e-15 3.322480e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad4f1e4.final.pdb | -6.015478e-16 4.743119e-15 2.121147e-15 5.248281e-15 6.271844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb2872.final.pdb | 5.068941e-16 3.509082e-15 2.049112e-15 3.509371e-15 5.926594e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c8w45d3135.final.pdb | 1.125166e-15 7.154897e-15 5.634003e-15 1.570263e-15 4.923059e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c8w45d3135.final.pdb | -4.713177e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7af057e0ad0f1e4.final.pdb | 3.162654e-15 1.650022e-15 -3.013494e-15 8.313600e-15 9.624919e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b2a64f7e1f2872.final.pdb | 5.765319e-15 7.642266e-15 -1.415519e-15 3.706055e-15 4.038449e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fba.final.pdb | 5.765319e-15 7.642266e-15 -1.415519e-15 3.706055e-15 4.038449e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eejcefe132f9.final.pdb | 3.564515e-16 7.798391e-15 -4.426565e-15 4.871575e-15 6.814007e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 3.993799e-15 1.409016e-14 1.462596e-15 4.154625e-15 5.461729e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -2.943648e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -6.015478e-16 4.743119e-15 2.121147e-15 5.248281e-15 6.271844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d45569ef569760.final.pdb | 3.993799e-15 1.409016e-14 1.462596e-15 4.154625e-15 5.461729e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d45569ef569760.final.pdb | -2.943648e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -6.015478e-16 4.743119e-15 2.121147e-15 5.248281e-15 6.271844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -2.943648e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d45569ef569760.final.pdb | -6.015478e-16 4.743119e-15 2.121147e-15 5.248281e-15 6.271844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d45569ef569760.final.pdb | -2.943648e-16 |
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-1.543801e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb
7.138046e-16 6.283977e-15 -3.122349e-16 -3.228283e-15 8.732611e-15
-3.455032e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
7.421354e-15 -5.995918e-15 2.995256e-15 -8.192465e-15 -1.103249e-15
6.358247e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb
-1.544573e-15 1.296622e-14 6.436747e-15 1.003268e-14 1.824227e-14
-3.372643e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
-1.570072e-15 3.759297e-15 1.584721e-15 5.241218e-16 5.351401e-15
-1.137863e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
-2.700157e-15 3.315197e-15 3.773738e-15 7.611338e-15 7.944920e-15
-1.269098e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
1.056445e-14 1.537163e-14 -4.294179e-16 2.100324e-16 1.004148e-14
7.679702e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb
4.529682e-15 7.914182e-15 6.969737e-15 -2.245022e-15 -7.205733e-16
-3.747082e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
2.862695e-15 2.022379e-14 5.330819e-15 8.012996e-15 9.309345e-15
-1.482713e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
-2.263026e-17 3.998751e-16 4.765847e-16 1.491020e-15 1.112838e-14
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2a.final.pdb
-3.028361e-15 1.624442e-15 4.997963e-15 4.561950e-16 -1.518366e-16
5.153908e-16
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5.765319e-15 7.642266e-15 -1.415519e-15 3.370605e-15 4.038449e-15
-2.056845e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
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-1.092971e-14
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4.364785e-17
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-4.713177e-16
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1.365629e-15 4.430002e-15 1.385624e-15 5.038118e-16 6.481745e-15
-1.945510e-15
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-3.042461e-16 4.993431e-15 4.057140e-15 8.156584e-16 5.375821e-15
-1.626210e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
1.101904e-15 4.677703e-15 1.955003e-15 1.113284e-15 6.068841e-15
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-9.775597e-16
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-1.570072e-15 3.759297e-15 1.584721e-15 5.241218e-16 5.351401e-15
-1.137863e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
1.178640e-15 8.077711e-15 3.342728e-15 4.845163e-15 7.966353e-15
-3.509495e-15
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-7.805624e-15 -3.318062e-15 3.184140e-15 5.654245e-16 -2.090326e-17
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-3.028361e-15 1.624442e-15 4.997963e-15 4.561950e-16 -1.518366e-16
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-5.033627e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-5.130456e-15 2.164221e-15 5.908894e-16 4.022822e-15 8.567966e-16
-1.737340e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-4.618802e-15 3.283268e-15 -4.678940e-15 1.309894e-15 -4.572341e-16
-5.948341e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
3.079050e-16 -1.946358e-15 2.238959e-15 -2.440883e-15 -1.935899e-15
-4.849148e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-3.330593e-15 2.250116e-15 -3.591213e-15 3.549810e-16 -7.989843e-17
4.053567e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
-6.037265e-15 6.347589e-15 -5.533661e-16 1.207249e-16 3.802202e-16
-4.426609e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
-4.972790e-16 2.199631e-15 -6.073836e-15 3.463108e-16 -1.346093e-15
-3.365283e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-3.158073e-15 2.296342e-15 -5.644275e-15 5.540146e-15 -6.905783e-16
6.391095e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
-6.266781e-15 2.706782e-15 -4.205089e-15 1.898885e-15 -1.563087e-15
-1.021345e-15
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9.825690e-15 1.296100e-15 -3.078516e-15 7.039532e-15 7.269907e-15
3.731576e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
-5.298314e-15 1.645939e-15 -3.869340e-15 2.981852e-15 -3.843322e-16
-8.440275e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551bea0a93.final.pdb
9.825690e-15 1.296100e-15 -3.078516e-15 7.039532e-15 7.269907e-15
3.731576e-15

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| File Path                                                                 | Values                        |
|--------------------------------------------------------------------------|-------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb     | 1.284102e-15 -6.222254e-17    |
|                                                                         | -5.774155e-15 7.147781e-15    |
|                                                                         | 4.99691e-15 -3.735451e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb     | -3.545265e-15 3.460519e-15     |
|                                                                         | -8.126431e-15 7.852022e-15    |
|                                                                         | 6.137784e-15 -3.916924e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb      | -4.497279e-15 2.199631e-15     |
|                                                                         | -6.073836e-15 5.463108e-15    |
|                                                                         | -1.346093e-15 -3.365283e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | -8.874285e-15 1.011662e-15     |
|                                                                         | -2.768333e-15 8.731834e-15    |
|                                                                         | -4.474615e-15 -1.078449e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | -1.577201e-15 1.541302e-15     |
|                                                                         | -4.598591e-15 5.385023e-15    |
|                                                                         | 9.209096e-16 -6.620116e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb      | -5.014227e-15 3.066559e-15     |
|                                                                         | -2.126256e-15 9.830275e-16    |
|                                                                         | -2.262027e-15 -1.446028e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc4.final.pdb      | 5.999992e-16 -1.02907e-14     |
|                                                                         | -1.351992e-14 6.549408e-17    |
|                                                                         | 3.998577e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb       | 4.120733e-16 -7.002899e-15    |
|                                                                         | -2.22721e-15 -2.646524e-15    |
|                                                                         | -2.672486e-16 -3.431852e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | -8.874285e-15 1.011662e-15     |
|                                                                         | -2.768333e-15 8.731834e-15    |
|                                                                         | -4.474615e-15 -1.078449e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | -4.301399e-15 2.111854e-15     |
|                                                                         | -2.776240e-15 3.179339e-15    |
|                                                                         | -3.363948e-15 8.307926e-16    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | -6.037265e-15 6.347589e-15     |
|                                                                         | -5.533661e-16 1.202749e-16    |
|                                                                         | 3.802202e-16 -4.426609e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb       | -4.454935e-15 -1.873935e-15   |
|                                                                         | -3.981770e-15 1.144349e-14    |
|                                                                         | 4.208678e-15 1.302157e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -3.744002e-15 1.704919e-15    |
|                                                                         | 3.031830e-17 8.636183e-15     |
|                                                                         | -5.182577e-15 3.093795e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | -3.744002e-15 1.704919e-15    |
|                                                                         | 3.031830e-17 8.636183e-15     |
|                                                                         | -5.182577e-15 3.093795e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12d3f9.final.pdb         | -5.298314e-15 7.616634e-16    |
|                                                                         | 4.542413e-16 -1.778663e-15    |
|                                                                         | -3.912711e-16 6.239933e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | -4.497279e-15 2.199631e-15    |
|                                                                         | -6.073836e-15 5.463108e-15    |
|                                                                         | -1.346093e-15 -3.365283e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | -8.874285e-15 1.011662e-15    |
|                                                                         | -2.768333e-15 8.731834e-15    |
|                                                                         | -4.474615e-15 -1.078449e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadcc62.final.pdb       | -8.726128e-15 1.854105e-15    |
|                                                                         | -3.862401e-15 -4.706443e-15   |
|                                                                         | 3.640226e-15 -5.940645e-15    |

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| File Path                                             | Coordinates                             |
|------------------------------------------------------|-----------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | -4.871531e-15 2.444895e-15 -3.004314e-15 1.256952e-15 -1.715326e-15 -1.300963e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | -6.040342e-15 3.396708e-15 -1.183779e-14 3.296270e-15 2.904752e-16 -1.624067e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | -8.726128e-15 1.854105e-15 -3.862401e-15 -4.706443e-15 3.640226e-15 -5.940645e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | -8.726128e-15 1.854105e-15 -3.862401e-15 -4.706443e-15 3.640226e-15 -5.940645e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | -1.488392e-14 3.043808e-15 -2.383716e-15 7.689307e-15 -1.008667e-14 5.511947e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | -6.296592e-15 -2.642370e-16 -3.683160e-15 1.743249e-15 -7.205499e-16 -8.860528e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -9.476516e-15 1.066600e-14 3.266543e-16 2.118798e-14 9.039609e-15 1.624528e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af80f0eef3.final.pdb | -9.476516e-15 1.066600e-14 3.266543e-16 2.118798e-14 9.039609e-15 1.624528e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | -1.058668e-14 1.413124e-14 -5.571614e-15 1.843588e-14 -1.889041e-15 -1.242197e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d84a82a50f43f2e9.final.pdb | -1.058668e-14 1.413124e-14 -5.571614e-15 1.843588e-14 -1.889041e-15 -1.242197e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -1.82628e-14 9.732117e-15 -1.277227e-14 -2.083300e-15 -1.582881e-14 -1.819222e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | -1.82628e-14 9.732117e-15 -1.277227e-14 -2.083300e-15 -1.582881e-14 -1.819222e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281flea2.final.pdb | -3.079050e-16 -1.946358e-15 2.238959e-15 -2.440883e-15 -1.935899e-15 -4.849148e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | -3.079050e-16 -1.946358e-15 2.238959e-15 -2.440883e-15 -1.935899e-15 -4.849148e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d999d00606.final.pdb | -7.44002e-15 1.704919e-15 3.031830e-17 8.636183e-15 -5.182577e-15 3.093795e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d999d00606.final.pdb | -7.44002e-15 1.704919e-15 3.031830e-17 8.636183e-15 -5.182577e-15 3.093795e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e698862e-16 -3.011270e-16 -9.172821e-15 -1.139722e-14 -1.165088e-14 -5.885770e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e744002e-15 1.704919e-15 3.031830e-17 8.636183e-15 -5.182577e-15 3.093795e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e744002e-15 1.704919e-15 3.031830e-17 8.636183e-15 -5.182577e-15 3.093795e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e841053e-15 2.280612e-15 -3.392833e-15 5.178686e-15 6.939940e-16 -2.559903e-15 |
|                                | Supplementary Text 10 |
|--------------------------------|-----------------------|
|                                | 8.750204e-16          |
|                                | 4.980489e-15          |
|                                | 9.898742e-16          |
|                                | -6.801687e-16         |
|                                | -4.58908e-15          |
|                                | 5.04236e-15           |
|                                | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb |
|                                | 4.169171e-15          |
|                                | 2.212146e-15          |
|                                | 4.55937e-15           |
|                                | 6.385902e-16          |
|                                | -1.537484e-15         |
|                                | 4.265986e-15          |
|                                | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f453d8d47579a.final.pdb |
|                                | -1.848343e-14         |
|                                | 7.606326e-15          |
|                                | -2.630716e-15         |
|                                | -8.010883e-15         |
|                                | -6.800747e-15         |
|                                | 9.163769e-15          |
|                                | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd391854336d.final.pdb |
|                                | 7.295046e-16          |
|                                | -4.050605e-16         |
|                                | 8.926155e-16          |
|                                | 2.642054e-15          |
|                                | -8.824735e-15         |
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|                                | -5.628473e-16         |
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|                                | 3.407707e-15          |
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|                                | 1.169747e-15          |
|                                | -5.838665e-15         |
|                                | 9.475956e-15          |
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|                                | 8.127996e-16          |
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|                                | -7.591310e-15         |
|                                | 1.174615e-14          |
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|                                | 6.763785e-15          |
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|                                | -1.365590e-14         |
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Supplementary Text 10

-6.902443e-15  9.764840e-15  3.627780e-15 -4.723131e-15 -8.351119e-15
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5.593563e-15

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Supplementary Text 10

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Supplementary Text 10

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Supplementary Text 10

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-2.866858e-15
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Supplementary Text 10

| PDB ID | File Path                          | Scores                              |
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| 86d50469ef569760.final.pdb    | -6.534341e-15 5.160529e-16 -1.036133e-15 6.398074e-15 3.732166e-16 |
| 89d0666e1402203d.final.pdb    | -7.801389e-15 -1.174860e-15 -6.379271e-15 5.226828e-16 -3.479232e-15 4.006296e-16 |
| 8b34852716dadc62.final.pdb    | -1.644504e-15 1.218080e-15 4.426403e-15 2.370620e-16 -4.33895e-16 1.201645e-15 |
| 8b6ef9ac3fe74395.final.pdb    | -2.522387e-15 -4.591080e-15 -7.804498e-15 4.289953e-15 1.675012e-14 7.238422e-15 |
| 98bbe0d5986c138f.final.pdb    | -4.582408e-15 -7.639936e-17 7.672088e-15 -1.119113e-15 8.221024e-15 -2.696610e-16 |
| 9c22f4909d67e2fa.final.pdb    | -2.182051e-15 1.026206e-14 3.177104e-16 6.342703e-15 -4.423687e-15 -5.164790e-15 |
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| 9f752b3616e6033b.final.pdb    | -9.051591e-16 -1.282989e-15 -2.802234e-15 -4.561309e-16 6.792433e-15 3.943505e-16 |
| a02c70083816d6ba.final.pdb    | 4.640747e-15 7.583541e-15 5.015139e-15 1.147642e-14 1.106673e-15 -1.594485e-15 |
| a0c997d891e4e082.final.pdb    | 7.917389e-15 -8.955055e-15 -9.491874e-15 -6.069323e-15 2.127900e-14 1.082787e-14 |
| ab8039a2d823c616.final.pdb    | 4.702213e-16 2.367486e-15 1.584986e-15 6.444909e-16 4.962838e-15 6.756521e-16 |
| acf4d74b9c71d4dc.final.pdb    | -4.909128e-16 -1.626866e-15 9.394651e-15 9.880189e-19 9.463208e-15 6.326556e-16 |
| ad8a823e4b4c668e.final.pdb    | -3.996872e-16 1.382526e-15 1.079856e-15 1.654955e-15 3.241488e-15 1.971137e-15 |
| b16ababd03b7b857.final.pdb    | -2.182051e-15 1.026206e-14 3.177104e-16 6.342703e-15 -4.423687e-15 -5.164790e-15 |
| b226923e697d3c63.final.pdb    | 6.841195e-15 3.789052e-15 4.396831e-15 -4.916976e-15 -3.899469e-15 1.989636e-15 |
| b28e48f6fa27a165.final.pdb    | -4.582408e-15 -7.639936e-17 7.672088e-15 -1.119113e-15 8.221024e-15 -2.696610e-16 |
| b42c4924e3cd1aec.final.pdb    | -3.773361e-15 3.194041e-15 1.019449e-14 5.349985e-15 -4.731734e-16 9.195472e-15 |
| b4dd239fcabff1df.final.pdb    | -4.582408e-15 -7.639936e-17 7.672088e-15 -1.119113e-15 8.221024e-15 1.082787e-14 |
| Filenames                                      | Values                        |
|----------------------------------------------|-------------------------------|
| b669942ef97459a2.final.pdb                 | -2.696610e-16                |
| b99f4d9d87c1017b.final.pdb                 | -4.582408e-15 -7.699363e-17  |
| b669942ef97459a2.final.pdb                 | 1.218080e-15 4.426403e-15    |
| b99f4d9d87c1017b.final.pdb                 | -1.201645e-15                |
| b669942ef97459a2.final.pdb                 | 7.672088e-15 -1.19113e-15    |
| b99f4d9d87c1017b.final.pdb                 | 1.218080e-15 4.426403e-15    |
| b669942ef97459a2.final.pdb                 | 2.370620e-15 -4.333895e-16   |
| b99f4d9d87c1017b.final.pdb                 | 1.201645e-15                |
| b669942ef97459a2.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 8.221024e-15    |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
| b669942ef97459a2.final.pdb                 | 1.201645e-15                |
| b99f4d9d87c1017b.final.pdb                 | 8.221024e-15 -4.333895e-16   |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
-1.594485e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
-4.909128e-16 -1.626866e-15  9.394651e-15  9.880189 e-19  9.463208e-15
6.326556e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-4.383555e-16  2.164483e-15  1.409204e-15  2.250467 e-15  3.613835e-15
9.878774e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
-5.824878e-17  2.497930e-15  2.084977e-15  3.121370e-15 1.048729e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-1.474842e-16  2.132125e-15  2.059812e-15  1.466293e-15 5.019299e-15
1.197600e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d49ad3a0ad.final.pdb
-1.986147e-15  1.186139e-15  1.388311e-15  4.43102e-15 6.808367e-15
4.789547e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-9.051591e-16 -1.282989e-15 -2.802234e-15 -4.561309e-16 6.792433e-15
3.943050e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f38584e22003fb92.final.pdb
6.414655e-15  4.414156e-16 -5.784737e-16  2.453550e-15 9.975046e-15
2.240484e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
5.742297e-15  7.194734e-15  6.065433e-15  2.787198e-15 3.336287e-15
7.062835e-16

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-6.074698e-15 -9.307826e-16 -2.461554e-16 -4.225360 e-16  3.338557e-15
4.008082e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-3.245655e-15 -1.978608e-15 -9.854429e-18 -1.477060 e-15  2.539679e-15
3.629983e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-5.133618e-15 -2.282342e-15  4.017876e-15 -2.705175e-15 2.870743e-15
1.688058e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-7.058858e-15 -3.161435e-15  2.130990e-15  1.895083e-16  2.721493e-15
4.694963e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-3.773367e-15 -5.190773e-15 -7.164501e-16  1.388905e-15  7.778501e-15
1.523863e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-4.614589e-15 -1.746599e-15 -2.368379e-15 -2.334351e-15 1.953301e-15
2.382634e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
-3.615441e-15 -4.060020e-15  8.430791e-16  4.568430e-16 1.943400e-15
3.538898e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0db59f3306825e8.final.pdb
-7.271437e-15 -4.698111e-15 -6.668286e-15 -2.358965e-15 1.252471e-15
5.923121e-15
| File Path                                               | Values                                                                 |
|---------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 1.278365e-15 4.455157e-15 -9.859744e-15 1.979361e-15 6.420212e-15 1.628597e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb     | -4.327492e-15 -2.349416e-15 -3.420489e-15 9.263112e-16 -3.226560e-16 3.906589e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb     | -6.994495e-15 1.109490e-15 -1.765349e-14 -4.345055e-15 2.356482e-15 4.556887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb     | -3.992217e-15 -2.117894e-15 -2.195955e-15 1.035386e-15 2.100479e-15 2.834015e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb     | -6.994495e-15 1.109490e-15 -1.765349e-14 -4.345055e-15 2.356482e-15 4.556887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb     | 1.302923e-14 4.294449e-16 -5.703767e-15 2.342054e-15 2.000852e-15 5.730375e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb     | -7.425327e-15 1.266358e-14 -8.319947e-15 -1.450883e-15 -1.110580e-15 6.713875e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb     | -3.053824e-15 -1.200328e-15 -9.634185e-16 -3.018817e-16 2.735302e-15 4.070590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fc3b46e33793b0.final.pdb      | -7.99068e-15 -5.330602e-15 7.331253e-16 -3.922917e-16 8.819494e-17 2.570337e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb     | -7.949188e-15 -1.015744e-14 6.390228e-15 -4.552844e-15 4.553566e-15 2.276568e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb     | -4.519814e-15 -3.790991e-15 -6.916005e-15 -4.347551e-16 5.254041e-15 5.070653e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb     | 1.278365e-15 4.455157e-15 -9.859744e-15 1.979361e-15 6.420212e-15 1.628597e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb     | -8.073371e-15 -3.166534e-15 -3.030791e-15 1.255045e-15 5.033896e-15 5.038538e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb      | 4.339280e-15 -1.803465e-15 -1.728761e-15 -7.076850e-16 5.245209e-15 4.692605e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4432df75a7fcfc.final.pdb       | -1.461246e-15 1.198409e-15 9.297174e-15 3.805162e-15 6.579020e-15 4.252450e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\444ef21dfe8cdfb.final.pdb      | -6.444249e-15 3.176482e-15 1.798245e-15 -1.122610e-15 7.138116e-15 1.002147e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\47240be3ef113c7.final.pdb      | -7.271437e-15 -4.698111e-15 -6.668286e-15 -2.358965e-15 1.252471e-15 5.923121e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb     | -9.748555e-15 3.748011e-16 2.165589e-15 -7.04814e-15 3.127349e-15 -2.150128e-15 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
-1.693276e-14  3.913924e-15  7.178710e-15  1.261186e-15 -8.678821e-15
9.178113e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ea45b62cb6a25f.final.pdb
-4.665748e-15  2.460085e-15 -1.887692e-15  1.449372e-15 -1.591639e-16
7.359942e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c37161d85ac96.final.pdb
1.278365e-15  4.455157e-15 -9.859744e-15  1.979361e-15  6.420212e-16
1.628597e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
-4.263692e-15 -4.252918e-16  1.772811e-15 -1.258062e-15  4.120781e-16
4.50704e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
-3.615441e-15 -4.060020e-15  8.430791e-16  4.568430e-16  1.943400e-15
3.538898e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
-4.665748e-15  2.460085e-15 -1.887692e-15  1.449372e-15 -1.591639e-16
7.359942e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
-7.986241e-15 -4.486595e-15  1.924845e-15  1.840077e-15 -5.173810e-16
1.092793e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
-7.271437e-15 -4.698111e-15 -6.668286e-15 -2.358965e-15  1.252471e-15
5.923121e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
-4.263692e-15 -4.252918e-16  1.772811e-15 -1.258062e-15  4.120781e-16
6.450704e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-8.558235e-16  6.389366e-15 -5.745508e-15  1.691398e-16 -2.058239e-16
5.839352e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
-3.354214e-16 -1.796786e-15 -2.178388e-15  6.297463e-16  2.999337e-15
2.856781e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc4.final.pdb
-8.670289e-15 -2.846833e-14 -3.323496e-15 -5.008244e-15  5.801174e-15
-3.669842e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-8.661265e-15  1.11076e-14 -3.985141e-15 -7.039322e-15  9.745679e-15
6.344743e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb
-4.263692e-15 -4.252918e-16  1.772811e-15 -1.258062e-15  4.120781e-16
6.450704e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f90fffb22872.final.pdb
-3.708712e-15 -3.608958e-15 -1.364866e-15 -1.682688e-15  2.630569e-15
3.449700e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\79f18c80dd5c3135.final.pdb
-3.615441e-15 -4.060020e-15  8.430791e-16  4.568430e-16  1.943400e-15
3.538898e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
-3.866383e-15 -1.299002e-14  1.317340e-14  1.820661e-14  2.012062e-15
6.155908e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
-7.799406e-15 -5.330602e-15  7.331253e-16 -3.922917e-16  8.819949e-17
2.570337e-15
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -4.091504e-15  -5.684307e-16  -6.250152e-15  -6.548067e-15  1.431167e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | -7.119582e-15  9.801552e-15  -4.661591e-15  2.013967e-16  -1.471602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -3.614775e-15  1.663861e-16  -4.127449e-15  -1.442613e-15  -1.746333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b876b.final.pdb | -1.029951e-14  1.496227e-14  -7.060756e-15  9.179547e-15  -4.802270e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -5.955296e-15  8.227936e-16  -3.878389e-15  3.126175e-15  -3.982840e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -1.029951e-14  1.496227e-14  -7.060756e-15  9.179547e-15  -4.802270e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 2.198603e-15  2.875863e-15  -1.156361e-14  -4.097279e-14  -6.152177e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | 4.923962e-15  -3.307736e-16  -6.222613e-15  4.187175e-14  -4.034297e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | -2.838925e-15  1.211396e-15  -5.003536e-15  -9.468616e-16  -1.419418e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -1.787714e-15  -4.046575e-15  -4.49980e-15  6.038775e-15  -2.893433e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -2.061476e-15  -3.665721e-15  -3.997082e-15  -3.060312e-14  8.860984e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287197b7ab.final.pdb | 6.764896e-15  -3.97736e-16  -6.222613e-15  4.187175e-14  -4.034297e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | -7.119502e-15  9.801552e-15  -4.661591e-15  2.013967e-16  -1.471602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -2.731621e-15  2.346748e-15  -3.546198e-15  -1.731421e-14  -1.271033e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | -4.286718e-16  9.474595e-16  -1.737390e-14  -1.161532e-15  -4.623699e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fccc.final.pdb | -1.430751e-14  3.479965e-15  3.074999e-15  -3.368783e-15  5.326652e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cddf.final.pdb | 1.764999e-15  8.596089e-15  -6.555501e-15  1.630660e-14  1.283781e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 2.016758e-14  |
| PDB File Path                                      | Data                  |
|--------------------------------------------------|-----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -2.453313e-15 -2.290338e-15 -4.089566e-15 1.794523e-14 -1.316778e-15 4.862035e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -1.276082e-14 1.034626e-14 8.379159e-16 4.856656e-15 -5.614846e-15 7.451023e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | -1.276082e-14 1.034626e-14 8.379159e-16 4.856656e-15 -5.614846e-15 7.451023e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5ab4e57c7c6682ce6.final.pdb | -1.276082e-14 1.034626e-14 8.379159e-16 4.856656e-15 -5.614846e-15 7.451023e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | -8.630728e-15 5.407526e-15 -1.836887e-15 3.241186e-15 -3.499622e-15 -4.306521e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | -1.817030e-14 5.149596e-15 -2.168296e-15 -4.232458e-16 4.128525e-15 3.612138e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 1.017033e-15 1.523319e-16 -2.240198e-15 3.345959e-17 -2.591860e-15 4.200390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 1.017033e-15 1.523319e-16 -2.240198e-15 3.345959e-17 -2.591860e-15 4.200390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -7.941439e-15 1.518510e-14 -1.578002e-15 -2.909548e-14 8.032261e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 1.017033e-15 1.523319e-16 -2.240198e-15 3.345959e-17 -2.591860e-15 4.200390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | -5.221961e-15 -9.736322e-15 5.997400e-15 6.070268e-15 -2.418316e-15 3.370972e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | 3.806805e-15 5.291843e-15 -4.733301e-15 -3.187096e-15 -6.763370e-15 4.946522e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 1.017033e-15 1.523319e-16 -2.240198e-15 3.345959e-17 -2.591860e-15 4.200390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb | -3.178473e-15 2.101028e-15 -2.935584e-15 3.850911e-15 -1.677817e-15 2.692975e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | -4.091504e-15 -5.684307e-16 -6.250152e-15 -6.548067e-15 1.431167e-15 3.862926e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 1.017033e-15 1.523319e-16 -2.240198e-15 3.345959e-17 -2.591860e-15 4.200390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -1.787714e-15 | -4.046575e-15 | -4.449980e-15 | 6.038775e-15 | -2.893433e-15 | 1.474198e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | -2.731621e-15 | 2.346748e-15 | -3.546189e-15 | 1.173412e-14 | -1.271033e-15 | 3.610076e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12df9.final.pdb | -2.731621e-15 | 2.346748e-15 | -3.546189e-15 | 1.173412e-14 | -1.271033e-15 | 3.610076e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -2.453313e-15 | -2.290338e-15 | -4.089566e-15 | 1.794523e-14 | -1.317786e-15 | 4.860235e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -1.898576e-15 | -1.113054e-14 | 9.255486e-15 | 6.540050e-15 | 7.128481e-15 | 1.936069e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d50469ef569760.final.pdb | -2.453313e-15 | -2.290338e-15 | -4.089566e-15 | 1.794523e-14 | -1.317786e-15 | 4.860235e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -4.091504e-15 | -5.684307e-16 | -6.250152e-15 | 3.862926e-15 | 3.862926e-15 | 3.862926e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | -1.056195e-14 | 5.157868e-15 | 9.372035e-16 | 9.364338e-16 | 9.364338e-16 | 9.364338e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a183e9d0d81fb3ef.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a183e9d0d81fb3ef.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a183e9d0d81fb3ef.final.pdb | -2.052292e-14 | 2.201908e-15 | 8.625716e-16 | 1.565009e-14 | -3.082353e-15 | 9.881176e-15 |
|ideon | path                                                                 | 1         | 2         | 3         | 4         | 5         |
|-------|----------------------------------------------------------------------|-----------|-----------|-----------|-----------|-----------|
|1      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | -1.787714e-15 | -9.606722e-15 | 1.057570e-14 | 1.156166e-15 | -5.510458e-15 |
|2      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e723072a1fbd.final.pdb | -8.630728e-15 | 5.407526e-15 | -1.836887e-15 | 3.241186e-15 | -3.499622e-15 |
|3      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | -1.787714e-15 | -4.046575e-15 | -4.449980e-15 | 6.038775e-15 | -2.893433e-15 |
|4      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb  | -4.91504e-15 | -5.684307e-16 | -6.250152e-15 | -6.548067e-15 | 1.431167e-15 |
|5      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb  | -3.45853e-15 | 1.383552e-15 | -3.363432e-15 | 2.177578e-15 | -1.436534e-15 |
|6      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862bc1cad2078.final.pdb  | -3.080160e-15 | 1.497625e-15 | -4.630787e-15 | 4.194500e-16 | -1.146632e-15 |
|7      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb  | -2.890617e-15 | 5.154903e-16 | -1.688479e-15 | 4.856656e-15 | -5.614846e-15 |
|8      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb  | -2.185431e-15 | -1.675668e-15 | -3.667909e-15 | 2.422963e-15 | -2.262707e-15 |
|9      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e14fcae8dec44fa3.final.pdb  | 1.936069e-15 | -4.508646e-15 | -3.173172e-15 | 1.021981e-14 | -2.152070e-15 |
|10     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb  | -9.356281e-15 | 4.043765e-15 | -1.688479e-15 | 4.856656e-15 | -5.614846e-15 |
|11     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52ca629.final.pdb  | -1.808252e-16 | 1.781058e-15 | -8.104150e-15 | -2.551533e-15 | 1.674050e-14 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb
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-2.118205e-15
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-6.217749e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4c.final.pdb
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-7.706697e-15
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-4.601762e-15 -6.051364e-15 -4.405290e-15  3.814612e-15  5.732074e-16
-2.980231e-16
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-9.014897e-16
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-3.028930e-15  3.188080e-15 -8.540959e-15  3.679759e-15 -3.111226e-15
-4.518587e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
-1.418138e-15 -4.418414e-15  1.717681e-15  7.805707e-16  1.268665e-15
-6.442895e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\913cc65a2298261a.final.pdb
-5.875049e-15 -3.966858e-15 -3.946705e-16 -7.264916e-15  2.770726e-15
3.750066e-15
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-3.671361e-15 -1.317460e-14 -6.351811e-15  3.441816e-15 -8.901614e-15
-9.871778e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b6ef9ac3fe74395.final.pdb
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-8.440647e-15
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-6.157917e-15 -3.182763e-15 -3.946705e-16 -7.264916e-15  2.770726e-15
3.750066e-15
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-1.441872e-14
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-4.000254e-15 -2.226245e-15  1.322492e-15  3.410081e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
-1.075437e-15 -9.805348e-16 -6.333834e-15  4.369001e-15  6.658762e-18
1.076379e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
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-4.031528e-15

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3.546167e-15

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2.993568e-15

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1.051937e-14

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1.076379e-14

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3.397950e-15

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2.513393e-16

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3.700339e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
-2.097018e-15 -4.755210e-15 -2.769915e-15  3.864514e-15 -2.910132e-15
6.082895e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb
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6.082895e-16

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2.335970e-15

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-8.032185e-16

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1.076379e-14

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-8.488782e-16

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5.231369e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98b8e0df5986c138f.final.pdb
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2.513393e-16

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-8.144264e-15  3.772257e-15  1.881096e-15  3.666159e-15  6.235438e-15
8.213751e-15

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| File Path                                      | Values                            |
|-----------------------------------------------|-----------------------------------|
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ce34248de3e81a3c.final.pdb | -3.612207e-15 9.124232e-15 2.792593e-15 -4.164473e-15 -3.296659e-15 -1.275245e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\d02e697772494a61.final.pdb | 3.515383e-15 3.885782e-15 -5.759913e-15 1.101429e-14 7.912221e-15 2.150474e-14 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\d04221245d015047.final.pdb | -3.089973e-15 3.398384e-16 -3.153506e-15 3.577392e-15 -2.526613e-15 1.349753e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\d678141e4018054a.final.pdb | 4.452526e-15 2.776203e-15 -2.678278e-15 1.050662e-14 -1.368550e-14 2.843717e-14 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\d71b40af0f0efe39.final.pdb | 6.678768e-15 4.073364e-15 -1.459775e-15 -1.715807e-15 3.750111e-15 6.463137e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\dc0809eff10197e2.final.pdb | -1.054661e-14 7.086264e-15 -7.059824e-15 4.433356e-17 -2.251842e-16 1.348337e-14 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\d284037b1f36312a.final.pdb | 3.874162e-15 5.812916e-15 1.271242e-14 -1.283620e-14 1.216964e-14 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\e1163918d3707839.final.pdb | -2.44301e-15 4.685202e-15 -3.951946e-15 3.116818e-15 1.235536e-15 1.253831e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\e529e19ad281f35e.final.pdb | -4.850544e-15 4.659222e-15 -3.583279e-15 3.495473e-15 -1.423666e-15 7.886011e-16 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\e5602082718ec3a1.final.pdb | -2.097018e-15 4.755210e-15 -2.769915e-15 3.864514e-15 -2.910132e-15 6.082895e-16 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\e5d589d9960a960.final.pdb | -1.840040e-14 -1.674896e-15 -1.010601e-14 -3.963276e-15 -7.343756e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\e9df9e72307a2fbd.final.pdb | -8.084322e-15 2.786712e-16 -3.013548e-16 -6.173203e-16 -2.543566e-16 -1.352081e-16 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ea00f8694090cae7.final.pdb | -2.097018e-15 4.755210e-15 -2.769915e-15 3.864514e-15 -2.910132e-15 6.082895e-16 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\eb217be32db5050.final.pdb | -3.256977e-15 -1.895173e-16 -1.291048e-15 1.006076e-15 -1.110022e-15 2.513393e-16 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ec04b9545899c29d.final.pdb | -5.255254e-15 4.033408e-16 -2.700253e-15 2.445193e-15 -2.882198e-15 3.019119e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ee6862cbcad52078.final.pdb | -4.545009e-15 6.68301e-16 -3.879255e-15 2.416406e-15 -1.008215e-15 3.117103e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | -3.955287e-15 3.893765e-16 -2.927809e-15 2.652740e-15 -2.306336e-15 3.102613e-15 |
| e:\r-3.1.2\scripts\mpds\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | -3.089973e-15 3.398384e-16 -3.153506e-15 3.577392e-15 -2.526613e-15 1.349753e-15 |
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| Filename                          | Link to File                                      |
|----------------------------------|--------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff286d.final.pdb | 3.609979e-15 -3.691845e-15 -1.78154e-15 -1.29360e-15 -2.248147e-15 -3.287012e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -3.427566e-15 -3.019237e-15 4.218982e-15 -3.509898e-15 -3.287012e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -1.299738e-15 4.836876e-15 -6.312225e-15 -1.797970e-15 7.062779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -3.675613e-15 -4.157960e-15 2.619229e-16 -2.663837e-15 -1.231365e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | 4.023185e-15 -1.661730e-14 -4.785455e-15 5.097127e-15 4.107934e-15 -7.648861e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -6.127305e-15 -1.460909e-14 6.931131e-15 -5.365202e-15 4.051014e-15 -7.227478e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | -2.567148e-15 -1.299738e-15 4.836876e-15 -6.312225e-15 -1.797970e-15 7.062779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | -6.949414e-15 -2.858398e-15 -3.691004e-15 -8.902006e-15 -3.663661e-15 -7.18564e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b899c49e633199.final.pdb | -4.106219e-15 2.946234e-15 -3.882103e-17 -1.661517e-15 3.386333e-15 -3.652431e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfef12d3f9.final.pdb | -4.468993e-15 -5.945996e-15 -2.128253e-16 4.544980e-15 1.413465e-15 -5.747977e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -3.019237e-15 4.218982e-15 -3.509898e-15 8.285949e-16 3.478514e-15 -3.287012e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -2.567148e-15 -1.299738e-15 4.836876e-15 -6.312225e-15 -1.797970e-15 7.062779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8bb6ef9ac3fe74395.final.pdb | 5.17863e-15 -1.895572e-15 -3.395225e-15 -1.008803e-14 4.943051e-15 7.022268e-15 |
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-3.106258e-15  9.600951e-16 -1.444855e-15 -3.251757e-15 -4.144616e-16
-2.11058e-16

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7.398891e-16

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-1.277599e-14

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-2.440512e-15

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-2.211058e-16

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-6.267973e-16  8.723177e-16 -9.815755e-16 -1.897514e-14 -3.724190e-15
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-5.461424e-17

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-5.649936e-15

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1.528937e-15

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-3.036829e-15

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-3.652431e-15

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-2.110581e-16

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-9.190250e-16

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| Filename                                           | Values                                                                 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -2.017412e-15 3.246927e-15 -1.976058e-16  -1.0.123055e-14 6.449697e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be0d5986c138f.final.pdb   | 2.683008e-15 5.263913e-15 4.211393e-16 -7.683813e-15 -2.557961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d7e2fa.final.pdb   | 9.369323e-15 3.386711e-15 -8.0.15968e-15 -5.460904e-15 -8.809072e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb   | 3.321584e-15 -3.798750e-16 4.877265e-15 -1.280361e-14 -1.364872e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb   | 3.802605e-15 -1.012243e-15 2.419300e-15 -1.299555e-14 -2.673965e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb   | 7.103554e-16 2.311395e-15 3.513226e-15 -8.629186e-15 -2.557963e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd4d74b9c71d4dc.final.pdb   | 3.027911e-16 1.160381e-15 -1.651352e-16 -1.058336e-14 -3.708617e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb   | 9.369323e-15 1.795832e-15 3.386711e-15 -8.015968e-15 -5.460904e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb   | 2.603008e-15 5.263913e-15 4.211393e-16 -7.683813e-15 -2.557961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb   | 4.112946e-15 4.976007e-15 -1.765478e-15 -1.407654e-14 -1.817934e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb   | 2.603008e-15 5.263913e-15 4.211393e-16 -7.683813e-15 -2.557961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb   | 8.336165e-16 4.678400e-15 8.618211e-16 -9.226805e-15 -4.232503e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb   | 2.603008e-15 5.263913e-15 4.211393e-16 -7.683813e-15 -2.557961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb   | 2.603008e-15 5.263913e-15 4.211393e-16 -7.683813e-15 -2.557961e-15 |
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-1.814253e-14
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-1.277130e-14
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-1.096310e-16

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-2.309341e-15

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| File Path                                           | Coordinates                 |
|----------------------------------------------------|-----------------------------|
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| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\1f305f9598641eeeb2.final.pdb | 4.902625e-15 2.447257e-15 -9.382946e-15 6.755294e-15 -6.028483e-15 -1.700208e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\1f8a00b551b0a39.final.pdb | 8.091554e-16 -1.580009e-15 -3.877148e-15 -8.438859e-16 -1.030372e-15 -7.246392e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\219f45328d47579a.final.pdb | 6.043383e-16 -1.393722e-15 -3.889773e-15 -2.488128e-16 -2.589505e-15 -3.738130e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\2b3027889e2fdc42.final.pdb | 2.242037e-15 -5.648803e-15 -3.174585e-15 -9.276377e-15 4.064511e-15 5.174228e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\34eb328251842006.final.pdb | -3.062659e-15 1.247148e-15 -8.688801e-15 -1.154716e-14 6.251001e-15 1.771960e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\354b32871797b7ab.final.pdb | -2.011102e-15 -3.955930e-15 -7.359714e-15 -8.993617e-15 -2.779356e-16 1.078389e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\3b307889e2f6424.final.pdb | -8.206050e-14 1.692313e-15 2.521337e-15 -1.189475e-14 -1.539461e-14 2.806050e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\3d307889e2f6424.final.pdb | -3.768204e-15 -9.473407e-15 1.680157e-16 -8.428100e-15 -1.305454e-15 1.111827e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\411fc3b46e33793b.final.pdb | -1.221308e-14 -1.692313e-15 2.521337e-15 -1.189475e-14 -1.539461e-14 2.806050e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\4234011c3d3f6eddd.final.pdb | -3.062659e-15 1.247148e-15 -8.688801e-15 -1.154716e-14 6.251001e-15 1.771960e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\4343251486257df8.final.pdb | -8.586107e-15 5.527586e-15 -1.169208e-14 3.836398e-15 -1.696901e-14 2.928688e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\443421df75a7fcfc.final.pdb | -5.420278e-15 1.944165e-15 -6.403929e-16 -6.432282e-16 -6.482498e-16 -3.309033e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\448ef21dffe8cfd8.final.pdb | -3.062659e-15 1.247148e-15 -8.688801e-15 -1.154716e-14 6.251001e-15 1.771960e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\4ab4a5c7c6682ce6.final.pdb | -4.123028e-15 -5.488722e-15 9.546827e-16 -5.947868e-15 4.866509e-15 1.121912e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\4eea45b62cb6a25f.final.pdb | -8.206050e-14 1.692313e-15 2.521337e-15 -1.189475e-14 -1.539461e-14 2.806050e-14 |
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-5.06255e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb

6.013848e-15 -1.158480e-15 -1.125489e-14 -5.930339e-15  4.785376e-15
1.762528e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb

1.318256e-15 -2.323934e-15 -5.179484e-15 -5.876140e-16  4.287448e-16
-7.288470e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb

4.880666e-15  1.753724e-15 -6.103985e-15  4.922549e-15 -1.322151e-15
-1.818975e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb

-1.148185e-15  2.744579e-15 -2.948312e-15  2.004336e-16  5.158338e-16
7.021779e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a3ab69a98d33b478.final.pdb

1.054046e-15 -1.466896e-15 -4.462622e-15 -1.176720e-15 -2.620329e-15
-9.504714e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd74b9c71d4dc.final.pdb

2.242037e-15 -5.648803e-15 -3.174585e-15 -9.276377e-15  4.064511e-15
5.174228e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb

6.471548e-16 -2.005246e-15 -4.303291e-15 -6.834825e-16 -1.783085e-15
-1.355233e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd0bb7bb57.final.pdb

1.560941e-15 -4.214401e-15 -5.183937e-15  3.799101e-15  1.615081e-15
-5.062025e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb

3.160878e-15  1.917510e-15 -1.602455e-15  7.042357e-15 -7.390865e-15
-7.499594e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a1df.final.pdb

3.864137e-16 -2.630688e-15 -9.677398e-16 -7.140869e-15 -1.585073e-16
9.347810e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1ae5.final.pdb

-6.435875e-16 -9.357646e-17  1.562006e-15 -2.585792e-15  1.587847e-15
-5.366313e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
| PDB Path | 5.408749e-15 | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb |
|----------|-----------------|------------------------------------------------------------------|
|          | 2.401293e-14    | 2.098330e-15 7.817856e-15 2.984169e-15 -1.636390e-18                                    |
|          | 6.325275e-15    | 7.021355e-15 2.371946e-15 3.641330e-15 1.200868e-16 3.700542e-15 |
|          | 3.630450e-15    | -2.582270e-15 7.372796e-16 3.783838e-15 -2.413914e-15 3.391810e-15   |
|          | 8.433422e-15    | -3.872874e-16 1.936891e-15 2.765586e-15 -4.333498e-16 8.341815e-16   |
|          | 3.630450e-15    | -2.582270e-15 7.372796e-16 3.783838e-15 -2.413914e-15 3.391810e-15   |
|          | 3.808335e-15    | -1.656846e-14 4.513786e-15 6.161783e-15 -1.275143e-14 1.699791e-14 |
|          | 3.550729e-15    | -1.00161e-15 1.364537e-14 7.227337e-15 2.642502e-15 1.854377e-14 |
|          | 6.823719e-15    | 1.349728e-15 3.407900e-15 3.779140e-15 5.812171e-16 3.449939e-15 |
|          | 5.003581e-15    | 2.121479e-15 3.213647e-15 -6.548303e-17 -4.308722e-15 6.867300e-16 |
|          | 1.443633e-14    | -6.122041e-15 2.703264e-15 -8.316974e-17 7.983719e-15 5.080644e-15 |
|          | 3.54b32871797b7ab.final.pdb | 4.850984e-15 -5.475079e-15 -1.200635e-15 -3.057750e-16 -1.042828e-14 |
|          | 8.339545e-16    | -4.631146e-15 -8.976008e-15 -2.363711e-16 -7.294514e-15 7.221549e-15 |
|          | 1.216066e-14    | 6.389138e-15 -4.350483e-15 6.664376e-15 5.241485e-15 -1.570999e-14|
|          | 1.344677e-14    | -8.686204e-15 3.952640e-15 -1.016111e-15 3.140181e-15 -2.886800e-15|
|          | 4.600499e-15    | 3.481625e-15 3.270184e-15 1.929337e-15 8.409182e-16 5.408749e-15 |
| Path                                      | Value                  | Value                  | Value                  | Value                  | Value                  |
|-------------------------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -3.999831e-15          | 1.023705e-14           | -1.560547e-14          | 1.224239e-14           | 1.363690e-18           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 9.332642e-15           | 5.010891e-15           | 4.113496e-15           | 5.729249e-15           | 6.726209e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 1.023705e-14           | 6.879016e-15           | 1.771164e-15           | 2.493926e-15           | -1.221916e-14          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 8.384171e-15           | 3.630979e-15           | 6.764990e-15           | -1.137960e-15          | 2.246136e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | 1.224239e-14           | 1.446641e-15           | 5.975764e-16           | 9.801638e-16           | 2.097505e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 9.332642e-15           | 4.113496e-15           | 6.879016e-15           | 1.771164e-15           | 2.493926e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 4.600499e-15           | 3.270184e-15           | 1.929337e-15           | 8.409182e-16           | 5.088749e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 3.223913e-15           | 7.265854e-16           | -1.449259e-15          | 2.232658e-15           | -6.202473e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 1.204104e-14           | 3.368545e-15           | 6.755592e-15           | 1.313555e-14           | -3.740772e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 4.600499e-15           | 3.270184e-15           | 1.929337e-15           | 8.409182e-16           | 5.088749e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcf.final.pdb | 1.224239e-14           | 1.446641e-15           | 5.975764e-16           | 9.801638e-16           | 2.097505e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | 8.384171e-15           | 3.630979e-15           | 6.764990e-15           | -1.137960e-15          | 2.246136e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 1.204104e-14           | 3.368545e-15           | 6.755592e-15           | 1.313555e-14           | -3.740772e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 3.223913e-15           | 7.265854e-16           | -1.449259e-15          | 2.232658e-15           | -6.202473e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 1.204104e-14           | 3.368545e-15           | 6.755592e-15           | 1.313555e-14           | -3.740772e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | 5.803581e-15           | 3.213647e-15           | 6.548303e-17           | -4.308722e-15          | 2.214798e-15           |

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6.867300e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
5.803581e-15 2.214798e-15 3.213647e-15 -6.548303e-17 -4.308722e-15
6.867300e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfe12d3f9.final.pdb
1.054068e-14 2.535071e-15 1.487598e-15 5.765790e-15 -3.983461e-15
1.069385e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
4.600499e-15 3.481625e-15 3.270184e-15 1.929337e-15 8.409182e-16
5.408749e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
8.384171e-15 -3.032145e-15 3.630979e-15 6.764990e-15 -1.137960e-15
2.246136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
9.075270e-15 -3.699401e-16 -8.436755e-15 7.164844e-15 4.534386e-17
-1.528512e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
5.640968e-15 -5.325267e-15 1.744926e-14 -5.34209e-16 1.039922e-14
1.005635e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be0d5986c138f.final.pdb
7.003696e-15 1.446641e-15 -5.975764e-16 9.801638e-16 1.722560e-16
2.097505e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
6.856992e-15 -3.748748e-15 1.505812e-15 3.678918e-15 3.798508e-15
4.432649e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9da8ed0d81fb3ef.final.pdb
1.706343e-14 2.042823e-14 8.162077e-15 -1.203464e-14 1.549023e-14
-4.518418e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
4.330330e-15 -5.318827e-16 2.236222e-15 -1.058291e-15 -6.894108e-16
6.389713e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
9.332642e-15 5.010891e-15 4.113496e-15 6.879016e-15 1.771164e-15
2.493926e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
1.179018e-14 8.277475e-15 5.228222e-15 6.744448e-15 -8.776450e-16
4.067918e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
6.257283e-15 5.315007e-16 2.182915e-15 3.766362e-15 -2.149807e-16
3.781913e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
5.803581e-15 2.214798e-15 3.213647e-15 -6.548303e-17 -4.308722e-15
6.867300e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
6.729730e-15 2.432540e-16 2.461236e-15 3.683748e-15 -4.312563e-16
2.663727e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
6.856992e-15 -3.748748e-15 1.505812e-15 3.678918e-15 3.798508e-15
4.432649e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
4.600499e-15 -6.896025e-15 7.938391e-16 3.826802e-15 -7.898611e-15
5.814462e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
7.003696e-15 1.446641e-15 -5.975764e-16 9.801638e-16 1.722560e-16
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcede41949d.final.pdb
2.066859e-15 -3.156211e-15 2.445986e-15 -4.341032e-16 -5.315917e-15
-2.374464e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
3.848469e-15 -3.548062e-15 1.593615e-15 2.407798e-16 -3.440273e-15
-3.738679e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-3.051394e-15 -4.596703e-15 2.830318e-16 4.454771e-15 9.558778e-15
-5.276209e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
1.954407e-15 -2.541562e-15 6.243458e-16 -2.470828e-16 -3.134132e-15
-1.588963e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
7.100783e-16 -1.714701e-15 -2.269356e-15 1.408526e-15 8.646766e-15
-5.364852e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb
2.832388e-15 -2.872598e-15 7.337267e-16 1.072134e-15 -2.637687e-15
-2.202901e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
7.100783e-16 -1.714701e-15 -2.269356e-15 1.408526e-15 8.646766e-15
-5.364852e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-1.759941e-15 -3.940306e-15 -4.776535e-15 6.036415e-15 -3.199137e-16
1.164372e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
8.928848e-16 -9.357413e-15 -6.115742e-15 4.417051e-15 5.265029e-15
-6.303630e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
2.111094e-15 -2.35073e-15 3.552193e-16 1.432277e-17 -2.60872e-15
-1.275083e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
8.907389e-15 2.099120e-15 -1.118958e-15 -2.889974e-15 -1.141902e-14
7.877628e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-6.406069e-15 -7.850516e-15 7.355501e-15 6.448222e-15 -2.935614e-15
-4.280041e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
3.797631e-15 2.235843e-16 1.778349e-15 3.727654e-15 -1.792431e-14
1.994100e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb
-3.051394e-15 -4.596703e-15 2.830318e-16 4.454771e-16 9.558778e-15
-5.276209e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
5.173397e-15 3.201536e-15 -8.075751e-16 -5.261341e-15 -7.650338e-15
1.568822e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357e3ee6642bf12.final.pdb
-1.415152e-16 -7.102562e-15 4.628905e-15 3.982181e-15 -6.60733e-15
-2.397025e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb
1.474622e-14 -8.954815e-15 1.705911e-15 -8.439420e-15 -2.645653e-15
-7.148705e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb
-9.550069e-15 4.545080e-15 9.428161e-15 8.670223e-15 5.567388e-15
3.518218e-15

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| File Path                                                                 | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 |
|--------------------------------------------------------------------------|---------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8cdfb.final.pdb       | 4.557493e-15 | 2.29457e-15 | -3.423550e-15 | -4.317283e-15 | -9.090690e-16 | -7.339740e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb     | 1.642875e-15 | 1.878308e-14 | -2.957781e-15 | 1.378046e-15 | -1.576455e-14 | -1.030299e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb     | 1.100643e-14 | -1.086664e-16 | -4.572175e-16 | 2.232517e-15 | -1.596935e-14 | 9.190174e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb      | -8.701730e-16 | -4.752223e-16 | -3.829700e-16 | -4.059161e-15 | -3.156076e-15 | -6.469283e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb      | -1.079482e-16 | 5.327957e-15 | 1.534052e-16 | -4.657805e-15 | -3.944247e-15 | -1.151549e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb      | 2.426487e-15 | -7.190066e-16 | -9.195785e-16 | -2.403085e-15 | -2.934562e-15 | 4.064930e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\60577f451d583d06.final.pdb      | 1.166006e-16 | -3.733094e-15 | 7.538686e-17 | -7.827841e-16 | -2.610833e-15 | -6.094270e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\61505f59b910a8b8.final.pdb      | -7.781574e-15 | 8.930401e-15 | 2.470205e-15 | -9.881874e-16 | -1.032565e-14 | -4.537841e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb       | 4.714494e-16 | 1.317276e-15 | -1.976835e-15 | -2.831141e-15 | -3.278113e-15 | -3.317313e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6359b0b3f8d9c8a2.final.pdb       | -1.045123e-14 | 7.957247e-15 | -1.334120e-14 | 2.520105e-15 | 1.902662e-15 | -1.678193e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6470e68bf992c94f.final.pdb       | -7.781574e-15 | 8.930401e-15 | 2.470205e-15 | -9.881874e-16 | -1.032565e-14 | -4.537841e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb       | -8.701730e-16 | -4.752223e-16 | -3.829700e-16 | -4.059161e-15 | -3.156076e-15 | -6.469283e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\669760178986bef01.final.pdb      | -4.800012e-15 | -1.251507e-15 | -3.758350e-15 | 4.389397e-15 | -8.049144e-15 | -1.407667e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\677f90d47926b1c8.final.pdb       | 4.714494e-16 | 1.317276e-15 | -1.976835e-15 | -2.831141e-15 | -3.278113e-15 | -3.317313e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\687f90d47926b1c8.final.pdb       | -1.045123e-14 | 7.957247e-15 | -1.334120e-14 | 2.520105e-15 | 1.902662e-15 | -1.678193e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\697f90d47926b1c8.final.pdb       | -7.781574e-15 | 8.930401e-15 | 2.470205e-15 | -9.881874e-16 | -1.032565e-14 | -4.537841e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb       | 4.714494e-16 | 1.317276e-15 | -1.976835e-15 | -2.831141e-15 | -3.278113e-15 | -3.317313e-15 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb         |
|----------------------------------------------|
| 6.098225e-16  6.703048e-16 -2.521618e-15 -1.123549e-15 -2.759359e-15 |
| -2.934111e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb         |
|----------------------------------------------|
| 9.528776e-15 -1.515250e-15 -4.493116e-15  8.211323e-15  1.936745e-15 |
| -3.288794e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb          |
|----------------------------------------------|
| 2.907488e-15 -2.50219e-15  1.443433e-15  2.842704e-15 -1.795625e-15 |
| 9.528776e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb          |
|----------------------------------------------|
| 2.426487e-15 -7.190066e-16 -9.195785e-16 -2.403085e-15 -2.934562e-16 |
| 4.064930e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb          |
|----------------------------------------------|
| 5.791451e-16  2.228224e-15  1.988093e-15  4.176112e-15 -1.918758e-15 |
| -3.437654e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb          |
|----------------------------------------------|
| 2.907488e-15 -2.50219e-15  1.443433e-15  2.842704e-15 -1.795625e-15 |
| 9.528776e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9df4f0d87c1017b.final.pdb          |
|----------------------------------------------|
| 2.426487e-15 -7.190066e-16 -9.195785e-16 -2.403085e-15 -2.934562e-16 |
| 4.064930e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb          |
|----------------------------------------------|
| 4.679845e-16  5.36739e-15  9.553572e-16  1.015621e-15  5.864389e-15 |
| -7.228025e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb          |
|----------------------------------------------|
| 2.907488e-15 -2.50219e-15  1.443433e-15  2.842704e-15 -1.795625e-15 |
| 9.528776e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb          |
|----------------------------------------------|
| 5.791451e-16  2.228224e-15  1.988093e-15  4.176112e-15 -1.918758e-15 |
| 3.222211e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb          |
|----------------------------------------------|
| 4.679845e-16  5.36739e-15  9.553572e-16  1.015621e-15  5.864389e-15 |
| -7.228025e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb          |
|----------------------------------------------|
| 2.677447e-15  1.267638e-15 -2.397602e-15 -5.226742e-15 -4.863185e-15 |
| -4.278122e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb          |
|----------------------------------------------|
| 7.252958e-15  1.415300e-14  1.168501e-14  1.874966e-14 -2.786125e-15 |
| -6.010932e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb          |
|----------------------------------------------|
| 1.273633e-14 -3.927808e-15  3.346773e-16 -1.08317e-14 -1.336470e-14 |
| 7.099707e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d80800eff10197e2.final.pdb          |
|----------------------------------------------|
| 8.451188e-15 -9.591100e-15  6.980665e-15 -4.699343e-15  4.943691e-16 |
| -2.462284e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb          |
|----------------------------------------------|
| 4.451188e-15 -9.591100e-15  6.980665e-15 -4.699343e-15  4.943691e-16 |
| -2.462284e-15 |
| File Path                                                                 | Values                                      |
|--------------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                              | -7.199446e-16 3.721739e-16 3.384158e-15 -6.252370e-16 -2.830383e-15 3.423215e-15 -1.707653e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb    | 5.768168e-17 5.305246e-15 6.992885e-16 7.203684e-16 5.720762e-15 -3.521917e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb     | -1.019283e-16 2.216910e-15 -3.316360e-15 -3.213508e-15 3.341505e-15 -1.668032e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb     | 3.522056e-16 3.715892e-15 -4.232725e-15 -2.191076e-15 5.741876e-15 -4.402782e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb      | -8.686607e-16 8.157817e-16 -4.234265e-15 9.285352e-15 3.691135e-15 2.389635e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb      | 7.719541e-16 -4.304255e-15 -4.858766e-15 -6.010359e-15 6.177211e-15 -4.306446e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | 1.950234e-17 3.293306e-15 -2.438590e-15 -2.608090e-15 3.117942e-15 -4.645679e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb      | 1.151682e-15 6.974669e-15 -1.034289e-15 -5.009355e-15 4.373507e-15 9.732017e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb      | 4.592282e-17 3.023439e-15 -2.749407e-15 -2.984778e-15 3.313541e-15 -1.332024e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb      | 1.151682e-15 6.974669e-15 -1.034289e-15 -5.009355e-15 4.373507e-15 9.732017e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb      | -6.868938e-16 -2.912486e-15 6.904199e-15 2.796254e-15 -7.966776e-15 -1.596479e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb      | 2.589565e-15 -2.137065e-15 -8.667546e-15 -1.724869e-15 -1.052018e-14 -2.213561e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2dca42.final.pdb      | -1.530327e-16 1.465956e-15 -3.102553e-16 -2.737947e-15 3.616189e-15 -2.027945e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb       | -6.653138e-16 6.336761e-15 -2.722216e-16 -1.881494e-15 2.050662e-15 -2.426176e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb       | 5.654468e-15 4.589797e-15 1.688262e-16 -3.843332e-15 -1.144478e-15 -3.109356e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb       | -5.985855e-15 1.467863e-14 -6.937229e-15 -9.922335e-15 1.459058e-14 1.278351e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb       | 7.719541e-16 -4.304255e-15 -4.858766e-15 -6.010359e-15 6.177211e-15 -4.306446e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb       | 8.755543e-16 4.420759e-15 6.818763e-16 -1.215360e-15 2.598618e-15 |

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-4.656961e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
-1.023977e-15 5.404911e-16 -1.786313e-15 -1.006364e-14 2.872829e-15 2.976967e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
-1.111970e-16 2.299590e-15 -2.781156e-15 -4.563658e-15 2.729748e-15 -1.731078e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
3.522056e-16 3.715892e-15 -4.232725e-15 -2.191076e-15 5.741876e-15 -4.027828e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
3.804289e-16 2.236784e-15 -4.170015e-15 -1.145328e-14 2.484982e-16 -1.338718e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
-6.653138e-16 6.336761e-15 -2.722216e-16 -1.881494e-15 2.050662e-15 -2.426176e-16  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
-6.653138e-16 6.336761e-15 -2.722216e-16 -1.881494e-15 2.050662e-15 -2.426176e-16  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
8.755543e-16 4.420759e-15 6.818763e-16 -1.215360e-15 2.598618e-15 -4.953963e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
-8.686607e-16 8.157817e-16 -4.234265e-15 9.285352e-16 3.691135e-15 2.389635e-16  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
-1.023977e-15 5.404911e-16 -1.786313e-15 -1.006364e-14 2.872829e-15 2.976967e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
3.522056e-16 3.715892e-15 -4.232725e-15 -2.191076e-15 5.741876e-15 -4.402782e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f490d598e1a.final.pdb
-2.366644e-15 -3.285750e-15 -8.869511e-15 -5.318794e-16 1.215176e-15 -3.862986e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
9.115404e-16 -5.940181e-16 -7.621056e-15 -9.787824e-15 1.300025e-14 -1.120244e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e033b.final.pdb
-1.980226e-15 2.544942e-15 -2.841246e-15 -3.093719e-15 6.814402e-16 1.357990e-15  
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7.049851e-17 -1.757872e-15 -1.834540e-15 -2.634328e-15 3.653043e-15 -3.176419e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-2.145649e-15 -9.433855e-15 -6.084019e-15 -9.135185e-15 5.697794e-16 -3.543990e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
2.232130e-17 2.291141e-15 -2.525233e-15 -2.330298e-15 3.622134e-15
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-1.667019e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
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-4.242176e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
-6.653138e-16  6.336751e-15 -2.722216e-16 -1.881494e-15  2.050662e-15
-4.242176e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\af4d74b9c71d4dc.final.pdb
-6.653138e-16  6.336751e-15 -2.722216e-16 -1.881494e-15  2.050662e-15
-4.242176e-16
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E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
1.719704e-15  2.051376e-15 -3.172800e-16  2.369319e-16 -1.055997e-15
3.567740e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
2.614003e-15 -2.188979e-16  9.722707e-16  1.791321e-15 -2.797266e-15
4.281680e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
3.827699e-15  2.466437e-15  4.568592e-16 -8.024922e-16 -1.609863e-15
2.951379e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-1.595256e-15  1.420533e-15  4.482756e-15  6.463851e-16 -8.274452e-16
8.635576e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
7.174265e-16  2.340347e-15  6.789029e-16  2.637470e-16 -1.004943e-15
2.439330e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
8.604284e-16 -7.888016e-16 -6.959781e-16  1.964777e-15 -2.437199e-15
4.573013e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
7.827762e-16  1.807376e-15 -1.364346e-15 -4.291434e-16 -9.176509e-16
7.195755e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-4.372115e-16  8.347718e-15  4.140040e-15 -9.271175e-15  8.926767e-16
-2.929374e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
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2.676554e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
2.821303e-16  3.274328e-15  6.566568e-15 -5.699968e-15 -7.540865e-15
-5.183123e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb
9.581533e-16  2.726731e-16  9.642772e-16  1.686763e-16 -1.686479e-15
2.789668e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
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-5.183123e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-5.790501e-15  5.638349e-15 -1.453293e-15 -5.265550e-15  3.519842e-15
7.423164e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
1.127484e-14  5.441458e-15  1.488147e-15 -7.318595e-15 -6.884596e-15
-3.097995e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
1.016554e-15  2.411763e-15  8.019556e-16  5.311206e-17 -2.700090e-15
2.498284e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fc3b3d4633793b0.final.pdb
6.724374e-15  1.380586e-15 -8.582667e-16  2.403000e-15  4.298832e-16
4.364797e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
4.867578e-15 -5.505090e-16 -1.637278e-15 -2.799082e-16  3.626738e-15
1.315847e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
5.167938e-15  7.264385e-15 -3.908743e-15  5.123635e-15  4.757459e-15
1.797732e-14

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
5.730626e-16  6.443873e-15  1.064094e-14 -7.782105e-15  8.182784e-16
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-6.299316e-15  7.392940e-15 -2.309242e-15  8.147890e-16 -3.391009e-15
2.426403e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb
-4.565281e-15  1.383677e-15 -7.143244e-15  3.820647e-15 -2.878992e-15
8.147890e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
1.130710e-14  5.922050e-17  9.366336e-15 -5.433984e-15  1.941940e-15
8.364025e-16

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-5.183123e-16

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8.635576e-16

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4.364797e-16

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-1.337646e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
2.769289e-15  3.150489e-15  4.284899e-15 -6.417184e-16 -4.988651e-15
-4.754062e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
6.724374e-15  1.380586e-15 -8.582667e-16  2.403000e-16  4.298832e-16
4.364797e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
8.604284e-16 -7.888016e-16  9.695781e-16  1.941940e-15 -2.437199e-15
4.573013e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
7.643205e-16  2.911973e-15  1.363731e-15 -6.175985e-16 -1.773404e-15
2.321116e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
1.495337e-15  2.456866e-15  5.186536e-16  4.174040e-16 -2.893431e-15
2.480937e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-5.331898e-16  2.047878e-15  9.628693e-16  1.321719e-16 -1.34096e-15
2.592914e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a8ad.final.pdb
1.250976e-16  2.436552e-15 -9.315925e-16  2.028089e-15 -1.277342e-15
2.893646e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
2.987173e-15  1.885376e-15 -3.172400e-15  1.282001e-15 -1.410897e-15
4.618853e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
4.040177e-15  1.038629e-14  1.487822e-15  4.362165e-15 -4.191872e-15
-2.993912e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa29.final.pdb
-1.595256e-15  1.420533e-15  4.827565e-15  6.463851e-16 -8.274452e-16
8.635576e-16

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| File Path                                                                 | Numbers                                                                 |
|--------------------------------------------------------------------------|-------------------------------------------------------------------------|
| E:\\R-3.1.2\\scripts\\40.1ns_data\\NAT0.pdb                       | -3.082224e-15  -1.700446e-15  1.350312e-15  2.491929e-15 -4.050201e-15 |
| E:\\R-3.1.2\\scripts\\40.1ns_data\\LJP6.pdb                       | -2.993554e-15  -4.962661e-16 -4.724211e-16  3.914347e-15 -7.607428e-16 |
| E:\\R-3.1.2\\scripts\\40.1ns_data\\3WY9.pdb                        | -4.388972e-15 -1.886893e-15  2.183733e-15  2.745943e-15 -3.387800e-15 |
| E:\\R-3.1.2\\scripts\\40.1ns_data\\ZSP9.pdb                       | -4.571149e-15 -2.091296e-15 -2.331323e-15  3.546617e-15  1.133203e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\013d855ad26c877c.final.pdb | -3.864948e-15 -8.310774e-16  2.320694e-15  9.384456e-15 -4.341363e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0a2a705342ca0d54.final.pdb | -3.877562e-15 -2.419269e-15  7.025253e-16  3.806045e-15 -2.57942e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0a59fcede4b194d9.final.pdb | -8.783506e-16  2.385302e-15  2.315716e-15 -9.591589e-17 -4.244270e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\0dba59f3306825e.final.pdb | -3.684537e-15 -4.668286e-15  2.483758e-15 -3.803025e-16 -1.642133e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\126f26a78b57339c.final.pdb | -3.822527e-15 -1.014481e-14 -2.766274e-15  8.357066e-15 -4.575417e-17 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\12f06f3e342df706.final.pdb | -7.26139e-15 -2.846011e-15  1.600028e-15  3.247464e-15 -3.383669e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\1f305f598641eeb2.final.pdb | -7.666454e-15 -7.585078e-15 -5.821828e-15  6.823339e-15  5.265107e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\1f8a00b551be0a39.final.pdb | -7.666454e-15 -7.585078e-15 -5.821828e-15  6.823339e-15  5.265107e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\219f45328d47579a.final.pdb | -9.512299e-17 -6.747505e-16  7.470447e-15  8.107591e-15 -5.509750e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\238dd3918e54336d.final.pdb | -1.391653e-14 -1.588220e-14  1.853900e-15  1.074480e-14  1.037313e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\2b3027889e2fdc42.final.pdb | -3.162114e-15 -2.805858e-15  2.046942e-15  4.144616e-15 -3.368776e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\2fcb3b46e33793b0.final.pdb | -2.798972e-16  1.713028e-15  4.504436e-16  7.126010e-17 -2.657168e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\34eb328251842006.final.pdb | -1.458735e-15 |

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| File Path                                                                 | Values                                                                 |
|---------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | -2.907092e-16 -1.401111e-15 5.467196e-15 9.660744e-16 -2.257922e-15 -5.181570e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb        | -5.08047e-15 4.955216e-15 1.444426e-15 -1.696349e-15 2.001994e-15 9.662181e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb        | -2.807082e-15 -2.633332e-15 9.304714e-16 2.153436e-15 -1.714434e-15 -4.572754e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c7id4dc.final.pdb        | -2.798972e-16 1.713028e-15 4.504436e-16 7.126010e-17 -2.657168e-15 -4.587335e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a8234b4c668e.final.pdb         | -3.535219e-15 -2.852267e-15 1.610490e-15 3.985931e-15 -1.997177e-15 -3.296901e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb        | -6.161477e-15 -3.336752e-15 6.072249e-15 4.550750e-15 -2.329522e-15 -3.412901e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e6973c63.final.pdb         | -2.895624e-15 2.633900e-15 5.787890e-15 1.525498e-16 1.031442e-15 -3.776686e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb        | -8.783586e-16 2.385302e-15 2.315716e-15 -9.591589e-17 -4.244270e-15 -3.344424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb        | -3.448134e-15 -2.664812e-15 3.026101e-15 -3.597055e-15 -6.724832e-15 -5.177648e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb        | -8.783586e-16 2.385302e-15 2.315716e-15 -9.591589e-17 -4.244270e-15 -3.344424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb        | -2.576671e-15 -1.263757e-15 6.534062e-16 4.083675e-15 -3.552286e-15 -1.252107e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb        | -8.783586e-16 2.385302e-15 2.315716e-15 -9.591589e-17 -4.244270e-15 -3.344424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb         | -8.783586e-16 2.385302e-15 2.315716e-15 -9.591589e-17 -4.244270e-15 -3.344424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88ca585f3a288.final.pdb         | -3.07831e-15 -2.484067e-15 5.466773e-16 3.851881e-15 -3.587785e-15 -4.001859e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb         | -1.489255e-16 1.612414e-15 1.263547e-14 8.584416e-15 -9.709361e-15 -8.056755e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb         | -2.576671e-15 -1.263757e-15 6.534062e-16 4.083675e-15 -3.552286e-15 -1.252107e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb         | -6.347302e-15 2.603266e-15 -1.061602e-14 9.315626e-15 -9.985086e-15 -8.344113e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb          | -2.576671e-15 -1.263757e-15 6.534062e-16 4.083675e-15 -3.552286e-15 -1.252107e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d052087e375403e7.final.pdb         | -8.783586e-16 2.385302e-15 2.315716e-15 -9.591589e-17 -4.244270e-15 -3.344424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d052087e375403e7.final.pdb         | -3.307831e-15 -2.484067e-15 5.466773e-16 3.851881e-15 -3.587785e-15 -4.001859e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 4.819349e-15 | 4.854681e-15 | 5.080485e-15 | 9.017020e-15 | -8.659791e-15 |
|-----------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -8.494359e-15 | -2.624936e-15 | -4.759235e-15 | 4.711227e-16 | 1.193909e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -2.429652e-15 | 3.462529e-15 | 8.375913e-15 | -7.199213e-15 | -1.857408e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 7.439798e-15 | 2.763379e-15 | -5.759886e-15 | -4.31776e-15 | 2.208427e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.373530e-15 | -6.665085e-15 | 6.555396e-15 | -1.099218e-14 | -7.792554e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | -2.907092e-16 | -1.401111e-15 | 5.467196e-15 | 9.660744e-16 | -2.257922e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | -2.5463449e-15 | 3.151936e-15 | 1.013806e-15 | 3.936449e-15 | -3.119301e-15 |

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-2.943562e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
5.950288e-16 9.548159e-15 -3.045937e-15 6.767467e-16 -6.389945e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
5.532494e-15 8.148985e-15 -1.491143e-16 -9.420897e-16 -1.060593e-15
-8.266052e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-5.471620e-15 8.015015e-15 1.085506e-14 -4.137125e-16 -1.041469e-15
4.736208e-16

[,217] [,218] [,219] [,220] [,221] [,222]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
5.331560e-16 -7.942865e-17 -4.03767e-15 -6.28510e-15 -4.218822e-16
-5.157976e-16
E:\R-3.1.2\scripts\40.1ns_data\LJ36.pdb
2.875535e-15 -8.965068e-16 -6.958700e-15 -4.467057e-15 -3.640165e-15
-1.580122e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
2.837331e-15 2.059161e-15 -7.022411e-15 -3.159445e-15 -1.159445e-15
-2.557268e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
9.150113e-16 -9.578049e-16 -5.259641e-15 -5.568262e-16 -9.596441e-16
-3.604911e-16
E:\R-3.1.2\scripts\40.1ns_data\L3P6.pdb
1.091298e-15 -3.098188e-15 -5.210807e-15 -2.638430e-15 -1.127733e-15
-3.823419e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
8.138347e-16 -2.764615e-15 -6.437572e-15 -3.405714e-15 -4.822105e-16
1.874222e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
3.725371e-15 -5.259857e-15 -4.256787e-15 -5.850800e-15 -2.884298e-15
-6.562590e-15
E:\R-3.1.2\scripts\40.1ns_data\L3P6.pdb
1.267625e-15 -2.483983e-16 -3.733138e-15 -3.974817e-15 -4.210615e-16
6.058375e-15

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| PDB File                          | Coordinates                  |
|----------------------------------|------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | 8.923155e-16 -2.967055e-15 -5.467646e-15 -4.139163e-15 -1.503150e-15 -7.780990e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 9.342615e-17 -2.135151e-15 -7.146702e-15 -6.022182e-15 -2.315052e-15 -1.494126e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | 1.570243e-15 1.627102e-15 -5.132978e-15 -3.330020e-15 -1.679456e-15 -2.530945e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 1.210687e-16 -6.212378e-15 -1.066900e-14 -9.057935e-16 1.845067e-15 -2.058795e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 1.204714e-15 -6.980609e-15 -8.728824e-15 5.191045e-16 1.664050e-15 9.000060e-15 |

[223] [,224] [,225] [,226] [,227] [,228]
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb | 2.936322e-15 -5.482694e-16 -3.605151e-15 9.057935e-16 1.845067e-15 -2.058795e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb | 2.894697e-15 3.204892e-16 -3.907434e-15 -1.639793e-15 1.763597e-15 -2.856312e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | 2.139327e-15 1.237876e-15 -2.839191e-15 -4.790808e-15 2.242899e-15 -2.024548e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | 2.141026e-15 -1.975491e-16 -3.991877e-15 1.435218e-15 1.606004e-15 -1.834378e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\13d855ad26c877c.pdb | 3.17911e-15 1.214248e-16 -3.51407e-15 4.079697e-15 -5.725813e-15 -2.328505e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\10349924ca0d54.pdb | 3.294822e-15 1.584917e-15 -3.782031e-15 3.129152e-15 3.158248e-15 -3.242812e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\10549feadb914d9.pdb | 3.205303e-16 2.039753e-15 -3.093375e-15 -9.030038e-16 4.674488e-15 -1.038002e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\16d59f3306825e8.pdb | 9.944751e-16 -1.084261e-15 -4.076522e-15 -5.589652e-15 8.637066e-15 -5.217986e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\16f26a78b57339c.pdb | 6.233557e-15 9.091531e-16 -5.824906e-15 4.827363e-15 1.974426e-15 -3.549960e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\12f06f3e342df706.pdb | 2.002751e-15 8.466833e-16 -3.417956e-15 1.459480e-16 2.953334e-15 -2.355332e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\18618a2a251b867b.pdb | 4.584086e-15 5.495175e-15 7.943032e-16 5.909860e-15 -4.449986e-15 2.069203e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\1f305f598641eeb2.pdb | 2.085571e-15 4.964637e-16 -3.551497e-16 6.878139e-16 2.472320e-15 -1.656000e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\1f8a00b551bea39.pdb | 2.085571e-15 4.964637e-16 -3.551497e-16 6.878139e-16 2.472320e-15 -1.656000e-15 |
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3.205303e-16  2.039753e-15 -3.093375e-15 -9.030038e-16  4.674488e-15
-1.038002e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
7.005779e-15  1.487718e-15 -3.669344e-15  2.945776e-15  6.751755e-15
1.782534e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
1.220179e-14  2.554898e-15 -2.376688e-15  2.129387e-15  6.461378e-15
-1.181526e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
9.944751e-16 -1.084261e-15 -4.076522e-15 -5.589652e-15  8.637066e-15
-5.217986e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
1.220179e-14  2.554898e-15 -2.376688e-15  2.129387e-15  6.461378e-15
-1.181526e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
2.145681e-15  2.013859e-16 -4.149163e-15  5.425957e-16  4.002318e-15
-1.743478e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc4.final.pdb
1.42725e-15  -8.014705e-15 -1.147422e-14  1.581428e-15 -4.36986e-15
-7.974212e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-4.792242e-15  6.865325e-15 -4.592146e-15  2.366828e-15  2.086622e-15
-4.809701e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70aad0f1be4.final.pdb
6.83120e-15  -3.038488e-15  1.449158e-15  1.750492e-15  2.041621e-15
-6.00164e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910d667f22872.final.pdb
1.298601e-15  3.732409e-16 -3.250011e-15 -1.266655e-15 -2.920854e-15
-2.75845e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
3.205303e-16  2.039753e-15 -3.093375e-15 -9.030038e-16  4.674488e-15
-1.038002e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f099.final.pdb
-2.009878e-15  3.689847e-15 -6.062530e-15 -3.838035e-15  2.218953e-15
-1.465668e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\80489c94a633196.final.pdb
-1.253772e-15  1.707301e-15 -2.316374e-15 -1.768554e-15  5.092620e-15
3.927089e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
-1.253772e-15  1.707301e-15 -2.316374e-15 -1.768554e-15  5.092620e-15
3.927089e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c00efcfe12d3f9.final.pdb
-8.541351e-16 -1.994186e-15 -3.291505e-15 -1.326200e-15  1.586310e-15
3.201660e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
9.944751e-16 -1.084261e-15 -4.076522e-15 -5.589652e-15  8.637066e-15
-5.217986e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
6.831207e-15 -3.038488e-15  1.449158e-15  1.750492e-15  2.041621e-15
-6.00164e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
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5.874207e-15 -1.977252e-15 -3.759664e-15 -4.002878e-15  1.889453e-15
-3.258884e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
2.074066e-15 -2.485464e-15 -5.521865e-15 -2.241811e-15  2.301504e-15
-3.602467e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
3.205303e-16  2.039753e-15 -3.093375e-15 -9.030038e-16  4.674488e-15
-1.038002e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f490d67e2fa.final.pdb
1.167794e-15  1.127795e-15 -8.089750e-15 -1.023491e-15  3.718286e-15
-6.121297e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
1.073003e-14  1.597348e-14 -5.04010e-15  1.847171e-14  5.840449e-15
-1.461260e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e033b.final.pdb
1.635529e-16  4.592906e-16 -4.209141e-16 -3.044060e-16  2.126872e-16
-2.365918e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9ac7f083816d6ba.final.pdb
7.005779e-15  1.487718e-15 -3.669344e-15  2.945776e-15  6.751755e-15
1.782534e-16

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8.178037e-15 -3.619799e-15  2.945776e-15  6.751755e-15  8.174365e-15
-9.120456e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
2.363570e-15  1.990405e-15 -3.699667e-15  3.834234e-16  2.844935e-15
-2.519400e-15

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3.927089e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
2.280086e-15  4.989283e-16 -2.511374e-15  6.249179e-16  2.310728e-15
-2.297856e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
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-6.121297e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
4.208007e-15 -2.020910e-15 -1.858959e-15  1.019621e-14  1.429264e-15
-9.135213e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
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-1.038002e-15

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3.078943e-15 -8.504710e-15 -1.213859e-15 -1.256358e-15  5.700830e-15
-1.858078e-15

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-1.038002e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
5.874207e-15 -1.977252e-15 -3.759664e-15 -4.002878e-15  1.889453e-15
-3.258884e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9f4d9d87c1017b.final.pdb
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-1.038002e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e.final.pdb
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 3.205303e-16 2.039753e-15 -3.093375e-15 -9.030038e-16 4.674488e-15 -1.038002e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 8.317212e-15 5.617042e-15 -2.788652e-15 4.248334e-15 5.034507e-15 -1.380253e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 5.874207e-15 -1.977252e-15 -3.759664e-15 -4.002878e-15 1.889453e-15 -3.258884e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 7.860537e-15 3.513707e-15 -6.799378e-16 2.470529e-15 4.700476e-15 2.290267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e6977249a461.final.pdb | 1.256491e-15 1.737894e-15 -3.698149e-15 -3.131994e-15 3.532536e-15 -2.087887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 4.939590e-15 -1.130471e-15 -3.122129e-15 5.563775e-15 1.743660e-14 -4.057787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -1.317911e-15 1.214248e-15 -3.351407e-15 4.079697e-15 -5.725813e-16 -2.332850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0e39.final.pdb | -1.253772e-15 1.707301e-15 -2.316374e-15 -1.768554e-15 5.092620e-15 3.927089e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d776735e15.1.697485e-15 -2.018017e-15 2.522445e-16 -4.471785e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8009eff10197e2.final.pdb | 4.939590e-15 -1.130471e-15 -3.122129e-15 5.563775e-15 1.743660e-14 -4.057787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d901f8a2e5.final.pdb | 4.584086e-15 5.495175e-15 7.943032e-16 5.909860e-15 -4.449986e-15 2.069203e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e0895f2d2e.final.pdb | -1.317911e-15 1.214248e-15 -3.351407e-15 4.079697e-15 -5.725813e-16 -2.332850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -1.276564e-14 -7.562755e-15 -8.274183e-15 -1.211429e-14 -8.447421e-16 6.218794e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e22c41e72d.final.pdb | 4.939590e-15 -1.130471e-15 -3.122129e-15 5.563775e-15 1.743660e-14 -4.057787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e30b56b0488.final.pdb | 5.874207e-15 -1.977252e-15 -3.759664e-15 -4.002878e-15 1.889453e-15 -3.258884e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 4.939590e-15 -1.130471e-15 -3.122129e-15 5.563775e-15 1.743660e-14 -4.057787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 5.874207e-15 -1.977252e-15 -3.759664e-15 -4.002878e-15 1.889453e-15 -3.258884e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d096.final.pdb | 6.879512e-15 -7.057171e-16 -1.462864e-14 -1.331301e-15 1.949767e-14 -1.019112e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d096.final.pdb | 6.879512e-15 -7.057171e-16 -1.462864e-14 -1.331301e-15 1.949767e-14 -1.019112e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6502087218ec3a1.final.pdb | -1.253772e-15 1.707301e-15 -2.316374e-15 -1.768554e-15 5.092620e-15 3.927089e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6502087218ec3a1.final.pdb | 6.879512e-15 -7.057171e-16 -1.462864e-14 -1.331301e-15 1.949767e-14 -1.019112e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e707301e-15 -2.316374e-15 -1.768554e-15 5.092620e-15 3.927089e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e707301e-15 -2.316374e-15 -1.768554e-15 5.092620e-15 3.927089e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93|
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682c4c527078.final.pdb         | 2.058333e-15 7.53402e-17 -3.774094e-15 -4.959747e-16 2.402877e-15 -2.237549e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb        | 2.253446e-15 7.534042e-17 -3.774094e-15 -4.959747e-16 2.402877e-15 -2.237549e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb        | 1.256491e-15 1.737894e-15 -3.698149e-15 -3.131994e-15 3.532536e-15 -2.087887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb         | 1.635529e-16 4.592906e-16 -4.209141e-15 -3.044060e-15 2.126872e-15 -2.365918e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb         | 5.626260e-16 6.918424e-16 -1.362569e-15 2.596302e-16 2.506672e-15 -4.182889e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb         | 1.186505e-16 4.675259e-15 -3.890328e-16 1.518499e-15 3.917119e-17 -2.180641e-16 |
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6.059261e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
-2.274993e-16 2.053919e-15 4.027641e-16 -1.054095e-15 2.446498e-15
1.146598e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f80b551be0a39.final.pdb
1.186505e-15 4.675259e-15 2.370665e-15 3.018739e-15 3.373711e-15
6.059261e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
5.503745e-15 4.769375e-16 2.101831e-15 -1.201765e-15 -3.217338e-15
1.245008e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
7.856897e-15 -2.371641e-15 7.440587e-15 7.818364e-15 8.976033e-15
8.127962e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
-6.458498e-16 1.822812e-15 2.626672e-16 2.430488e-15
1.438705e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
7.664973e-16 1.162272e-15 9.860648e-16 1.391865e-15 1.457706e-15
-2.271675e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb32871797b7ab.final.pdb
-6.459655e-15 9.263803e-17 1.098379e-14 -9.143185e-15 3.204381e-15
3.387632e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
-7.345936e-15 2.394183e-15 6.716843e-15 -6.673375e-15 3.423994e-15
-1.597289e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc3d25de.final.pdb
3.056060e-15 2.439738e-15 -1.685772e-15 -1.295084e-15 7.059477e-15
5.990301e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
2.357672e-15 -1.280917e-16 4.571847e-15 -2.732006e-15 5.438896e-15
-5.884507e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb
-4.034987e-15 7.022572e-15 1.672132e-15 8.105610e-15 -1.094116e-14
1.018098e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\443242d1f75a7fcf.final.pdb
5.274968e-17 -3.785232e-15 4.093594e-15 6.883543e-15 1.395006e-14
4.199376e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb
2.096511e-16 1.036671e-14 -1.843793e-15 -1.788785e-14 1.873902e-14
1.053102e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb
-5.430571e-16 1.537953e-15 1.251440e-15 3.446637e-16 -3.286414e-15
-2.705759e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951e153.final.pdb
-4.542039e-15 4.669493e-15 2.896208e-15 -3.579528e-15 8.830750e-15
-1.666125e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab45b62cb6a25f.final.pdb
1.997718e-15 3.369640e-16 -3.599720e-15 4.123814e-15 6.433739e-15
1.888799e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
3.056060e-15 2.439738e-15 -1.685772e-15 -1.295084e-15 7.059477e-15
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5.990301e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
4.621444e-16  4.680991e-15 -2.442194e-15 -4.680991e-15  3.80164e-15
-2.716928e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
4.621444e-16  4.609095e-15 -2.442194e-15 -4.680991e-15  3.801064e-15
-2.716928e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
1.997718e-15  3.369640e-16 -3.599720e-15  4.128314e-15  6.433739e-15
1.888799e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
8.373532e-16  3.007743e-16 -4.365437e-15 -1.562097e-15  5.064515e-15
7.660655e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
-5.430571e-16  1.537953e-15  1.251440e-15  3.446637e-16 -3.286414e-15
-2.705759e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
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-2.716928e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
5.010820e-15 -3.280925e-16  2.368735e-15 -1.538200e-15  4.455578e-15
2.370727e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
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1.198995e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982f4c.final.pdb
-1.175304e-14 -1.381061e-14  8.382569e-15 -1.142653e-14  1.095756e-14
1.209324e-14
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-5.293393e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
-6.637820e-15 -8.409248e-15  4.192474e-15 -4.171982e-15  6.975350e-15
-5.694951e-15
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7.664973e-16  1.162272e-15  9.860648e-16  1.391865e-15  1.457706e-15
-2.716754e-15
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-5.884587e-16
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-5.430571e-16  1.537953e-15  1.251440e-15  3.446637e-16 -3.286414e-15
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-2.71675e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
-2.693257e-15 2.928102e-15 -3.890328e-16 1.518499e-15 3.917119e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-2.180641e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
-2.389841e-16 1.601038e-15 1.350705e-16 2.530178e-15 2.659471e-15 1.771989e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-4.389841e-16 1.601038e-15 1.350705e-16 2.530178e-15 2.659471e-15 1.771989e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
3.558266e-15 4.269913e-15 -2.583671e-16 2.780369e-15 -5.180421e-15 -8.039302e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
3.656495e-15 1.604185e-15 -5.232470e-15 1.231794e-16 6.576017e-15

[,235]        [,236]        [,237]        [,238]        [,239]        [,240]
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcedb4194d9.final.pdb
3.046888e-16

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### Supplementary Text 10

| Path                                                                 | Number of Atoms | Numbers | Numbers | Numbers | Numbers | Numbers |
|----------------------------------------------------------------------|-----------------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb  | 5.431310e-15    | 2.480360e-15 | -3.282649e-15 | -2.395735e-16 | 6.439207e-15 | 7.18576e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 3.768568e-15    | 2.924406e-15 | -3.411811e-15 | -4.007116e-15 | -6.855260e-15 | 3.836934e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | -1.507070e-15   | 2.353007e-15 | 3.805941e-16  | -2.722855e-15 | -2.127129e-15 | 5.346888e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 2.054298e-15    | 2.580788e-15 | -2.886987e-15 | -1.119988e-15 | 6.683667e-16 | 2.182799e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 1.226854e-15    | 2.250659e-15 | -1.900784e-15 | -3.801112e-16 | 9.589441e-16 | 2.809855e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 0.130998e-15    | 1.663654e-16 | -8.541060e-16 | -2.440704e-15 | -1.622341e-15 | 3.213757e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 1.96878e-15     | 2.480905e-15 | -7.206899e-16 | 1.084293e-15 | -1.364717e-15 | -1.425058e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 1.364021e-15    | 1.386572e-15 | -3.209861e-15 | -4.246749e-16 | 2.977114e-15 | 1.533098e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 2.083837e-15    | 1.054919e-15 | -5.842792e-15 | -2.724825e-15 | 3.368529e-15 | -1.762642e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | -2.053755e-16   | -6.485787e-16 | -1.876678e-15 | -1.201227e-15 | 3.003719e-15 | -9.361091e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | -1.728885e-16   | 2.846266e-15 | -3.289882e-15 | -9.263143e-16 | 2.094474e-15 | 1.728885e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | 3.558266e-15    | 4.269913e-15 | -2.583671e-15 | 2.780369e-15 | -5.180421e-15 | -8.39302e-16 |

| Path                                                                 | Number of Atoms | Numbers | Numbers | Numbers | Numbers | Numbers |
|----------------------------------------------------------------------|-----------------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb                            | 9.577049e-16    | 2.846266e-15 | -3.289882e-15 | -9.263143e-16 | 2.094474e-15 | 1.728885e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb                            | 1.364021e-15    | 1.386572e-15 | -3.209861e-15 | -4.246749e-16 | 2.977114e-15 | 1.533098e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                            | 2.083837e-15    | 1.054919e-15 | -5.842792e-15 | -2.724825e-15 | 3.368529e-15 | -1.762642e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                            | -2.053755e-16   | -6.485787e-16 | -1.876678e-15 | -1.201227e-15 | 3.003719e-15 | -9.361091e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                            | -7.070808e-16   | -2.463310e-16 | -9.378834e-15 | 1.812542e-15 | 9.161101e-15 | -9.902243e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                            | 1.624002e-15    | 1.411686e-15 | -3.270914e-15 | -2.366741e-15 | 2.246393e-15 | -1.826893e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                            | 2.556243e-16    | 1.247237e-15 | -5.938303e-15 | 2.782492e-15 | 5.970575e-15 | -6.986539e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                            | 0.130855ad26c877c.final.pdb | -7.070808e-16 | -2.463310e-16 | -9.378834e-15 | 1.812542e-15 | 9.161101e-15 | -9.902243e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                            | 0.130855ad26c877c.final.pdb | -7.070808e-16 | -2.463310e-16 | -9.378834e-15 | 1.812542e-15 | 9.161101e-15 | -9.902243e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                            | 0.130855ad26c877c.final.pdb | -7.070808e-16 | -2.463310e-16 | -9.378834e-15 | 1.812542e-15 | 9.161101e-15 | -9.902243e-16 |
| Path                                                                 | Coordinates              | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb |
|----------------------------------------------------------------------|--------------------------|---------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb  | 8.155911e-15 4.624772e-15 4.210293e-15 -1.336027e-14 -3.174951e-15  | -8.767532e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb  | 3.554548e-15 2.462491e-15 -3.014769e-15 -1.392440e-14 -3.844191e-15  | -8.665505e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb   | 2.019670e-15 5.50309e-16 -3.07218e-15 -2.412012e-15 2.645133e-15     | -1.803075e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb   | 3.554548e-15 2.462491e-15 -3.014769e-15 -1.392440e-14 -3.844191e-15  | -8.665505e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb   | 5.431547e-16 2.597719e-15 1.99190e-15 -4.910140e-15 7.542234e-15     | 1.115818e-14                                                       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e2fdc42.final.pdb   | 2.078060e-15 -1.781590e-15 4.267455e-15 -2.012285e-14 -6.453298e-15  | -1.240988e-14                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b30278892fdec42.final.pdb   | 2.078060e-15 -1.781590e-15 4.267455e-15 -2.012285e-14 -6.453298e-15  | -1.240988e-14                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb   | 3.554548e-15 2.462491e-15 -3.014769e-15 -1.392440e-14 -3.844191e-15  | -8.665505e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb   | 8.155911e-15 4.624772e-15 -3.07218e-15 -1.392440e-14 -3.844191e-15  | -8.767532e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6eddd.final.pdb  | 8.155911e-15 4.624772e-15 -3.07218e-15 -1.392440e-14 -3.844191e-15  | -8.767532e-15                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb    | 3.339772e-15 4.893772e-15 -6.725669e-15 8.425602e-15 1.048211e-14     | 7.336685e-16                                                       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcdc.final.pdb    | 4.271314e-15 4.05050e-15 -1.375516e-14 -4.08922e-15 -1.781762e-15    | -1.093520e-14                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cfdb.final.pdb    | 3.339795e-15 1.713832e-14 3.314690e-15 -1.486212e-14 -4.798566e-15  | -2.490438e-14                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb     | 8.108747e-16 -2.554381e-15 -5.473104e-15 -2.146097e-15 1.113719e-15   | 1.750205e-15                                                       |

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| Path |
|-------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6474221e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982f1c8.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6da9d87d47926b1c.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6e68614e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6f60752431cf2dcb.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb |
Supplementary Text 10

-3.489812e-15 -2.948039e-15 -8.051652e-15 3.772277e-15 6.450249e-15
1.899693e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
-3.489812e-15 -2.948039e-15 -8.051652e-15 3.772277e-15 6.450249e-15
1.899693e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
-4.208204e-15 6.844720e-16 -3.210693e-17 -1.406686e-15 5.623219e-15
-4.067214e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
8.108747e-16 -2.554381e-15 -5.473104e-15 -2.146097e-15 1.113719e-15
1.750205e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
1.518077e-15 3.434967e-15 3.925811e-15 -1.421979e-15 -2.740166e-15
6.474221e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
2.980707e-15 1.334126e-15 1.806348e-15 -3.140596e-15 8.063257e-16
2.755779e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
5.561408e-15 1.056704e-15 -1.612044e-15 3.583736e-15 -1.270239e-16
1.221407e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
2.556243e-16 1.247237e-15 -5.938303e-15 2.782492e-15 5.970575e-15
-6.986539e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\99c22f4909d67e2fa.final.pdb
9.523975e-15 5.777865e-16 -9.197247e-15 -1.173398e-14 2.899486e-15
-3.997825e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b6ef9ac3fe74395.final.pdb
9.875231e-16 -3.050965e-16 -5.330999e-16 3.533205e-15 5.705335e-15
-1.525590e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
4.967888e-17 1.665390e-15 -3.954991e-15 3.452272e-17 3.164793e-15
3.051507e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
2.945443e-15 -9.960803e-16 -1.070587e-15 -4.437924e-15 2.871123e-16
-1.533322e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-1.789565e-15 2.610686e-15 -5.089122e-15 -9.339137e-15 -3.086511e-15
-2.868326e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
1.813130e-15 1.310511e-15 -2.541193e-15 -1.198568e-15 3.175623e-15
-2.004293e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac4ad74b9c71d4dc.final.pdb
-3.489812e-15 -2.948039e-15 -8.051652e-15 3.772277e-15 6.450249e-15
1.899693e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
8.374263e-16 1.688794e-15 -3.439280e-15 -2.339680e-15 2.682773e-15
-2.177410e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
9.523975e-15 5.777865e-16 -9.197247e-15 -1.173398e-14 2.899486e-15
-3.997825e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
3.993690e-15 3.454049e-15 -2.082892e-15 -1.354295e-14 -4.794729e-15
-1.646562e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
|                | 2.556243e-16 | 1.247237e-15 | -5.938303e-15 | 2.782492e-15 | 5.970575e-15 | -6.986539e-16 |
|----------------|--------------|--------------|---------------|--------------|--------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 2.477271e-15 | 1.400137e-15 | -1.322556e-14 | 2.159182e-15 | 7.90693e-15 | 8.606195e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabf1df.final.pdb | 2.556243e-16 | 1.247237e-15 | -5.938303e-15 | 2.782492e-15 | 5.970575e-15 | -6.986539e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 2.980707e-15 | 1.334126e-15 | -3.140596e-15 | 8.063257e-16 | 2.755779e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 2.556243e-16 | 1.247237e-15 | -5.938303e-15 | 2.782492e-15 | 5.970575e-15 | -6.986539e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 2.556243e-16 | 1.247237e-15 | -5.938303e-15 | 2.782492e-15 | 5.970575e-15 | -6.986539e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 1.625514e-15 | 1.346116e-15 | -3.535765e-15 | 2.858698e-15 | 2.755779e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.215880e-14 | 7.746776e-16 | -1.178123e-14 | 3.781034e-15 | -1.916540e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 1.935812e-15 | 2.432053e-15 | 2.065224e-15 | 7.615061e-15 | -4.897684e-15 | 6.556231e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 1.058851e-15 | 2.965649e-16 | -4.856699e-15 | 1.794318e-15 | -1.713000e-15 | 0.010164e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 1.058851e-15 | 2.965649e-16 | -4.856699e-15 | 1.794318e-15 | -1.713000e-15 | 0.010164e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 1.935812e-15 | 2.432053e-15 | 2.065224e-15 | 7.615061e-15 | -4.897684e-15 | 6.556231e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 1.935812e-15 | 2.432053e-15 | 2.065224e-15 | 7.615061e-15 | -4.897684e-15 | 6.556231e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 1.935812e-15 | 2.432053e-15 | 2.065224e-15 | 7.615061e-15 | -4.897684e-15 | 6.556231e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 1.935812e-15 | 2.432053e-15 | 2.065224e-15 | 7.615061e-15 | -4.897684e-15 | 6.556231e-16 |
| File Path                                                      | Values                      |
|---------------------------------------------------------------|-----------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb | -7.835917e-16               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -5.405752e-15 1.991396e-15 -7.49792e-16 -7.263660e-15 4.181825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | -1.144559e-15 4.181825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -1.222477e-15               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -1.965551e-15 3.053165e-15 -9.314439e-15 -1.790168e-15 8.121491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\19f45328d47579a.final.pdb | 9.637770e-15 -1.380196e-14 -1.038445e-15 -5.188476e-15 2.646066e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1b3027889e2f3d42.final.pdb | -2.260131e-15 -1.025073e-15 -2.620093e-15 -7.489254e-16 -7.378284e-15 3.219045e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb3b46e33793b0.final.pdb | -2.339928e-15 -2.906815e-15 -3.706030e-15 -1.962365e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | -1.767621e-15 5.639333e-15 -5.108058e-15 9.562717e-15 7.433012e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | -9.327672e-16 8.915816e-16 -5.116563e-15 -1.760249e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -1.386103e-14               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 1.032935e-15 -4.663656e-15 1.244871e-15 -1.636144e-14 1.933602e-14 |

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| PDB Path                                                                 | Values                                                                 |
|------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb    | -9.288311e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb    | 4.375487e-15 9.523132e-15 -1.601146e-15 -8.228145e-15 7.857925e-15 5.467116e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb     | -6.300906e-15 -6.179034e-15 -3.888224e-15 -1.241708e-14 -3.245718e-15 4.060045e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb     | 1.351680e-15 2.991477e-15 -7.986917e-15 3.657244e-15 4.793165e-16 -3.027404e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb     | 1.965551e-15 3.053165e-15 -9.314439e-15 -1.790168e-15 8.121491e-15 -7.215657e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb     | 7.189502e-16 7.815728e-16 -1.003924e-14 -6.494865e-15 8.981631e-16 -2.418357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb     | -5.405752e-15 1.991396e-15 -6.285984e-15 -5.749792e-15 7.263660e-15 4.181825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb     | 1.351680e-15 2.991477e-15 -7.986917e-15 3.657244e-15 4.793165e-16 -3.027404e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb     | -9.445083e-17 9.584075e-15 -7.942523e-15 -1.916049e-16 2.404692e-15 2.160234e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb     | -4.366189e-16 2.997220e-16 -7.460020e-16 -5.848671e-15 -1.144559e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb     | 7.189502e-16 7.815728e-16 -1.003924e-14 -4.694865e-15 8.981631e-15 -2.418357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb     | 2.586532e-15 7.813918e-16 2.774841e-16 -3.953179e-15 1.074347e-14 -6.55149e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb     | 2.388806e-15 -6.351962e-15 -5.103174e-16 -3.703986e-15 1.290349e-15 -9.573436e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb     | 7.189502e-16 7.815728e-16 -1.003924e-14 -4.694865e-15 8.981631e-16 -2.418357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb     | -2.144664e-15 6.394038e-16 -5.406195e-15 -1.981219e-15 -1.368426e-15 -9.876470e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb     | 5.405752e-15 1.991396e-15 -6.285984e-15 -5.749792e-15 7.263660e-15 -5.405752e-15 |
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| Path                                      | Value       |
|-------------------------------------------|-------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 4.181825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -2.260131e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb | -2.620093e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb | -2.339928e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -4.366189e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | 7.189502e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 2.239934e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 2.260030e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b6e9ac3fe74395.final.pdb | 2.630995e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b8be0d5986c138f.final.pdb | -5.405752e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 6.287003e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d8ed0d81fb3ef.final.pdb | -2.662714e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e033b.final.pdb | -2.228861e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 1.351680e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.896614e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | -6.614233e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf474b9c71d4dc.final.pdb | -2.260131e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | -1.089536e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 2.329948e-15 |
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-7.433012e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb
9.524728e-16 -1.291017e-15 4.589369e-15 -7.415281e-16 -2.350601e-15
3.148164e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
-2.260131e-15 -1.025073e-15 -2.620093e-15 -7.489254e-16 -7.378284e-15
3.219045e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
1.901677e-15 2.991477e-15 -7.986917e-15 8.463452e-15 -5.751500e-15
3.182137e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
1.351680e-15 2.991477e-15 -7.986917e-15 3.657244e-15 4.793165e-16
-3.027404e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
-2.260131e-15 -1.025073e-15 -2.620093e-15 -7.489254e-16 -7.378284e-15
3.219045e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
-5.405752e-15 1.991396e-15 -6.285984e-15 -5.749792e-16 -7.263660e-15
4.181825e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-9.446496e-16 7.794044e-16 -5.39004e-16 -1.507311e-15 -9.753382e-16
-1.129024e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862bcad52078.final.pdb
-8.625109e-16 6.847158e-16 -5.254691e-15 -2.724302e-15 -1.695197e-15
-1.756134e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-9.902058e-16 7.458724e-16 -5.354370e-15 -1.568788e-15 -1.010639e-15
-1.745287e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-2.632936e-15 1.274539e-15 -5.231847e-15 5.543513e-15 -1.819424e-15
-7.579151e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-2.228861e-15 2.349455e-16 -6.343311e-15 -2.542586e-15 -3.044675e-15
-5.679991e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
4.375487e-15 9.523132e-15 -1.601146e-15 -8.228145e-15 7.859252e-15
5.467116e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
9.524728e-16 -1.291017e-15 4.589369e-15 -7.415281e-16 -2.350601e-15
-3.148164e-15

[,] [253] [254] [,255] [256] [,257] [258]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
5.274630e-15 -2.440283e-16 4.348793e-15 -3.798746e-15 1.540038e-15
-3.981575e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
6.422916e-15 5.956632e-15 5.109090e-15 -2.954917e-15 2.246143e-15
-2.756152e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
5.756084e-15 9.141924e-16 4.771762e-15 -1.760196e-15 2.673831e-15
-2.870898e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
2.833860e-15 -3.293564e-16 3.952578e-15 -1.979444e-15 1.616409e-15
-2.979867e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-2.295226e-15  1.619429e-15 -1.402173e-15  4.937522e-15  8.456392e-15
-6.294969e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
2.774645e-15 -4.447790e-17  4.947623e-15 -1.441527e-15  2.031294e-15
-3.110523e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
3.345867e-15  1.793807e-15  6.528700e-15  2.166893e-15  1.119596e-15
1.392785e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
-3.627438e-16  7.173727e-16  5.025411e-15  1.288688e-16 -7.706019e-16
-1.959896e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
2.296154e-15 -3.630712e-15  4.400911e-15 -4.775086e-15  9.155493e-16
-4.901119e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
2.612665e-15 -8.650021e-16  4.931360e-15 -1.133831e-15  1.885144e-15
-2.074893e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
-1.679261e-16 -5.546785e-15 -6.158830e-16 -1.607892e-15  2.623241e-15
-1.012531e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
2.474992e-15  4.550736e-16  3.724286e-15 -1.736307e-15  2.241383e-15
-2.504573e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
-1.679261e-16 -5.546785e-15 -6.158830e-16 -1.607892e-15  2.623241e-15
-1.012531e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
6.391174e-15 -6.408774e-16  2.364241e-16 -2.122759e-14  8.217651e-15
1.047797e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
-5.660021e-15 -1.230683e-15  5.852158e-15 -1.442997e-14  8.973990e-15
1.242683e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fcd42.final.pdb
1.366331e-15 -4.058224e-16  4.666040e-15 -1.255608e-15  2.863427e-15
-1.690686e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
1.711714e-15  1.471622e-15  9.079622e-16  8.519002e-16  2.310772e-15
-2.599983e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
4.169610e-15  2.746698e-15  7.442381e-15  5.720383e-15  7.142644e-15
1.171873e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
6.144675e-15 -9.851947e-16 -7.143909e-15  3.902878e-16  7.638084e-15
-3.058065e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb
2.296154e-15 -3.630712e-15  4.400911e-15 -4.775086e-15  9.155493e-16
-4.901119e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
1.040589e-16 -3.672701e-15 -1.877136e-15  3.771331e-15  2.451284e-15
-9.520662e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb
8.555535e-15 -4.665828e-15  7.990624e-15 -3.362055e-15  6.361421e-15
9.113020e-15
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb      | 9.931633e-16 4.563423e-15 -1.126570e-15 2.017630e-15 -1.979405e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb      | 3.885181e-15 -1.499517e-15 5.839199e-15 8.182894e-16                  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb      | 7.570219e-15 -9.460786e-15 3.814426e-15 1.356013e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb       | 6.528700e-15 2.166893e-15 1.119596e-15 1.392785e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | 6.921478e-16 -6.617682e-15 3.33907e-15 2.448889e-15                |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb       | 2.166893e-15 1.119596e-15 1.392785e-15                              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb       | 6.740970e-15 -5.962094e-15 -3.39938e-15 4.583343e-15             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb       | 6.528700e-15 2.166893e-15 1.119596e-15 1.392785e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb       | 1.9.93087e-15 6.528700e-15 2.166893e-15 1.119596e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb       | 4.696398e-15 -1.719755e-15 2.409461e-15 -1.539332e-15             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | 6.917402e-15 8.199747e-15 1.378351e-14 -1.084111e-14 7.113566e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | 6.740970e-15 -5.962094e-15 -3.39938e-15 4.583343e-15             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 9.983308e-16 9.179178e-15 7.793535e-15 -4.774484e-15 4.327101e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb        | 8.925407e-15 1.391732e-14 -2.358584e-14 1.101576e-14 1.112155e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 2.810422e-15 1.381482e-15 1.101576e-14                                |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | 1.084111e-14 7.113566e-16 1.235247e-14                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f7ee39.final.pdb        | 2.160907e-15 -4.916771e-15 -2.589852e-15 1.256116e-14              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8090eff10197e2.final.pdb        | 7.729600e-15 -2.566952e-15 -1.242398e-15 1.087657e-14 1.256116e-14  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d824808e-14 1.150641e-14 -6.306082e-15 -7.023368e-15 1.243381e-14 |
3.20525e-15  2.813994e-15  2.201469e-15  -2.778396e-15  8.808601e-16
1.474498e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
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3.873153e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
1.358541e-15  4.759859e-15  3.357828e-15  -7.809132e-15  2.424808e-15
1.063359e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
2.170288e-15  1.206245e-15  3.90490e-15  -1.253412e-15  2.578361e-16
3.873153e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d9.final.pdb
2.052431e-15  2.891561e-15  3.533035e-15  2.713701e-15  1.977249e-15
2.031335e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
9.949326e-15  5.962889e-15  -6.121135e-15  -6.346326e-15  9.355477e-16
4.728288e-15
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2.031335e-15
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2.400897e-15  2.117842e-15  2.579073e-15  -1.453339e-15  1.050605e-15
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9.840992e-15  8.653242e-15  -6.491788e-15  -3.827049e-15  3.956855e-15
7.251050e-15
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2.780456e-15  2.64950e-15  1.211644e-15  -2.806360e-15  5.359418e-16
9.483940e-16
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7.224055e-15  9.034252e-15  -1.280563e-14  -1.978739e-15  1.803429e-15
1.185153e-15
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2.384394e-15  2.166481e-15  2.235552e-15  -2.611479e-15  9.724963e-16
8.093548e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
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8.093548e-16
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4.569741e-15  -6.845236e-15  3.765696e-15  -7.812450e-15  -1.939608e-16
3.322411e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-4.069967e-15  1.659342e-16  3.026165e-16  6.353316e-16  -1.104076e-15
-6.093877e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-2.543235e-15  7.172292e-15  1.490691e-15  -5.433831e-15  -1.293511e-14
7.942434e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
9.949326e-15  5.962889e-15  -6.121135e-15  -6.346326e-15  9.355477e-16
4.728288e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
### Supplementary Text 10

| Path                                                        | File Name                        | 100 | 140 | 160 | 190 | 210 |
|-------------------------------------------------------------|----------------------------------|-----|-----|-----|-----|-----|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb |                                  | -4.518806e-15 | 1.140325e-15 | -1.648881e-15 | 1.968168e-16 | -8.020800e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb  |                                  | 4.618306e-15  | 1.140325e-15 | -1.648881e-15 | 1.968168e-16 | -8.020800e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb |                                  | -1.097630e-15 | -2.911882e-16 | 7.860995e-15  | -4.272911e-15 | 4.260584e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb |                                  | -4.069967e-15 | 1.659342e-16  | 3.026165e-15  | 6.353316e-16  | -1.104067e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\79d0666e1402203d.final.pdb |                                  | 2.052431e-15  | 2.891561e-15  | 3.533035e-15  | 2.713701e-15  | 1.977249e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b889c94a633196.final.pdb |                                  | 1.493545e-14  | 8.587583e-15  | -1.166228e-15 | 5.475232e-15  | 1.040409e-14  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb |                                  | 3.512468e-15  | 2.351062e-15  | 1.874065e-15  | 3.113939e-16  | 3.990503e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\922f4909d67e2fa.final.pdb |                                  | 1.711176e-15  | -2.917537e-15 | -1.060410e-15 | 3.139741e-16  | -4.513666e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 2.032571e-15  | 8.670726e-15  | 5.609941e-15  | 2.385419e-15  | 3.880477e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb |                                  | 6.492026e-15  | 2.032571e-15  | 8.670726e-15  | 5.609941e-15  | 2.385419e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 4.442566e-16  | 3.674342e-16  | 1.080895e-14  | -5.579305e-15 | 5.038533e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | -9.215140e-16 | 5.79305e-15   | 5.038533e-15  | 5.038533e-15  | 5.038533e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be0d5986c138f.final.pdb |                                  | 1.493545e-14  | 8.587583e-15  | -1.166228e-15 | 5.475232e-15  | 1.040409e-14  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be0d5986c138f.final.pdb |                                  | 3.990503e-15  | 3.990503e-15  | 3.990503e-15  | 3.990503e-15  | 3.990503e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 6.492026e-15  | 2.032571e-15  | 8.670726e-15  | 5.609941e-15  | 2.385419e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 1.266192e-15  | 1.266192e-15  | 1.266192e-15  | 1.266192e-15  | 1.266192e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 2.130124e-15  | 2.548046e-15  | 4.707171e-15  | -1.342479e-15 | 2.136243e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 3.512468e-15  | 2.351062e-15  | 1.874065e-15  | 1.823362e-16  | 3.113939e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 3.113939e-16  | 3.113939e-16  | 3.113939e-16  | 3.113939e-16  | 3.113939e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | -5.004066e-15 | 3.358150e-15  | 5.609941e-15  | 2.385419e-15  | 3.880477e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |                                  | 4.161080e-15  | 4.161080e-15  | 4.161080e-15  | 4.161080e-15  | 4.161080e-15  |
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1.860452e-15  2.109582e-15  2.267996e-15 -2.483083e-15  2.670479e-16
4.719195e-16

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-4.069967e-15  1.659342e-16  3.026165e-15  6.353316e-16 -1.104067e-15
-6.093877e-16

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6.609874e-16

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3.990503e-15

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-2.123756e-16

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-3.396807e-15

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-1.809816e-16

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-1.097630e-15 -2.911882e-16  7.860995e-15 -4.272911e-15  4.260584e-16
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-4.323485e-15

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-1.809816e-16

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-4.771679e-15  2.515398e-15  1.847486e-15 -5.462322e-15 -3.227899e-15
-6.224070e-16

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2.510522e-15

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1.342154e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0e39.final.pdb

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb |
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| 6.058883e-15 1.032105e-14 -1.857786e-15 4.600281e-17 6.064568e-16 |
| 7.46052e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb |
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| 7.746052e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 8.400992e-15 8.653242e-15 -6.491788e-15 -3.827049e-15 3.956855e-15 |
| 7.251050e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb |
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| 9.840992e-15 8.653242e-15 -6.491788e-15 -3.827049e-15 3.956855e-15 |
| 7.251050e-15 |
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| 1.358541e-15 4.759859e-15 3.357828e-15 -7.809132e-15 3.956855e-15 |
| 7.251050e-15 |
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| 3.512468e-15 2.351062e-15 1.874065e-15 1.823362e-16 4.123290e-15 |
| 3.113939e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e689d94009cae7.final.pdb |
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| 2.232172e-15 1.994310e-15 2.632538e-15 -2.841764e-15 1.008926e-15 |
| 9.400012e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6a517be32db050e.final.pdb |
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| 2.7121253e-15 1.928153e-15 2.959853e-15 -2.135260e-15 4.260584e-16 |
| 9.665189e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e8e2bf87e52caa29.final.pdb |
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| 5.340958e-15 1.817715e-15 2.456214e-15 -2.256701e-15 -2.007175e-15 |
| 1.342154e-16 |
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| 2.130124e-15 2.454046e-15 4.707171e-15 -1.342479e-15 2.136243e-15 |
| 7.868299e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e2bf87e52caa29.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
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| 1.063359e-15 |

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
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-1.344256e-15
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3.341240e-15
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5.836061e-15  3.319346e-15  1.622495e-14  1.202127e-14  9.631597e-15
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | 9.462232e-16 |
|---------------------------------------------------------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -4.384902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 1.416202e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 2.710310e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -2.686876e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb | 5.307025e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb | -2.446270e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -4.331002e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | 1.416202e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -1.864305e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.928149e-15 |

**Supplementary Text 10**
| Path                                      | Scores                                      |
|-------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 4.350161e-16 -6.230261e-16                   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | -2.194192e-15 2.559379e-15 -1.037507e-15 1.604348e-15 1.045330e-15 2.809774e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd474b9c71d4dc.final.pdb | -2.868687e-15 5.307025e-15 8.477768e-15 -1.421688e-15 3.291962e-15 3.341240e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | -2.449117e-15 2.381812e-15 -5.964774e-16 1.323420e-15 8.819369e-16 1.388334e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | -6.097333e-15 4.274214e-15 -3.389909e-15 -4.725035e-15 -5.099010e-16 6.169706e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | -3.537410e-15 5.620695e-15 -8.931229e-15 -5.972170e-16 -8.425853e-15 -5.184770e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | -1.864305e-15 5.344767e-15 1.995654e-15 -2.358439e-15 4.424901e-15 2.889771e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -1.325902e-14 -4.403404e-15 9.414772e-15 -3.343718e-15 -1.114428e-15 6.728443e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | -1.864305e-15 5.344767e-15 1.995654e-15 -2.358439e-15 4.424901e-15 2.889771e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | -2.451834e-15 2.719263e-15 -2.536315e-16 3.681125e-16 6.672370e-16 2.331623e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | -4.125683e-15 1.532527e-14 -1.200238e-14 -2.446910e-15 -1.236967e-15 9.849922e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd8a823e4b4c668e.final.pdb | 1.068571e-15 -3.608575e-15 5.056791e-15 -5.361121e-16 -1.032871e-14 4.402883e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 1.166821e-15 2.453405e-15 -8.991764e-15 1.887297e-15 -1.610366e-15 -5.658506e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 4.713320e-15 -2.032921e-16 -6.838244e-15 1.552524e-15 3.057208e-15 3.213820e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\df0221245d015047.final.pdb | 1.068571e-15 -3.608575e-15 5.056791e-15 -5.361121e-16 -1.032871e-14 4.402883e-15 |
| File Name                                                                 | Values                                      |
|---------------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb      | -2.666856e-15 -5.460956e-15 -3.908378e-15 6.863225e-15 9.718239e-15 1.527438e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb      | -6.003351e-15 8.163177e-16 3.238034e-15 1.516684e-15 3.551497e-15 3.534038e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb      | -6.299572e-15 4.763714e-15 -1.404424e-15 -6.134897e-15 -6.576467e-15 1.680703e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb      | -1.025274e-14 1.664658e-15 6.83017e-15 -2.083875e-15 5.070729e-15 5.675466e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb      | -2.224781e-15 1.922725e-15 -8.704582e-15 4.778200e-15 -1.595883e-15 9.786225e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb      | -4.275490e-15 3.361343e-15 1.171044e-14 -1.357106e-15 4.210196e-15 9.896963e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb      | -2.686867e-15 5.307025e-15 8.477768e-15 -1.421688e-15 3.291962e-15 3.341240e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb      | 1.494546e-15 5.012406e-15 -1.083752e-14 -1.198886e-16 -5.494590e-16 -1.768803e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb      | -2.075037e-15 2.321880e-15 -1.106615e-14 -2.879316e-15 -4.198703e-15 -1.595883e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5e6862cbcad52078.final.pdb     | -2.376048e-15 3.491215e-15 2.457520e-16 6.540324e-17 7.065211e-16 2.081389e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e667693099c839a.final.pdb      | -1.866343e-15 3.280580e-15 -9.221793e-16 1.238497e-15 9.875339e-16 2.932788e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e8642fc83b81e5d.final.pdb       | -1.864305e-15 5.344767e-15 1.995654e-15 -2.358439e-15 4.424901e-15 2.889717e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb      | -2.476518e-15 3.100576e-15 2.357111e-16 1.088934e-15 1.131389e-15 2.510029e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbbd52078.final.pdb       | -2.376048e-15 3.491215e-15 2.457520e-16 6.540324e-17 7.065211e-16 2.081389e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb      | -1.866343e-15 3.280580e-15 -9.221793e-16 1.238497e-15 9.875339e-16 2.932788e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0.final.pdb        | -1.152382e-15 2.926706e-15 1.490419e-15 1.554041e-15 4.471192e-15 5.264842e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae83b81e5d.final.pdb       | -2.928149e-15 5.724572e-15 4.503828e-15 2.623483e-16 1.159145e-15 2.936183e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb     | 7.113540e-15 4.361612e-15 8.448821e-16 5.331590e-15 1.121417e-14 4.666127e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa29.final.pdb     | -4.275490e-15 3.361343e-15 1.171044e-14 -1.357106e-15 4.210196e-15 |

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9.896963e-15

[,271]        [,272]        [,273]        [,274]        [,275]        [,276]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.014296e-15 -1.008829e-15 -1.780005e-16  1.167532e-15  2.642532e-16
-4.161912e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
3.104699e-16 -9.999192e-16 -2.044181e-15  7.668618e-16  3.916358e-15
-5.073136e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-3.039367e-16  1.079657e-15 -3.795633e-15  1.583719e-15 -6.638684e-16
-1.206250e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
1.830857e-16 -2.567689e-15 -4.223516e-16 -1.343173e-15  5.157419e-16
-4.609083e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-7.009163e-15  1.645293e-15  4.197798e-15  4.278150e-15 -2.033380e-15
-5.263727e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
8.986295e-15 -1.985607e-15 -3.671149e-15 -4.167730e-17  1.340980e-15
-4.622689e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
6.413976e-15 -4.970416e-15  5.600297e-16 -2.657846e-15  3.838051e-15
-6.498951e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0db59f3306825e.final.pdb
3.705356e-15 -1.046998e-15 -7.392249e-16 -3.966990e-15  3.000787e-15
1.397611e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a708b57339c.final.pdb
-2.843225e-15 -3.001597e-15 -2.174709e-16  7.140834e-15  7.239628e-16
-7.019918e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
8.160133e-16 -1.126485e-15  1.975376e-16  4.900154e-16  1.151028e-15
-3.557135e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618ca251b867b.final.pdb
-8.759534e-15  7.168895e-15 -1.931846e-16  4.388353e-15  2.258743e-15
-4.588619e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
6.306956e-16 -1.316312e-15 -3.704619e-16  1.341863e-15  9.631566e-16
-4.520134e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551b0a39.final.pdb
-8.759534e-15  7.168895e-15 -1.931846e-15  4.388353e-15  2.258743e-15
-4.588619e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-1.546236e-15 -8.138888e-15 -1.019436e-15 -1.357746e-16  1.171375e-14
5.665779e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238d3918e54336d.final.pdb
-7.008013e-15 -2.926478e-15 -7.100076e-15 -2.584012e-15 -1.05455e-14
3.312211e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdcc42.final.pdb
7.002307e-16 -2.554813e-15 -2.630688e-17  2.512856e-16  8.413158e-16
-3.444970e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
8.458013e-16  2.000479e-15  2.193459e-15 -1.367775e-15  2.916455e-15
-9.257868e-16

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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb     | -4.902384e-15 -1.944815e-15 -3.419968e-15 -1.684277e-15 -1.92950e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb     | -4.449355e-15  3.793661e-15 -2.038772e-15  2.149065e-15  2.512680e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb      | -1.566343e-15 -6.494511e-15  1.474859e-15  4.913053e-15  1.199205e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb      | -1.566343e-15 -6.494511e-15  1.474859e-15  4.913053e-15  1.199205e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb       | -1.566343e-15 -6.494511e-15  1.474859e-15  4.913053e-15  1.199205e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb       | -1.566343e-15 -6.494511e-15  1.474859e-15  4.913053e-15  1.199205e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb      | -2.277568e-15 -3.709363e-15 -4.774925e-15 -1.131745e-15 -3.694576e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb      | 1.861724e-15 -1.354338e-14 -1.796599e-15  2.423226e-15  1.302490e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb       | 6.413976e-15 -4.970416e-15  5.600297e-16 -2.657846e-15  3.838051e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | 1.046595e-14 -1.592516e-14  1.923011e-16 -5.006812e-15  9.967434e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb       | 6.413976e-15 -4.970416e-15  5.600297e-16 -2.657846e-15  3.838051e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb       | 5.392512e-15 -3.321653e-15 -1.425174e-15 -8.091945e-16  5.667727e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb       | 6.413976e-15 -4.970416e-15  5.600297e-16 -2.657846e-15  3.838051e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb       | 6.413976e-15 -4.970416e-15  5.600297e-16 -2.657846e-15  3.838051e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb       | 5.905095e-16 -1.737325e-15 -2.977633e-17  1.069783e-16  1.186526e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | 4.994393e-15 -1.655239e-14 -1.295762e-14 -1.045393e-14 -9.479879e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2af5f5f9d681.final.pdb         | 5.392512e-15 -3.321653e-15 -1.425174e-15 -8.091945e-16  5.667727e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 1.317668e-16  2.435329e-15  1.396912e-15  7.465273e-15  8.688896e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 1.335031e-15 | -1.646402e-15 | -8.896944e-16 | -1.886187e-15 | 1.866680e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\43342d1f75a7fcfc.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 1.298035e-14 | -1.328379e-14 | 1.206953e-14 | 2.611309e-15 | -4.226612e-15 |
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-1.030456e-14  1.090538e-14  -5.704843e-15  5.039897e-15  -2.207193e-15
6.321357e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb

-1.078201e-14  -1.189031e-14  1.493224e-14  -1.553000e-15  4.737159e-15
3.486020e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b36166e033b.final.pdb

-3.193089e-15  -3.853780e-15  3.519696e-15  2.228588e-15
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Supplementary Text 10

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Supplementary Text 10

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| File Path | Values |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -1.252119e-15 |
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| File Path                                                                 | Values                                                                 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb      | -4.31776e-16 8.383145e-15 -3.550055e-15 -1.124431e-14 -2.301490e-15 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb      | 4.487942e-16 6.392013e-15 -2.676132e-15 -9.718692e-15 5.144910e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb      | -8.359239e-16 -2.878998e-15 1.216389e-15 -4.351024e-15 -3.591157e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb      | -2.525679e-15 -2.057761e-15 2.784553e-15 1.357449e-15 -8.376086e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a8234e4b4c668e.final.pdb     | -7.368159e-18 -2.254931e-15 1.544747e-15 -3.783823e-15 -3.339658e-15 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb      | 3.526917e-16 -2.933912e-15 3.854940e-15 8.214515e-16 -7.041740e-15 |
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| ee6862cbcad52078.final.pdb     | -6.987675e-16 -2.549888e-15 1.415269e-15 -3.709646e-15 -3.879339e-15 -2.057700e-15 |
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| ef8e88d4ad93a0ad.final.pdb     | -3.788243e-16 -1.195666e-15 1.400487e-15 -4.158036e-15 -4.807198e-15 -1.016271e-15 |
| f14fcae8deec4fa3.final.pdb     | 2.360633e-16 -3.814811e-15 4.417563e-15 -1.474831e-15 -4.718928e-15 -5.481124e-16 |
| f83584e22003fb92.final.pdb     | -3.211731e-15 9.910631e-15 -4.04512e-15 -1.350455e-14 1.516519e-15 1.827360e-15 |
| f8e2bf87e52caa29.final.pdb     | -3.622216e-15 2.054050e-15 2.101737e-15 3.992862e-15 -1.039002e-14 -5.630861e-16 |
| 013d855ad26c877c.final.pdb     | -3.390420e-15 -2.019331e-15 1.356135e-17 3.697899e-15 2.567197e-16 2.096838e-15 |
| 0a2a705342ca0d54.final.pdb     | -6.935746e-15 -3.224066e-15 2.113072e-15 5.043687e-15 2.949472e-15 8.261183e-15 |
| 0a59fceedb4194d9.final.pdb    | -6.935746e-15 -3.224066e-15 2.113072e-15 5.043687e-15 2.949472e-15 8.261183e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 1.286833e-16 | 6.684102e-15 | 8.371025e-15 | 5.940029e-15 | 1.825777e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | 3.131817e-15 | 0.000000e+00 | 0.000000e+00 | 0.000000e+00 | 0.000000e+00 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 1.508204e-16 | -2.537787e-15 | 4.072357e-15 | 6.126405e-15 | 2.863105e-15 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | -2.502242e-15 | -6.151442e-15 | 8.653106e-16 | 8.431959e-15 | 4.584855e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 8.122074e-16 | 6.214826e-16 | 6.085358e-15 | 4.764051e-15 | 8.854617e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 5.146660e-15 | -1.590289e-15 | 6.359112e-15 | 5.772031e-15 | -3.908447e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -2.962594e-15 | -7.821477e-16 | 2.596131e-15 | 6.563074e-15 | 3.393405e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982f7ef.final.pdb | -5.327134e-15 | -2.793784e-15 | 4.127579e-15 | 2.817018e-15 | 2.410555e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 | 2.949472e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 8.122074e-16 | 6.214826e-16 | 6.085358e-15 | 4.764051e-15 | 8.854617e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | -2.977285e-15 | -5.418741e-15 | 4.072750e-15 | 6.126405e-15 | 2.863105e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 2.256836e-15 | 7.604814e-16 | -9.490271e-16 | 1.380483e-15 | -4.917814e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -1.627860e-15 | -5.211846e-15 | -2.55815e-15 | 5.447543e-15 | 4.260019e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298f7ef.final.pdb | -1.627860e-15 | -5.211846e-15 | -2.55815e-15 | 5.447543e-15 | 4.260019e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfe12d3f9.final.pdb | 2.256836e-15 | 7.604814e-16 | -9.490271e-16 | 1.380483e-15 | -4.917814e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 3.250784e-15 | 2.50784e-15 | 1.825777e-15 | 6.684102e-15 | 8.371025e-15 |

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|                |        |        |        |        |        |
|----------------|--------|--------|--------|--------|--------|
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\89d0666e1402203d.final.pdb |        | -2.502242e-15 | -6.151442e-15 | 8.653106e-16 | 8.431959e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b34852716dadc62.final.pdb |        | -2.148277e-15 | -1.572396e-15 | 4.828903e-15 | 6.224699e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b6ef9ac3fe74395.final.pdb |        | -9.183463e-15 | -2.827166e-15 | 1.006285e-14 | 7.735708e-16 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\98bbe0d5986c138f.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\9c22f490d7e2fa.final.pdb |        | -3.222505e-15 | -2.085170e-15 | 7.536156e-15 | 1.403963e-14 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\9dda8ed0d81fb3ef.final.pdb |        | -1.208809e-15 | -6.566019e-15 | 9.714833e-15 | -9.137589e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\9f752b3616e6033b.final.pdb |        | -2.636291e-15 | -1.247119e-15 | 2.027665e-15 | 6.596829e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb |        | 1.508204e-16 | -2.537787e-15 | 4.072750e-15 | 6.12405e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a0c997d891e4e082.final.pdb |        | -5.793787e-15 | -4.59470e-15 | -4.039326e-15 | -3.287022e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\ab8039a2d823c616.final.pdb |        | -2.916965e-15 | -2.971928e-15 | 1.966178e-15 | 6.693095e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\acf4d74b9c71d4dc.final.pdb |        | -1.627800e-15 | -5.211846e-15 | -2.55815e-15 | 5.447543e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\ad8a823e4b4c668.final.pdb |        | -2.607660e-15 | -3.728379e-16 | 2.379678e-15 | 6.978417e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\ad8abab03b7b857.final.pdb |        | -3.222505e-15 | -2.085170e-15 | 7.536156e-15 | 1.403963e-14 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b16ababd03b7b857.final.pdb |        | -2.916965e-15 | -2.971928e-15 | 1.966178e-15 | 6.693095e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b226923e697d3c63.final.pdb |        | -1.222879e-14 | 4.646528e-16 | 8.559994e-17 | 1.090671e-14 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b28e48f6fa27a165.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b42c4924e3cd1aec.final.pdb |        | -7.568892e-15 | -6.845797e-15 | -2.162766e-17 | 1.042749e-14 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b4dd239fcabff1df.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b669492ef97459a2.final.pdb |        | -9.183463e-15 | -2.827166e-15 | 1.006285e-14 | 7.735708e-16 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b694b07405f66fda.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b85c997d52b666b7.final.pdb |        | -9.183463e-15 | -2.827166e-15 | 1.006285e-14 | 7.735708e-16 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b9229e6e2e6d69b9.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b991f2e9f6e35eef.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b9f4d250f66f6e6d.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
|                |        |        |        |        |        |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\b9fda3e0d8aca5de.final.pdb |        | -6.935746e-15 | -3.224066e-15 | 2.113072e-15 | 5.043687e-15 |
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-1.627860e-15  -5.211846e-15  -2.555815e-15  5.447543e-15  4.260019e-16
3.312584e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb

-6.935746e-15  -3.224066e-15  2.113072e-15  5.043687e-15  2.949472e-15
3.312584e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb

-2.605198e-15  -7.029788e-16  3.095562e-15  6.971487e-15  3.450086e-15
5.087708e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682cbbcad5207e.final.pdb

-3.010067e-15  -8.101981e-16  3.075843e-15  5.896304e-15  2.943401e-15
3.832000e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb

-2.523248e-15  -8.427300e-16  2.065403e-15  6.416056e-15  3.163987e-15
5.026978e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb

1.597431e-14  4.006587e-15  7.375030e-15  -7.420734e-15  -2.146904e-15
9.077777e-16  -1.446101e-15  1.004205e-16  -1.469041e-15  -2.046460e-17
5.087708e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb

1.597431e-14  4.006587e-15  7.375030e-15  -7.420734e-15  -2.146904e-15
9.077777e-16  -1.446101e-15  1.004205e-16  -1.469041e-15  -2.046460e-17
5.087708e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb

1.597431e-14  4.006587e-15  7.375030e-15  -7.420734e-15  -2.146904e-15
9.077777e-16  -1.446101e-15  1.004205e-16  -1.469041e-15  -2.046460e-17
5.087708e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb

1.993575e-15  -2.637406e-15  -2.820683e-15  -8.631575e-15  3.851054e-15
2.554400e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb

1.993575e-15  -2.637406e-15  -2.820683e-15  -8.631575e-15  3.851054e-15
2.554400e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcelandb419d4.final.pdb

1.993575e-15  -2.637406e-15  -2.820683e-15  -8.631575e-15  3.851054e-15
2.554400e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0bda59f3306825e.final.pdb

1.993575e-15  -2.637406e-15  -2.820683e-15  -8.631575e-15  3.851054e-15
2.554400e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb

1.993575e-15  -2.637406e-15  -2.820683e-15  -8.631575e-15  3.851054e-15
2.554400e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb

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-3.591437e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
2.785026e-15 -1.608792e-15 5.138190e-16 1.537733e-15 2.487118e-15 -5.306840e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea0f8694090cae7.final.pdb
1.069302e-15 3.356230e-15 -1.050081e-14 -7.467718e-15 5.932139e-15 -3.073588e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
1.176859e-15 -4.533359e-16 -2.228465e-15 -5.78940e-15 2.982245e-15 5.244846e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
7.124739e-17 -2.100819e-15 1.002609e-15 -2.025406e-15 6.093685e-16 -7.504354e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
4.135807e-16 -2.349822e-15 -2.625894e-16 -2.125973e-15 1.169155e-16 -6.09888e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-1.847876e-16 -1.864451e-15 1.309254e-15 -2.305117e-15 2.714195e-16 -7.878973e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-2.416441e-15 -9.891329e-16 -8.020826e-16 -2.495552e-15 1.086236e-16 -6.809187e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-5.299610e-17 -1.617280e-15 -5.311832e-16 -1.92803e-15 1.099128e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-7.530531e-15 -4.422817e-15 -6.248253e-15 -3.674431e-153.304244e-15 -5.548349e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
1.993575e-15 -2.637406e-15 -2.820683e-15 -8.631575e-153.851054e-15 2.554400e-15

[,307] [,308] [,309] [,310] [,311] [,312]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
1.677986e-15 -2.031532e-15 -1.640750e-15 -5.766136e-16 7.054827e-16 4.076707e-16
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
3.026929e-15 -1.875297e-15 -1.324503e-17 -2.915430e-15 -6.544817e-16 1.810309e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
2.889347e-15 -1.159361e-15 -1.776836e-15 -2.432970e-15 -2.097165e-15 3.048159e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
2.665908e-15 -1.110514e-15 -1.534805e-15 -2.738140e-15 2.514053e-16 2.171465e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
6.891432e-15 -3.578437e-15 -2.999269e-15 1.720922e-15 7.956751e-15 3.739181e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a70342ca0d54.final.pdb
4.413548e-15 -1.871678e-15 -2.152924e-15 -2.065968e-158.303382e-16 2.346216e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
-4.428864e-16 -2.665069e-15 -4.755747e-15 -1.900480e-15 4.594944e-15 2.916125e-15

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| File Path                                                                 | Values                  |
|---------------------------------------------------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb        | 2.783606e-15 -3.083174e-15 -2.267216e-15 -2.168328e-15 -2.555674e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb        | 5.733504e-15 1.284426e-15 6.336145e-15 -6.732819e-15 -4.020143e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb        | 4.704953e-15 1.778926e-15 9.210642e-15 -3.365209e-15 1.164981e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb        | 3.562548e-15 -1.296614e-15 -1.197343e-15 -1.753178e-15 7.570614e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb        | 2.080099e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb        | 2.080099e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb        | 1.229458e-15 1.081783e-14 5.849104e-15 -3.588515e-15 1.397912e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb        | 3.885249e-15 -9.901933e-16 -1.281963e-15 -2.203623e-15 1.311979e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb        | 7.814831e-15 -1.325429e-15 8.442463e-15 1.662425e-15 -1.006737e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb        | 2.338462e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb        | 2.338462e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb        | 5.733504e-15 1.284426e-15 6.336145e-15 -6.732819e-15 -4.020143e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | 3.885249e-15 -9.901933e-16 -1.281963e-15 -2.203623e-15 1.311979e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb        | 2.783606e-15 -3.083174e-15 -2.267216e-15 -2.168328e-15 -2.555674e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fccf.final.pdb        | 1.229458e-15 -1.400060e-15 1.788795e-15 -4.984286e-15 1.341995e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb        | 1.229458e-15 -1.400060e-15 1.788795e-15 -4.984286e-15 1.341995e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | 1.229458e-15 -1.400060e-15 1.788795e-15 -4.984286e-15 1.341995e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | 1.229458e-15 -1.400060e-15 1.788795e-15 -4.984286e-15 1.341995e-14 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb     | 1.166895e-14 -2.973416e-15  5.698131e-15 -3.064913e-15  1.023366e-14 |
|                                                                           | 4.467458e-16                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb     | -4.463201e-15  7.608361e-15 -7.802719e-15 -3.730013e-15 -5.894149e-15 |
|                                                                           | -3.828550e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb     | 6.558202e-15 -3.147710e-15  4.269787e-15 -5.656140e-15 -2.153309e-15 |
|                                                                           | 1.029343e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb     | 6.558202e-15  1.284426e-15  6.336145e-15 -6.732819e-15 -4.020143e-16 |
|                                                                           | 2.080099e-17                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb     | -2.228521e-15 -1.612564e-15 -1.770423e-15 -2.398171e-16 -4.175355e-15 |
|                                                                           | 2.824656e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb     | -4.428864e-16 -2.665669e-16 -4.755747e-16 -1.900480e-16  4.594944e-15 |
|                                                                           | 2.916125e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb     | 6.558202e-15 -3.147710e-15  4.269787e-15 -5.656140e-15 -2.153309e-15 |
|                                                                           | 1.029343e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb      | 3.827211e-15 -3.092056e-15  2.706037e-15 -4.373584e-15 -8.329869e-15 |
|                                                                           | 5.272695e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb      | 2.783606e-15 -3.083174e-15 -2.267216e-15 -2.168328e-15 -5.556747e-15 |
|                                                                           | 5.295228e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | -2.228521e-15 -1.612564e-15 -1.770423e-15 -2.398171e-16 -4.175355e-15 |
|                                                                           | 2.824656e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | -1.364253e-15  3.831475e-15 -5.788151e-15 -1.493220e-15 -2.344482e-15 |
|                                                                           | 2.658930e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb      | 2.923252e-15 -1.166890e-15 -7.935685e-16 -1.951921e-15  1.735165e-15 |
|                                                                           | 2.310636e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc.final.pdb       | 2.279234e-14  8.068385e-15 -5.834935e-15 -4.829745e-15 -4.811890e-15 |
|                                                                           | 4.654974e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb       | 5.290450e-15  1.456389e-15 -2.198460e-15 -8.317880e-17 -1.026897e-14 |
|                                                                           | -1.968041e-14                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | -2.228521e-15 -1.612564e-15 -1.770423e-15 -2.398171e-16 -4.175355e-15 |
|                                                                           | 2.824656e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | 4.381861e-15 -1.199160e-15 -1.195964e-15 -1.821955e-15 -1.488073e-15 |
|                                                                           | 1.781195e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | -4.428864e-16 -2.665609e-16 -4.755747e-15 -1.900480e-15  4.594944e-15 |
|                                                                           | 2.916125e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb       | 9.195179e-15 -2.114635e-15 -1.012960e-14  2.154276e-15  5.818142e-15 |
|                                                                           | 1.439607e-15                                                           |
| File Path                                      | Coordinates                  |
|-----------------------------------------------|-------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | -4.428864e-16, -2.665069e-15, -4.755747e-15, -1.900480e-15, 4.594944e-15, 2.916125e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 6.510852e-15, -8.177191e-15, -1.022156e-14, 4.041697e-15, 2.763791e-16, 1.773414e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | -4.428864e-16, -2.665069e-15, -4.755747e-15, -1.900480e-15, 4.594944e-15, 2.916125e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 2.167831e-15, -7.760544e-19, 1.245166e-16, -4.025665e-15, -4.742012e-15, -4.818071e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -9.136887e-15, 7.408904e-15, -6.059825e-15, -1.357729e-15, -6.271798e-15, 1.745186e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 3.075173e-15, -3.117080e-15, -2.000268e-15, -3.484331e-15, 7.516397e-16, 2.039792e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 2.167831e-15, -7.760544e-19, 1.245166e-16, -4.025665e-15, -4.742012e-15, -4.818071e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | -4.428864e-16, -2.665069e-15, -4.755747e-15, -1.900480e-15, 4.594944e-15, 2.916125e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd02e697772494a61.final.pdb | -3.726718e-16, -5.771334e-15, 6.243754e-15, 1.250191e-14, 1.894606e-15, 3.658110e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ba2a1f55fc9d0681.final.pdb | 3.640268e-15, 2.817470e-15, -1.638511e-15, -5.063971e-15, 4.271180e-15, 1.582493e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b71b40af0f0efe39.final.pdb | -3.508306e-15, -5.523964e-15, -1.367103e-15, -3.661236e-15, -1.020339e-15, 9.263290e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4b4806824ef848.final.pdb | 1.035646e-14, -4.280135e-15, -6.667548e-15, -7.667686e-15, 2.514172e-15, -2.300584e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b529e19ad281fe2a.final.pdb | 4.704953e-15, 1.778926e-15, 9.210642e-15, -3.365209e-15, 1.164981e-15, 5.438860e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b529e19ad281fe2a.final.pdb | 6.891432e-15, -3.578437e-15, -2.999269e-15, 1.720922e-15, 7.956751e-15, 3.739181e-15 |
Supplementary Text 10

-6.601067e-15 -1.313993e-15 3.411302e-15 -5.256657e-15 1.444956e-14
5.818862e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb
4.285464e-15 -9.141886e-16 1.904315e-15 8.276390e-15 -4.947846e-15
-4.175805e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
5.952679e-15 -1.530907e-14 -1.996263e-15 1.624737e-14 -3.204291e-16
-8.219239e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
-5.274813e-15 2.409975e-15 -1.704777e-15 -1.858949e-15 -2.963120e-15
7.204518e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb
3.629943e-15 -2.257478e-15 3.018321e-15 1.160268e-14 -4.999140e-15
-3.864060e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
5.469847e-15 -1.611114e-14 3.062243e-15 7.966525e-15 -4.306966e-15
-1.807908e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
1.517425e-15 -4.340249e-15 -5.246713e-15 4.567842e-15 1.051091e-15
-1.631363e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
-5.609907e-16 -1.129007e-15 6.334313e-15 2.586441e-16 -6.944518e-16
-2.881062e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
3.629943e-15 -2.257478e-15 3.018321e-15 1.160268e-14 -4.999140e-15
-3.864060e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
7.224872e-15 -7.010583e-15 4.388245e-15 6.986814e-15 -2.856315e-15
-5.480289e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
4.285464e-15 -9.141886e-16 1.904315e-15 8.276390e-15 -4.947846e-15
-4.175805e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
1.517425e-15 -4.340249e-15 -5.246713e-15 4.567842e-15 1.051091e-15
-1.631363e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
1.322169e-15 -2.034460e-16 7.358087e-16 1.426864e-16 -1.174534e-14
-1.424396e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
9.673721e-16 -2.957259e-15 2.812443e-15 5.777304e-15 -2.80056e-15
-2.706494e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc.final.pdb
9.094870e-16 -1.154081e-14 -5.566970e-15 2.639768e-14 2.497298e-15
-9.817493e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-3.756511e-15 8.524851e-16 1.942718e-15 8.952473e-15 -4.631127e-15
-1.056310e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
1.517425e-15 -4.340249e-15 -5.246713e-15 4.567842e-15 1.051091e-15
-1.631363e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
2.792624e-16 -1.570393e-15 2.327052e-15 5.801390e-15 -3.531506e-15
-2.212535e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80ddc53135.final.pdb
| File Path | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|-----------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fccc.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfeefedeb.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b38f113c7.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5a4b4a5c7c6682ce6.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5aa551611d85ac96.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\611d124e8f113c7.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffef.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6e170625423cf2dcb.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\68760178986bef01.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1be4.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad6f1be4.final.pdb | -1.301625e-14 | 9.845627e-15 | 4.404223e-15 | 1.779254e-15 | -1.727847e-15 |
Supplementary Text 10

-1.428122e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
3.18818e-15 -2.379781e-16 1.230186e-15 2.268154e-15 -2.10859e-15
-1.809238e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
-1.034495e-15 -5.230731e-15 9.093729e-17 -1.147800e-15 -7.215710e-17
-1.163577e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
2.985761e-16 2.436450e-15 6.489029e-15 5.177870e-15 4.311564e-15
-6.055655e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
4.853416e-15 -5.914584e-16 1.186637e-15 2.259672e-15 -2.451338e-15
-2.344014e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
3.709042e-15 -8.110343e-15 -3.488177e-16 7.642479e-15 -1.433406e-15
6.98683e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
4.853416e-15 -5.914584e-16 1.186637e-15 2.259672e-15 -2.451338e-15
-2.344014e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
2.085405e-15 -4.791575e-15 3.033462e-15 3.944264e-15 -9.347484e-16
-3.577981e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
4.853416e-15 -5.914584e-16 1.186637e-15 2.259672e-15 -2.451338e-15
-2.344014e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9df2cbf3975403e7.final.pdb
2.085405e-15 -4.791575e-15 3.033462e-15 3.944264e-15 -9.347484e-16
-3.577981e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9f88c8a05f3a288.final.pdb
2.085405e-15 -4.791575e-15 3.033462e-15 3.944264e-15 -9.347484e-16
-3.577981e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
5.916542e-15 -9.805684e-15 2.500902e-15 6.427304e-15 -1.744431e-15
-1.212529e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55f9d60681.final.pdb
2.085405e-15 -4.791575e-15 3.033462e-15 3.944264e-15 -9.347484e-16
-3.577981e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
7.242014e-15 -2.431205e-15 5.346125e-15 2.524463e-15 -1.246696e-14
2.150747e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb
3.516811e-15 6.930859e-17 8.764343e-15 1.392961e-15 6.074135e-16
-6.287908e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
3.247062e-15 -8.18035e-16 -6.129724e-16 1.827817e-15 -4.081722e-16
-1.524418e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
6.892611e-15 1.231366e-14 1.17992e-16 -6.099297e-15 1.479702e-14
-1.00308e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
-7.341839e-16 -4.578306e-15 5.067898e-15 -6.534467e-16 1.118037e-15
1.123836e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb
-1.162616e-15 -1.288155e-14 2.145546e-15 3.564907e-15 -1.401970e-14
Page 267
| File Name                                                                 | Scores                |
|--------------------------------------------------------------------------|-----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb      | -6.070713e-15 6.556988e-15 8.613949e-15 9.316562e-15 4.015662e-15 5.131621e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb      | 7.451332e-15 -5.250804e-15 -2.601904e-15 2.622520e-15 -1.573620e-16 1.582468e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb      | 8.640613e-15 4.965566e-15 1.115671e-14 1.698627e-14 4.112163e-15 1.845647e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb      | -3.985631e-15 -8.475483e-16 1.805239e-15 -2.458180e-15 6.63134e-16 -4.044802e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feaa2.final.pdb      | 1.219351e-15 -3.459694e-15 5.075000e-15 7.911795e-15 2.378156e-15 2.095660e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb      | 1.790310e-15 2.127790e-15 3.528754e-15 7.376184e-15 2.561769e-15 4.192057e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb      | -7.386500e-16 -1.049228e-14 4.073243e-15 1.493040e-15 6.178340e-15 2.628500e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb       | -3.527850e-16 -4.706862e-16 1.125212e-15 7.704415e-15 6.254117e-16 2.849029e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb       | 1.125212e-15 7.704415e-15 6.254117e-16 2.849029e-16 1.790310e-15 2.127790e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb       | 3.528754e-15 7.376184e-15 2.561769e-15 4.192057e-15 1.790310e-15 2.127790e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb0589d996d0a960.final.pdb       | -7.386500e-16 -1.049228e-14 4.073243e-15 1.493040e-15 6.178340e-15 2.628500e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | -9.089314e-16 -2.594626e-16 1.142038e-15 4.620941e-15 1.021102e-15 1.121833e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | -1.333773e-16 -6.884929e-16 8.993645e-16 4.512603e-16 5.957829e-16 8.663322e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef3a42fc83b8e5d.final.pdb        | -8.624784e-16 -3.525558e-16 8.210006e-16 4.177787e-15 1.192212e-15 3.731954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb       | -6.921868e-16 -1.215375e-15 -1.241163e-15 3.632361e-15 3.672668e-15 3.485860e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef9e42fc83b8e5d.final.pdb        | -8.624784e-16 -3.525558e-16 8.210006e-16 4.177787e-15 1.192212e-15 3.731954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | 2.165896e-15 -2.443317e-16 1.616959e-15 2.961739e-15 1.048096e-15 1.069207e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f38358a2e203fb92.final.pdb       | 6.657131e-16 -5.292449e-15 7.881254e-16 -3.216241e-15 6.656527e-15 3.262419e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52ca29.final.pdb        | 1.219351e-15 -3.459694e-15 5.075000e-15 7.911795e-15 2.378156e-15 2.095660e-15 |

[,331] [,332] [,333] [,334] [,335] [,336]
Supplementary Text 10

2.487561e-15  8.477914e-15  -2.718894e-15  -1.807997e-15  2.105116e-15  4.634855e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb

-2.656175e-15  3.313434e-15  -2.718894e-15  -1.807997e-15  2.105116e-15  4.634855e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb

-2.608127e-15  5.790425e-16  -1.345102e-15  -6.122348e-15  2.930115e-15  2.682211e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb

8.100658e-15  4.891311e-15  -9.828999e-15  -8.152150e-15  6.169328e-15  1.054808e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb

-2.811431e-15  -4.067822e-15  -1.824969e-16  -1.370240e-14  -7.888208e-16  1.057605e-14
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1.874146e-17  2.557528e-15  -9.394405e-15  -9.506045e-16  4.912851e-16  7.065175e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb

-9.540328e-15  7.295961e-16  -9.002106e-16  -5.903145e-15  -3.418628e-16  1.831827e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb

-2.988320e-15  7.372686e-15  -3.721081e-15  -2.060740e-15  -4.913246e-15  3.519834e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb

-4.120813e-15  2.567277e-15  -2.649126e-15  -3.447077e-15  -2.330739e-15  3.779636e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb

1.831827e-15  -1.013870e-14  -6.768540e-15  -2.662986e-15  -9.466806e-16  5.250017e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f0482230a.final.pdb

5.250017e-15  -2.642743e-15  -8.102822e-15  -4.181548e-15  -2.514179e-15  3.447077e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff286d.final.pdb

-5.553260e-15  6.946526e-16  -2.649126e-15  -3.447077e-15  -2.330739e-15  3.779636e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb

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-5.658871e-16  5.752455e-15  -4.371404e-15  3.447007e-15  8.815979e-16
5.218562e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffec.final.pdb

-6.896917e-15  3.854494e-15  -3.862572e-15  1.382667e-14  1.457880e-16
8.771837e-15

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-2.943782e-16  3.059406e-15  -3.155601e-15  -6.733498e-16  5.005988e-15
8.310006e-15

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5.250017e-15

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5.254222e-15

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5.866279e-15

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1.117900e-14

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6.515083e-15

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6.515083e-15

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2.682211e-15

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7.065175e-15

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6.951723e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
Supplementary Text 10

7.511249e-16  6.252362e-15 -4.514409e-15  1.722634e-15  1.772504e-15 
4.695458e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb

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4.294426e-16  8.129253e-15 -1.041136e-14 -4.216813e-15  1.406037e-15 
3.891676e-15

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5.674204e-15  1.050057e-14 -3.135032e-15 -2.503121e-15  3.630521e-14 
1.385736e-14

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6.419873e-15  8.089189e-16 -2.474720e-15 -3.698453e-15  1.203805e-14 
4.381354e-15

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-8.125957e-15 -5.176974e-16 -5.057522e-15  3.578656e-15  2.812667e-15 
5.370753e-16

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-3.402730e-15  5.001753e-15 -5.104434e-15  1.788910e-15  3.385671e-15 
5.827016e-15

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-6.434718e-16  2.852831e-15 -6.822383e-15  1.897564e-15  3.961408e-15 
6.515083e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb 
-2.935037e-15  7.728749e-15  2.683597e-15  1.113079e-14  2.455904e-15 
2.635911e-16

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-4.120813e-15  2.567277e-15 -2.649126e-15  3.447077e-15  2.330739e-15 
3.779636e-15

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-6.434718e-16  2.852831e-15 -6.822383e-15  1.897564e-15  3.961408e-15 
6.515083e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb 
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5.633824e-15

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-6.097008e-16  5.872834e-15 -4.509411e-15  3.083602e-15  3.283381e-15 
4.747816e-15

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-2.939246e-16  5.145958e-15 -4.067103e-15  2.249071e-15  3.239842e-15 
5.486241e-15

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7.511249e-16  6.252362e-15 -4.514409e-15  1.722634e-15  1.772504e-15 
4.695458e-15

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-3.418628e-16

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-4.820633e-15  6.879914e-15 -6.389571e-15  4.761708e-15  4.209823e-15 
6.951723e-15

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-9.540328e-15  7.295961e-16 -9.002106e-16  1.531766e-15 -5.903145e-15 
-3.418628e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb 
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-3.402730e-15  5.001753e-15 -5.104434e-15  1.788910e-15  3.385671e-15
5.827016e-15

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 2.599943e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-1.164624e-15  4.156895e-15  6.814344e-17  2.914916e-15 -2.948139e-15
 2.990301e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-6.331658e-16  4.997560e-15  1.846777e-15  1.766267e-15 -1.527606e-15
 1.781405e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
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 3.440180e-15
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 1.756216e-15
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-7.642945e-16  4.546171e-15  1.720305e-15  2.600302e-15 -1.999872e-15
 2.840887e-15
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 -5.924479e-16
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 1.450875e-14
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-1.037789e-15  5.028591e-15  1.755669e-15  3.214445e-15 -1.259170e-15
 2.981082e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
 2.397490e-15  2.109124e-15  2.703175e-15  5.154639e-15 -3.896787e-15
| File Path                                                                 | Coordinates |
|--------------------------------------------------------------------------|-------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb     | 4.190968e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa29.final.pdb    | -1.276314e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb     | 1.366827e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb     | -2.612523e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb     | 2.133139e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb      | 1.437084e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb      | 1.605850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | 1.816502e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb      | 1.605850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb      | 1.750564e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551be0a39.final.pdb       | 1.605850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb       | 6.882347e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb      | 7.652785e-15 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb
4.406425e-15 -7.500181e-15 2.33587e-15 -9.826855e-15 -6.161861e-15
4.488545e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
5.545696e-16 1.695360e-15 -1.932462e-15 -6.234800e-15 -4.106408e-15
-1.602004e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
6.407467e-15 -3.117691e-15 2.786236e-15 -4.667154e-15 -5.725138e-15
-9.662011e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
2.557407e-15 -1.457011e-15 -1.089508e-15 -5.465326e-15 -5.582369e-15
7.139086e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
4.711333e-15 -3.468144e-15 -3.349135e-15 1.829522e-15 -9.580942e-15
-1.095342e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
1.146853e-15 3.416190e-15 3.703889e-15 -1.621801e-15 -2.993978e-15
-5.146326e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
1.605850e-15 -7.486274e-15 -2.213435e-15 -3.705299e-15 -9.126225e-15
-1.388052e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb
1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15
-8.581627e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
1.779242e-16 1.084852e-15 5.702311e-16 -4.891547e-15 -1.709023e-15
-4.660874e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
2.921327e-16 -4.427475e-16 3.775726e-16 -6.132561e-15 -5.662254e-15
-8.331360e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
1.141280e-15 -2.558676e-15 -5.123405e-15 -6.732579e-15 -7.065012e-16
-2.515221e-15 7.390641e-16 -4.491996e-15 -6.846798e-15
-1.500890e-15
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad_final.pdb      | 2.557407e-15 -1.457011e-15 -1.089508e-15 -5.465326e-15 -5.582369e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3_final.pdb      | 1.810553e-15 -3.085193e-15 1.674397e-15 -5.881705e-15 -5.935805e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8358e42003fb92_final.pdb       | 1.095310e-15 -8.069459e-15 -6.653262e-15 -8.855210e-15 -8.929172e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29_final.pdb       | 1.366827e-15 2.016202e-15 -3.580534e-16 -1.419161e-16 -4.742652e-15    |

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E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 8.704329e-16 5.413606e-15 -2.051666e-15 -5.883462e-15 -5.442054e-15    |
| -2.966244e-15                                                       |

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| -2.247161e-16 6.166899e-15 2.516945e-17 -5.512208e-15 -6.741806e-15    |
| -1.665839e-15                                                       |

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 2.856430e-15 5.101578e-15 -6.553178e-15 -5.905213e-15 -5.379643e-15    |
| -3.525953e-15                                                       |

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 1.459179e-17 4.655806e-15 -1.677958e-15 -6.986109e-15 -4.104027e-15    |
| -4.276501e-15                                                       |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fced4b1949d_final.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| -3.345888e-15 3.808341e-15 -5.941472e-15 -5.702466e-15 -3.731616e-15    |
| -2.383149e-15                                                       |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0db59f3306825e8_final.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 4.140877e-15 5.093932e-15 -1.239264e-15 -2.295258e-15 -4.528052e-15    |
| -4.232093e-15                                                       |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c_final.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 3.017946e-16 7.510464e-15 1.282157e-15 -5.879197e-15 -3.691698e-15    |
| -1.222347e-15                                                       |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2_final.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 4.233040e-15 1.106754e-14 4.970025e-15 -7.471646e-15 -7.301070e-15    |
| 2.083006e-15                                                       |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39_final.pdb

| Values                                                                 |
|----------------------------------------------------------------------|
| 4.233040e-15 1.106754e-14 4.970025e-15 -7.471646e-15 -7.301070e-15    |
| 2.083006e-15                                                       |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682e.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb

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| Path                                                                 | Values                                      |
|----------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 7.699776e-15  5.390085e-15  2.081076e-15  -5.111001e-15  -1.414262e-15  -3.114716e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 5.522493e-15  4.120876e-15  -1.095203e-15  -3.718018e-15  2.045644e-15  -1.587401e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 2.522493e-15  4.120876e-15  -1.095203e-15  -3.718018e-15  2.045644e-15  -1.587401e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 8.805662e-15  1.309547e-15  -1.332847e-14  -1.161535e-14  4.041443e-15  -7.440110e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 6.984648e-15  8.573614e-15  -2.851833e-15  -1.429247e-15  3.251683e-15  1.888461e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | 1.765924e-14  9.338046e-15  -6.312514e-15  -1.680161e-15  1.267598e-15  -7.298816e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 4.245492e-15  2.521413e-15  -2.465633e-15  -3.593560e-15  4.041443e-15  -7.440110e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 1.765924e-14  9.338046e-15  -6.312514e-15  -1.680161e-15  1.267598e-15  -7.298816e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0e2939.final.pdb   | 5.688097e-15  9.110274e-15  1.913116e-15  1.427334e-16  1.565543e-15  -6.621858e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d9269772494a61.final.pdb   | 8.805662e-15  1.309547e-15  -1.332847e-14  -1.161535e-14  4.041443e-15  7.443787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 7.123282e-16  5.443702e-15  -5.700121e-16  -2.851116e-16  -2.095101e-15  -1.147083e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 8.563658e-15  6.642496e-16  -5.950868e-16  5.571765e-15  3.709262e-15  -3.470357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2.final.pdb   | 6.984648e-15  8.573614e-15  -2.851833e-15  -1.429247e-15  3.251683e-15  1.888461e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 6.984648e-15  8.573614e-15  -2.851833e-15  -1.429247e-15  3.251683e-15  1.888461e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 9.800407e-15  5.122746e-15  -9.321208e-17  -3.455033e-16  2.482633e-15  -2.522169e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 9.800407e-15  5.122746e-15  -9.321208e-17  -3.455033e-16  2.482633e-15  -2.522169e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 9.800407e-15  5.122746e-15  -9.321208e-17  -3.455033e-16  2.482633e-15  -2.522169e-15 |
| File Path                                                                 | Values                  |
|---------------------------------------------------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | 1.740152e-15 -3.114716e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | 2.364634e-15 -2.043193e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb       | 4.143238e-15 -2.369664e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb       | 4.245492e-15 -1.941375e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | 5.114305e-15 -9.889118e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb       | 4.832347e-15 1.691661e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa9.final.pdb       | 8.573614e-15 3.251683e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb       | 7.407243e-16 1.269333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb       | -5.704270e-17 -1.360004e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d9.final.pdb        | -2.229840e-15 -1.561821e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb       | -2.083508e-15 -2.083508e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb       | 3.559113e-15 5.370290e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb       | -5.509114e-17 3.936667e-15 |

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| File Path                                                                 | Coordinates          |
|---------------------------------------------------------------------------|----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb       | 2.470840e-15 -9.733991e-15 -8.062502e-15 5.392861e-15 5.623832e-15 4.376648e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb       | -1.668964e-16 6.292732e-17 -1.642430e-15 1.513502e-15 2.783403e-15 4.178557e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb       | 9.019833e-15 7.377776e-15 -8.650182e-15 -7.717373e-15 -8.717713e-15 1.000257e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd391854336d.final.pdb         | 5.568384e-15 -3.109278e-15 -7.797566e-15 3.816803e-15 2.761820e-15 5.681810e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb       | -8.546467e-16 4.419724e-16 -2.276808e-15 4.228367e-15 3.125244e-15 4.079793e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb        | -4.059616e-15 5.921088e-15 -2.772025e-16 8.951996e-15 6.295351e-15 2.679756e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb        | 1.083728e-14 7.364521e-16 -1.557670e-15 6.558913e-15 -7.674272e-15 3.504692e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb        | 6.723683e-15 -1.550812e-15 -9.403009e-15 1.627149e-14 -1.372680e-15 2.053316e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb        | 3.559113e-15 -8.665750e-15 -2.570633e-15 -4.851482e-15 2.561811e-15 5.370290e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | 1.382645e-15 -7.411712e-16 2.137243e-16 7.678275e-15 8.823276e-15 1.307590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb        | 5.020112e-15 -5.512815e-15 -2.089136e-15 9.032576e-15 -6.954636e-15 8.056684e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | -6.721900e-15 7.898557e-15 2.074473e-15 1.299010e-14 3.942383e-15 -1.129500e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21df8e8cdfb.final.pdb        | 7.127616e-15 -5.978247e-15 -7.160585e-15 -2.316768e-15 -6.718545e-15 1.519752e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | -2.083508e-15 1.980194e-15 -8.220314e-16 2.936993e-15 7.416868e-15 3.956490e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb        | -1.885129e-16 -1.018278e-14 1.041725e-14 1.348832e-14 1.170211e-15 1.923532e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c662ce6.final.pdb         | -9.654275e-15 5.126169e-15 5.296338e-15 1.120512e-14 4.458731e-15 3.115149e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb        | -4.811144e-15 -3.921773e-17 7.884915e-16 3.935650e-16 7.820487e-15 -4.834525e-16 |
| File Path                                                                 | Lines         |
|---------------------------------------------------------------------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb       | 15 8 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83db81e5d.final.pdb      | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d49.final.pdb       | 15 5 15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb       | 15 5 15       |
## Supplementary Text 10

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 3.512445e-15 | 6.279676e-15 | 1.103850e-15 | -8.007382e-16 | 5.879230e-15 |
| 4.234793e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -1.976038e-15 | -2.433430e-15 | 5.637683e-16 | -5.576086e-15 | 4.344012e-15 |
| 4.099835e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea0f8694090cae7.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -7.731263e-15 | 4.247781e-16 | -3.320540e-15 | -1.308393e-15 | 5.828217e-15 |
| -2.171680e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -5.480934e-15 | -8.302190e-15 | -5.701056e-15 | -3.148997e-15 | 7.640028e-15 |
| 2.653387e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -2.923750e-15 | -3.025710e-15 | -6.541812e-17 | -3.193637e-15 | 4.897167e-15 |
| -1.578129e-16 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682cbcad52078.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -3.022831e-15 | -3.116234e-15 | -4.657878e-16 | -3.405302e-15 | 5.452541e-15 |
| 2.980665e-16 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -2.471616e-15 | -2.776132e-15 | -4.198534e-16 | -3.145784e-15 | 5.003589e-15 |
| 2.577382e-16 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -2.675949e-15 | -2.321855e-15 | -1.473938e-15 | -1.782944e-15 | 3.620251e-16 |
| 3.271188e-16 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 2.481953e-16 | -2.088845e-15 | -1.161810e-15 | -2.936579e-15 | 2.999991e-15 |
| -1.246983e-16 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 2.035623e-15 | 6.111194e-15 | 2.429376e-15 | -3.958029e-15 | -1.039661e-15 |
| 2.006769e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| -5.042902e-15 | 6.882978e-15 | 2.658705e-15 | -2.855707e-16 | 8.370611e-15 |
| -1.293885e-15 |           |           |           |           |

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 2.936254e-15 | 4.103013e-15 | 4.538489e-15 | 2.987438e-15 | 1.164889e-15 |
| 5.321202e-15 |           |           |           |           |

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 2.093810e-15 | 1.580440e-15 | 5.070715e-15 | 3.542618e-15 | -8.329069e-16 |
| 4.600105e-15 |           |           |           |           |

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 2.437362e-15 | 4.412126e-15 | 5.509850e-15 | 2.457727e-15 | 6.258335e-16 |
| 5.039683e-15 |           |           |           |           |

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 3.921120e-15 | 2.048079e-15 | 2.980872e-15 | 1.966760e-15 | 5.029583e-16 |
| 5.234649e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 3.083988e-15 | 8.236863e-15 | 6.478100e-15 | 1.681830e-15 | -2.574941e-15 |
| 2.744457e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 1.734100e-15 | 3.673439e-15 | 3.850240e-15 | 2.168849e-15 | 9.022116e-16 |
| 3.829136e-15 |           |           |           |           |

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59feadb4194d9.final.pdb

|           |           |           |           |           |
|-----------|-----------|-----------|-----------|-----------|
| 1.483973e-15 | 4.571282e-15 | 2.853922e-15 | 4.559063e-15 | 6.558881e-17 |

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2.744457e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
-1.605512e-15  4.038973e-15  2.659837e-15 -4.285897e-15  1.359479e-15
5.547409e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
7.748355e-16  1.911863e-16  2.522774e-15 -3.474802e-15  8.739161e-15
1.136021e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
4.545884e-15 -9.569347e-16  4.876427e-15  6.032060e-16  2.342737e-16
7.857257e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
-1.605512e-15  4.038973e-15  2.659837e-15 -4.285897e-15  1.359479e-15
5.547409e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
1.483973e-15  4.571282e-15  2.853922e-15  4.559063e-15  6.556881e-17
8.840183e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
2.117815e-15  2.998308e-15  4.146159e-15  1.951697e-15  5.037984e-16
3.567259e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
1.951481e-15  3.633664e-15  3.692228e-15  1.878698e-15  5.205000e-16
3.317402e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
2.095169e-15  3.092208e-15  4.483276e-15  1.752960e-15  5.129999e-16
3.932473e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
1.660545e-15  4.683886e-15  2.529548e-15  1.608662e-15 -1.021264e-15
2.497396e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
5.545287e-17  4.548238e-15  3.063657e-15  4.033663e-15  3.634037e-15
2.726906e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
4.774309e-15  4.009232e-15  9.839058e-15 -7.045587e-15 -2.982774e-15
6.646336e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
3.083988e-15  8.236863e-15  6.478100e-15  1.681830e-15 -2.574941e-15
2.744457e-15

[,379]        [,380]        [,381]        [,382]        [,383]        [,384]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
3.441226e-15 -2.775875e-15 -3.154402e-15 -3.409216e-15  1.794918e-15
2.781986e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
3.052546e-15 -6.215171e-15 -3.132960e-15 -3.215251e-15 -6.321638e-16
1.652117e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
3.012395e-15 -5.158294e-15 -1.562470e-15 -3.269999e-15  1.794162e-16
5.560601e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
2.480146e-15 -4.104481e-15 -4.005864e-15 -2.286746e-15 -6.72996e-16
7.760043e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
5.364017e-15 -7.535191e-15 -1.513216e-15 -3.188974e-16  4.101895e-15
7.279758e-16

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| File Path                                                      | w, x, y, z, t          |
|---------------------------------------------------------------|------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -2.407227e-15, -1.958721e-15, -2.495484e-15, 5.686483e-17, 1.047416e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb   | -2.607285e-15, -4.047227e-15, -3.758721e-15, -2.495484e-15, 5.686483e-17, 1.047416e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dbaf933068258e.final.pdb | -5.722066e-16, -2.783784e-15, -7.525398e-16, -6.656710e-16, 3.055550e-15, 1.519010e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb  | -2.499289e-15, -4.628779e-15, -1.800351e-15, -2.437579e-15, 3.116690e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb  | -3.055605e-15, -3.433244e-15, -3.042790e-15, 7.179300e-16, 1.416912e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -3.092685e-15, -3.433244e-15, -3.042790e-15, 7.179300e-16, 1.416912e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb  | -3.057050e-15, -3.219863e-15, -2.371968e-15, 3.846545e-16, 1.659974e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb  | -3.057050e-15, -3.219863e-15, -2.371968e-15, 3.846545e-16, 1.659974e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb  | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb  | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb3282518797b.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb   | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\43432df75a7fccc.final.pdb    | -2.181086e-15, -3.842335e-15, -2.608658e-15, 7.568635e-16, 6.212452e-15 |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
7.224002e-16 -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-16
2.434758e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
-3.613462e-15 -8.362305e-15 -1.111083e-15 1.001402e-15 -2.922280e-15
-3.185082e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
4.183159e-15 -4.823798e-15 -1.519834e-15 -4.459707e-15 3.685824e-15
-6.263918e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
4.183159e-15 -4.823798e-15 -1.519834e-15 -4.459707e-15 3.685824e-15
-6.263918e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\830eefcfe12d3f9.final.pdb
6.965872e-15 -7.217716e-15 -3.263444e-16 -4.293174e-15 4.072234e-15
-2.881207e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
-5.722066e-16 -2.783784e-15 -7.525398e-16 -6.656710e-15 3.005550e-15
1.519010e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
5.038475e-15 -5.478797e-16 -7.13881e-16 7.319166e-16 1.370428e-15
4.423692e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
2.215982e-15 -1.652723e-15 -5.939910e-15 -2.451765e-15 -3.556646e-15
1.195068e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
-1.029078e-14 5.035807e-15 2.686210e-15 9.737314e-16 5.866382e-15
1.344644e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
7.224002e-16 -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-15
2.434758e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9b2e4909d67e2fa.final.pdb
-4.067592e-17 -1.904258e-15 -2.978737e-15 -3.414536e-15 -5.983741e-15
1.574105e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c2f4909d67e2fa.final.pdb
2.542621e-15 2.440999e-15 -4.546783e-15 -3.621928e-15 2.843910e-15
2.212455e-19

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9da8ed08d81fb3ef.final.pdb
2.284385e-15 9.432852e-15 -2.220662e-15 -1.766569e-14 5.752773e-15
-7.377632e-15

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6.879343e-16 -4.312170e-15 -2.733816e-15 -2.615509e-15 1.127580e-15
2.152420e-15

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2.542621e-15 2.440999e-15 -4.546783e-15 -3.621928e-15 2.843910e-15
2.212455e-19

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-3.679612e-15 -1.908074e-15 -9.918138e-15 -6.687436e-15 7.243844e-15
-1.713826e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
3.662389e-15 -3.542035e-15 -3.204975e-15 -2.383587e-15 2.539922e-16
1.910011e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac84d74b9c71d4dc.final.pdb
4.183159e-15 -4.823798e-15 -1.519834e-15 -4.459707e-15 3.685824e-15
-6.263918e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
2.595875e-15 -4.111677e-15 -3.794046e-15 -3.072656e-15 -7.473522e-16
3.046707e-16

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| File Path                                                                 | Line 1                                                                 | Line 2                                                                 | Line 3                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb      | -4.067592e-17 -1.904258e-15 -2.978737e-15 -3.414536e-15 -5.983741e-15 | 1.574105e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb      | -4.900885e-16 -7.564836e-15 -8.277666e-15 -4.853026e-15 7.516336e-15    | 1.288828e-14                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb       | -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-16                 | 2.434758e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | -1.469628e-14 5.778798e-15 1.569788e-15 -2.795294e-15                  | 4.129656e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb       | -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-16                 | 2.434758e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb       | -1.65273e-15 -5.939910e-15 -2.451765e-15 -3.556646e-15                 | 1.195068e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb       | -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-16                 | 2.434758e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb       | -4.047281e-15 -4.217903e-15 -3.057120e-15 3.014346e-16                 | 2.434758e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb       | -2.48509e-15 -3.325171e-15 -2.527162e-15 9.144425e-16                  | 1.385684e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | -8.40501e-15 2.289436e-15 -9.719872e-15 5.380310e-16 -8.407584e-15      | 5.648537e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | -1.65273e-15 -5.939910e-15 -2.451765e-15 -3.556646e-15                 | 1.195068e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | -3.40077e-15 -6.278226e-15 -1.210083e-15 2.917822e-15                 | -2.934684e-15                                                          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d0e697772494a61.final.pdb       | -5.948538e-15 -1.379618e-15 7.831739e-15 -5.873741e-17 8.354502e-15    | 2.484153e-15                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | -2.634775e-15 -1.745856e-15 -2.073071e-15 -1.857383e-15 -2.602005e-15   | 1.900844e-14                                                           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af00f3e39.final.pdb        | -2.848744e-15 -3.768455e-15 -5.323853e-18 2.488153e-15                | -2.602005e-15                                                          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | -1.299991e-14 -2.848744e-15 -3.768455e-15 -5.323853e-18 2.488153e-15  | -4.067592e-17 -1.904258e-15 -2.978737e-15 -3.414536e-15 -5.983741e-15 |
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|-----------------------|
| -2.216006e-15 -2.73997e-15 -2.813873e-15 4.009687e-16 -6.139132e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb |
| -2.362856e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb |
| -2.233577e-15 -3.411097e-15 -1.956825e-15 -9.510450e-16 -6.620652e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb |
| -2.009794e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb |
| -4.388509e-15 -7.724801e-15 -4.860078e-15 -6.220849e-15 -7.604817e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb |
| -2.687002e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb |
| -1.383968e-15 -4.709852e-15 1.669421e-15 3.799781e-15 -4.356981e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb |
| -2.115291e-15 -2.699508e-15 -1.750447e-15 -1.021247e-15 -6.768537e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb |
| -4.595798e-15 -4.572269e-17 -2.562328e-15 2.861079e-15 -7.765279e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb |
| -1.719724e-15 1.841386e-15 -2.562328e-15 2.861079e-15 -7.765279e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b30278518e2fdd.final.pdb |
| -1.851916e-15 -2.834723e-15 -1.837340e-15 -7.893024e-16 -6.778031e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb |
| -1.118485e-14 4.442365e-16 1.882734e-15 -1.596030e-14 -1.510448e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb |
| -3.973437e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb |
| -2.505756e-15 1.640852e-15 1.001015e-14 -1.022892e-14 -1.326224e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | -8.126249e-15 | 1.221247e-15 | -5.140086e-15 | -4.603064e-15 | -7.777900e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cfd8.final.pdb | -5.338179e-15 | -2.080740e-15 | -1.722066e-15 | -8.038589e-16 | -9.502220e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -1.754771e-15 | 4.667956e-15 | -1.327264e-14 | -1.937339e-14 | -1.672511e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -1.383968e-15 | 3.799781e-15 | -4.356981e-15 | -3.817339e-15 | -7.284910e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -5.207027e-15 | 6.494782e-15 | -3.193768e-15 | -1.164728e-14 | -5.179240e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 1.263417e-15 | 3.403337e-15 | -2.784910e-15 | -3.817339e-15 | -7.284910e-15 |

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-1.012150e-15 -1.520404e-15 -5.886741e-15 3.683437e-15 -1.028198e-14
6.866651e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
-2.281840e-15 -3.112741e-15 -2.301206e-15 -7.060379e-16 -6.869478e-15
-1.613846e-15
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-2.403735e-15 -3.235488e-15 4.054143e-16 -3.326907e-15 -6.151999e-15
-2.687002e-15
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-9.719235e-15
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-3.959670e-15
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-2.182299e-15
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-4.238298e-16
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-9.666674e-16 -5.830959e-15 -6.777777e-15 3.921638e-15 -8.158883e-15
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-2.687002e-15
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-1.052520e-15
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1.376524e-16
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-1.159799e-15
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-1.884462e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd474b9c714dc.final.pdb
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-2.241115e-15
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-7.338391e-17 -1.171111e-14  1.095550e-15  4.307867e-15 -7.958555e-15 -3.463630e-15
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-1.130403e-15 -4.024692e-15  6.341683e-16  2.492523e-15 -4.526395e-15 -4.043665e-15
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-1.186716e-15 -6.409564e-15 -4.166909e-15 -1.384873e-14 -8.052404e-15
Page 328
5.887876e-15  -1.828290e-15  2.642613e-15  5.542108e-15  -2.588073e-15  4.411117e-16
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cfd.b.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb
5.544622e-15  -3.760150e-15  1.517804e-16  6.014290e-16  -8.897897e-16  -2.294997e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\525656dd6ff2868d.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\546752341cf2dbc.final.pdb
6.461832e-15  -9.952283e-15  -3.203184e-15  1.239551e-14  -1.949486e-15  -9.941055e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\568353ff3c8f7ef.final.pdb
7.587966e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
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| File Path                                      | Values                                      |
|------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | -1.320762e-14 -1.329474e-14 -2.316514e-14 2.509009e-14 -8.468867e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 3.954110e-15 -1.328137e-15 5.458568e-15 3.858355e-15 1.661079e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 2.986196e-15 -5.028421e-15 -3.515517e-16 9.582813e-15 -6.816972e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 3.445436e-15 -3.165713e-15 -1.197131e-16 8.116393e-15 -3.619302e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | 5.887876e-15 -1.828290e-15 2.642613e-15 5.542108e-15 -2.588073e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 4.511117e-16 -3.019448e-15 3.116935e-15 4.722376e-15 -5.325093e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 3.971440e-15 -2.040293e-15 7.252013e-15 5.16338e-16 1.66401e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 8.118034e-15 -1.226360e-15 2.469145e-15 4.671775e-15 2.480471e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 5.544622e-15 -3.760150e-15 1.517804e-15 6.014290e-15 -8.97879e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b3492424e3cd1aeec.final.pdb | 3.627102e-15 -2.230923e-15 2.415740e-15 4.669337e-15 -3.218828e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b7551e5f9757f992.final.pdb | -2.908039e-15 -1.045877e-14 7.714836e-15 -1.346662e-16 1.146145e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -5.181718e-17 -6.590974e-15 -4.771595e-15 7.235198e-15 -7.167402e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf397575083e7.final.pdb | -1.367531e-15 -2.069222e-16 6.897403e-15 -5.368724e-16 3.354574e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf397575083e7.final.pdb | -6.959646e-16 -2.94997e-15 |

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3.954110e-15 -1.328137e-15  5.458568e-15  3.858355e -15  1.661079e-15
6.660103e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
8.266620e-15 -4.543506e-15 -8.295960e-15  1.031402e-14 -8.465109e-15
3.238771e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
9.254462e-15  3.786660e-15  8.548036e-15  3.115077e -15 -2.176502e-15
1.083103e-15
[.409]  [.410]  [.411]  [.412]  [.413]  [.414]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
2.938602e-15  4.186516e-15 -9.487381e-16  1.460247e -15 -1.823364e-15
-4.717062e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.829167e-15  5.134185e-15 -1.156597e-15  2.491220e -15 -1.119059e-15
-3.858728e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
2.399002e-15  7.698710e-15 -2.232831e-15  1.106732e-15 -1.502182e-15
-2.389986e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
2.376563e-15  5.902574e-15 -4.052324e-15  1.914708e-15 -1.790823e-15
-2.941987e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
6.285408e-16  4.660030e-16  4.358225e-15 -1.716597e-15 -7.290207e-15
-9.261984e-15
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2.584241e-15  5.061542e-15 -1.957375e-15  1.507545e-15 -1.790680e-15
-3.858728e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
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-9.30323e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
4.201204e-15  4.538376e-15 -3.187823e-15  2.845726e-15 -2.457268e-15
1.441477e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
4.888154e-15  3.617671e-15 -6.548253e-15  9.982454e-16 -2.367062e-15
-7.076666e-16
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-4.648027e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
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-8.370489e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
2.412714e-15  5.113111e-15 -4.228466e-15  1.635421e-15 -1.738355e-15
-3.533209e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
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-8.370489e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
8.620853e-15  3.845004e-15  1.401185e-15 -8.430858e-15  4.469471e-15
-1.932677e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
9.401913e-15 -5.758859e-15 -3.812689e-15  4.220481e-15  9.111195e-16
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| Index | Path                        | Value 1                          | Value 2                          | Value 3                          | Value 4                          | Value 5                          |
|-------|-----------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|----------------------------------|
| 1     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb | -1.230960e-14                   | 5.398761e-15                     | 1.238925e-15                     | -2.477229e-15                   | -4.279566e-15                   |
| 2     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -3.498328e-16                   | 6.105373e-15                     | 3.950939e-16                     | -1.846775e-15                   | -3.321790e-15                   |
| 3     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb3287197b7ab.final.pdb | 4.730285e-15                    | 5.934039e-15                     | 7.210572e-15                     | 1.228430e-15                    | 2.837263e-15                    |
| 4     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287197b7ab.final.pdb | -4.279566e-15                   | -3.498328e-16                    | 6.105373e-15                     | 3.950939e-16                     | -1.846775e-15                   |
| 5     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc3270d.final.pdb | -3.321790e-15                   | 4.730285e-15                     | 5.934039e-15                     | 7.210572e-15                     | 1.228430e-15                    |
| 6     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca3cd3df6edd.final.pdb | 1.633823e-15                    | 4.583587e-15                     | -1.866376e-17                    | -1.795862e-15                   | 2.747917e-16                    |
| 7     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 1.959392e-15                    | 8.015954e-15                     | -2.127799e-15                    | 2.398374e-15                     | 4.909570e-15                    |
| 8     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7f4fc.final.pdb | -3.884614e-14                   | 6.548253e-15                     | -2.637062e-15                    | 9.982454e-15                     | -7.076666e-15                   |
| 9     | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8941df.final.pdb | 1.008136e-14                    | -3.753794e-15                    | 1.930324e-15                     | -1.344573e-15                   | -7.832071e-16                   |
| 10    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 4.201204e-15                    | -3.187823e-15                    | 2.845726e-15                     | -2.457268e-15                   | -2.441477e-16                   |
| 11    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4826225951ea153.final.pdb | -9.769380e-16                   | 3.844570e-15                     | -1.706030e-15                    | -4.182520e-15                   | 3.203557e-15                    |
| 12    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -5.99827e-14                    | 5.182392e-15                     | -6.804862e-15                    | 1.147432e-15                     | 1.130169e-14                    |
| 13    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4aa45b62cb62a5f.final.pdb | 2.590521e-15                    | 4.708039e-15                     | -2.486070e-15                    | 1.704391e-15                     | -5.331833e-15                   |
| 14    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 4.888154e-15                    | 3.617671e-15                     | -6.548253e-15                    | 9.982454e-15                     | -7.076666e-15                   |
| 15    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59467f048223d0.final.pdb | -3.55688e-15                    | 1.236788e-14                     | -2.469315e-15                    | -4.894663e-17                    | -2.349889e-15                   |
| 16    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe38530d.final.pdb | 2.085716e-15                    | 7.16473e-15                      | -1.636316e-15                    | 4.436454e-15                     | -3.984704e-15                   |
| 17    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 2.590521e-15                    | 4.708039e-15                     | -2.486070e-15                    | 1.704391e-15                     | -5.331833e-15                   |
| 18    | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dc.final.pdb | 5.458013e-17                    | 6.775449e-15                     | -8.171479e-15                    | 1.735423e-16                     | -3.901839e-15                   |
| Path                                                                 | Values                                      |
|----------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb   | 4.201204e-15  4.538376e-15  -3.187823e-15  2.845726e-15  -2.457268e-15  1.441477e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb   | 3.355688e-15  1.236788e-14  -2.469315e-15  -4.894663e-17  -2.349889e-15  6.878444e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb   | 7.341078e-15  4.391273e-15  -4.401566e-15  7.193485e-15  4.310259e-15  -4.631025e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb   | 2.800415e-15  5.583371e-15  -2.142055e-15  1.636624e-15  -2.009709e-15  -3.568621e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff6c.final.pdb   | 7.630718e-15  1.243212e-14  1.322052e-15  -5.078487e-15  2.682605e-15  -1.512529e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb   | 8.443703e-15  -6.938365e-16  4.492327e-15  1.310416e-16  -7.923469e-16  -9.027337e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0aad0f1be4.final.pdb   | 3.355688e-15  1.236788e-14  -2.469315e-15  -4.894663e-17  -2.349889e-15  6.878444e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb   | 2.682791e-15  5.058189e-15  -2.040893e-15  1.524516e-15  -1.823698e-15  -4.212140e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c70ad0f1be4.final.pdb   | 2.085716e-15  7.716473e-15  -1.636316e-15  4.436454e-15  -3.984704e-15  -9.300323e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb   | 2.085716e-15  7.716473e-15  -1.636316e-15  4.436454e-15  -3.984704e-15  -9.300323e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\80d0666e1402203d.final.pdb   | 4.201204e-15  4.538376e-15  -3.187823e-15  2.845726e-15  -2.457268e-15  1.441477e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb   | 3.355688e-15  1.236788e-14  -2.469315e-15  -4.894663e-17  -2.349889e-15  6.878444e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb   | 1.633823e-15  4.583587e-15  -1.866376e-17  -1.795862e-16  2.747917e-16  -1.210426e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb   | 4.201204e-15  4.538376e-15  -3.187823e-15  2.845726e-15  -2.457268e-15  1.441477e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\886ee9ac3fe74395.final.pdb   | 5.825409e-15  2.408075e-15  -3.617188e-15  1.072071e-15  -3.067163e-15  1.658285e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bb0d5986c138f.final.pdb   | 2.800415e-15  5.583371e-15  -2.142055e-15  1.636624e-15  -2.009709e-15  -3.568621e-15 |
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9.300323e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
6.095099e-15  7.045593e-15 -1.331145e-15  5.293953e-15 -1.056159e-14
-1.856266e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
2.488327e-15  2.734525e-15 -7.340689e-15  6.911631e-15 -7.111271e-15
5.991567e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
2.206292e-15  5.610313e-15 -2.121310e-15  1.817509e-15 -1.630845e-15
-3.405977e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
2.590521e-15  4.708039e-15 -2.486070e-15  1.704391e-15 -5.31833e-15
-3.446832e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-1.345704e-16  8.493585e-16  7.810994e-16  1.216127e-16 -7.776419e-16
-1.193673e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
2.491801e-15  5.383226e-15 -1.959059e-15  1.167988e-15 -1.619018e-15
-3.764668e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
-3.498328e-16  6.105373e-15  6.003615e-16  3.950939e-16 -1.846775e-15
-3.321790e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
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-9.300323e-16
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-1.856266e-16
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7.432722e-15  4.984461e-15 -7.011851e-15  5.174406e-15 -4.929857e-15
-8.431814e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
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-9.300323e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
4.083405e-15  3.146955e-15  1.093103e-15  4.810114e-16 -1.819497e-15
-7.272151e-15
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2.085716e-15  7.716473e-15 -1.636316e-15  4.436454e-15 -3.984704e-15
-9.300323e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
3.396302e-15  5.555466e-15 -7.469572e-15  4.549757e-15  3.543878e-15
-1.751648e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
2.085716e-15  7.716473e-15 -1.636316e-15  4.436454e-15 -3.984704e-15
-9.300323e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
2.516361e-15  4.966069e-15 -1.777533e-15  1.063284e-15 -1.916046e-15
-3.296195e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
3.344261e-15  5.927998e-15 -6.644277e-15  7.890834e-15 -5.699162e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4aad93a0ad.final.pdb
8.854470e-16 -4.215826e-15 4.829849e-15 -1.296305e-16 1.663686e-15 -8.774241e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
2.066292e-15 5.610313e-15 -2.121310e-15 1.817509e-15 -1.638045e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-1.769380e-16 3.845470e-15 -1.706030e-15 -4.182520e-15 3.203557e-15 -7.599827e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
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E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-3.477605e-18 1.233621e-16 -2.157887e-15 2.948752e-15 -3.338856e-16
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-6.383400e-16 2.166692e-16 -5.068050e-16 2.872994e-15 1.555856e-15 -9.575476e-17
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-1.273044e-15 8.130249e-16 -1.137198e-15 1.750761e-15 2.804070e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
5.387904e-16 1.219659e-15 -6.274681e-16 8.404160e-15 7.224209e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
4.298759e-15 -1.053995e-16 -3.760402e-16 3.499380e-15 3.068512e-15 1.288880e-14
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
2.721393e-16 -1.276094e-15 3.353230e-16 1.751491e-15 4.396170e-15
4.590460e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
-2.735741e-15 -8.379982e-16 -1.222850e-15 9.159255e-16 -5.712687e-16
3.469788e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
-2.115235e-16 -1.197678e-15 1.754921e-16 1.120924e-15 3.874891e-15
-1.708879e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
-1.435819e-15 6.831136e-16 3.153987e-15 7.589218e-15 8.312720e-17
2.764799e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-9.259252e-15 -4.875075e-15 -5.568588e-17 7.104648e-15 9.256859e-15
1.672943e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
6.086754e-16 5.912558e-16 -1.009975e-15 3.206929e-15 4.789958e-15
7.693907e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb
-1.298601e-14 1.782268e-16 -1.257496e-14 1.240177e-14 4.806901e-15
6.530796e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
8.251041e-16 -5.730192e-16 -8.548718e-16 2.834963e-15 1.045550e-14
4.248462e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
-1.435819e-15 6.831136e-16 3.153987e-15 7.589218e-15 8.312720e-17
2.764799e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
-8.974964e-16 8.521679e-16 -1.561207e-15 3.244357e-15 3.10072e-15
6.609524e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
5.387904e-16 2.930544e-15 -2.196617e-15 -6.487478e-16 3.617676e-15
-3.831048e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
-6.419519e-15 -1.692739e-15 -3.076255e-15 1.473251e-14 7.962213e-15
-1.199771e-14

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1.018651e-15 -6.153728e-17 -2.229499e-15 -1.965547e-15 2.367575e-15
-8.812578e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb
1.018651e-15 -6.153728e-17 -2.229499e-15 -1.965547e-15 2.367575e-15
-8.812578e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
4.510975e-15 2.482001e-15 -1.856751e-15 -2.941328e-15 3.840789e-15
-2.747335e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
-2.115235e-16 -1.197678e-15 1.754921e-16 1.120924e-15 3.874891e-15
-1.708879e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
-1.435819e-15 6.831136e-16 3.153987e-15 7.589218e-15 8.312720e-17
2.764799e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716ddac62.final.pdb
-2.671105e-15 2.342331e-16 2.624257e-15 4.210069e-15 2.554058e-15
7.603110e-15
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| Path                                                                 | Description                        | Score   |
|----------------------------------------------------------------------|------------------------------------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | 1.627323e-15 7.172054e-16 7.592662e-16 -4.021944e-15 -2.224416e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 2.803895e-15                     |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | 1.102997e-16 4.638577e-17 -3.478865e-16 -5.680693e-15 -1.337885e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 2.296485e-15 9.783660e-16 -1.535974e-16 -3.315398e-15 -1.845508e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 5.871609e-15 2.790244e-15 -1.031077e-14 -4.385645e-15 -2.500664e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 3.674297e-15 -1.198580e-15 5.125565e-15 -8.920803e-15 1.781060e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 3.281322e-15 -1.130422e-14 -2.692987e-15 1.612803e-15 -4.203402e-16 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 1.161853e-15 -9.833106e-16 -2.462311e-15 2.169879e-15 2.229087e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 3.762979e-15 -1.198580e-15 5.125565e-15 -8.920803e-15 1.781060e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 2.537798e-15 2.312667e-15 -1.130422e-14 -2.692987e-15 1.612803e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 4.646441e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cddf.final.pdb | 1.084087e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 4.015040e-15 -9.163069e-16 3.954431e-15 -4.628069e-15 -1.163165e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | 1.795629e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 1.984546e-15 -3.171768e-16 5.968445e-15 -9.764585e-15 4.492399e-16 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | -3.59993e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 1.161853e-15 -9.833106e-16 -2.462311e-15 2.169879e-15 2.229087e-15 |         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 6.446414e-15 |         |
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-6.161350e-15  3.102839e-16  -2.407627e-15  -6.595609e-15  -3.427223e-15
  6.670122e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
2.782649e-15  -2.439991e-15  -2.057925e-15  -7.537248e-16  4.168040e-15
8.958694e-15  

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-5.740453e-15  4.651617e-15  -3.127246e-15  -5.858711e-15  -4.611308e-15
1.220220e-14  

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2.721150e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
3.221100e-15  2.167217e-15  -4.287912e-15  5.375921e-15  -6.797749e-15
2.092658e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
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-2.004669e-16  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
8.155054e-16  1.957094e-15  -1.113211e-15  -3.155734e-15  -1.348273e-15
5.128855e-15  

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1.779018e-16  -1.854629e-15  3.346642e-15  -2.335709e-15  -3.557556e-15
2.462681e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
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1.464388e-14  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
1.921422e-15  7.929929e-16  6.351098e-17  -2.730062e-15  -2.358026e-15
2.963118e-15  

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2.721150e-15  

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3.806371e-15  2.942944e-15  3.591914e-15  -2.734961e-16  -2.734961e-16
9.857677e-16  

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2.721150e-15  

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3.221100e-15  2.167217e-15  -4.287912e-15  5.375921e-15  -6.797749e-15
2.092658e-15  

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2.628494e-15  -1.754208e-14  5.427252e-15  -1.363250e-15  -3.949267e-16
-2.004669e-16  

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5.038215e-15  1.183497e-15  -8.767795e-17  -4.005818e-15  -2.436181e-15
2.721150e-15  

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7.218138e-15  1.082076e-14  -2.585436e-15  -3.479612e-15  -6.951965e-15
-2.462330e-15  

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2.721150e-15  

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2.782649e-15  -2.439991e-15  -2.057925e-15  -7.537248e-16  4.168040e-15
8.958694e-15  

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
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| File Path                                             | Values                                                                 |
|-------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbb3975403e7.final.pdb | 5.038215e-15 1.183497e-15 -8.67795e-17 -4.00581e-15 -2.436181e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb   | 1.468588e-15 1.088629e-15 1.347806e-15 -3.661475e-15 -1.745978e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e6af4ef427e.final.pdb  | -1.367366e-15 1.238447e-15 -3.607779e-15 -2.779261e-15 -5.864117e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | -2.628112e-15 1.051306e-14 -2.876246e-15 -5.283008e-15 1.088126e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb  | 1.315263e-14 5.343367e-15 2.889351e-15 -8.996248e-17 -1.773381e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb   | -2.474864e-15 6.028061e-15 -6.880456e-15 4.734073e-15 -1.842737e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 5.561943e-16 -2.862220e-16 -8.047181e-16 -5.023366e-15 -2.436181e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.659572e-16 1.121053e-15 7.682062e-15 -2.856671e-15 3.198075e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 1.506605e-14 1.857822e-15 6.282188e-15 -4.766336e-15 1.809857e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d2f02212450d015047.final.pdb | 5.561943e-16 -2.862220e-16 -8.047181e-16 -5.023366e-15 -2.436181e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d2f02212450d015047.final.pdb | 5.561943e-16 -2.862220e-16 -8.047181e-16 -5.023366e-15 -2.436181e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d2f02212450d015047.final.pdb | 5.561943e-16 -2.862220e-16 -8.047181e-16 -5.023366e-15 -2.436181e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d2f02212450d015047.final.pdb | 5.561943e-16 -2.862220e-16 -8.047181e-16 -5.023366e-15 -2.436181e-15 |
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5.740653e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
-5.313014e-15  5.847265e-17  2.844564e-15 -1.228128e-15  6.867873e-15
5.407265e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
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3.527032e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
1.697222e-15 -4.364413e-15 -3.014531e-15 -2.77007e-15  4.180453e-15
2.553193e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
4.180453e-15  2.553193e-15 -1.75789e-15  5.034076e-15  3.040409e-15
5.740653e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
-2.952854e-15 -1.75789e-15  5.034076e-15  3.040409e-15  9.76758e-15
6.757004e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
1.162275e-15 -2.591317e-15  1.639365e-15 -7.549819e-16  2.950055e-16
-2.935849e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
-1.886849e-15 -5.785150e-15 -2.093870e-15 -2.569511e-16  2.531831e-15
3.527032e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-5.564208e-15 -6.727447e-16  9.632322e-15 -2.468643e-15  4.364700e-15
-4.004146e-15
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-4.004146e-15
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-5.334976e-16  1.341522e-16  4.891141e-15 -7.352490e-16  2.950055e-16
-2.935849e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-4.188570e-16 -3.439837e-15 -6.003102e-15 -3.848611e-15 -2.156813e-15
2.079756e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
-1.886849e-15 -5.785150e-15 -2.093870e-15 -2.569511e-16  2.531831e-15
3.527032e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
7.611738e-16 -3.124645e-15 -7.059562e-16 -3.957263e-16  2.899019e-15
2.348922e-15
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2.553193e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
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4.895663e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a3633196.final.pdb
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-1.083136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
3.758227e-15 -6.329343e-15 -3.316034e-15 -7.905129e-16  9.257631e-16
-1.083136e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
5.884531e-16 -7.845058e-15 -6.89070e-15 -5.431332e-15  2.273643e-15
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1.914466e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
1.162275e-15 -2.959317e-15 1.639365e-15 -7.549819e-16 2.950055e-16
-2.935849e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
-1.886849e-15 -5.785150e-15 -2.093870e-15 -2.569511e-16 2.531831e-15
3.527032e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
1.287980e-15 -1.250506e-15 1.766705e-15 1.568711e-15 1.002959e-14
1.862425e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
4.760691e-15 1.025468e-15 3.116478e-15 -9.294004e-15 1.053089e-14
3.891426e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
1.697222e-15 -4.364413e-15 -3.014531e-15 -2.770007e-15 4.180453e-15
2.553193e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
-3.877159e-15 3.487891e-15 7.431662e-15 4.053269e-15 3.740352e-15
1.626502e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9da8ed0d81fb3ef.final.pdb
3.869831e-15 1.007933e-14 -9.450495e-16 4.420731e-15 1.621985e-16
8.408978e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
2.959637e-15 -4.177094e-15 2.426520e-16 -2.700239e-15 5.916383e-15
-4.214195e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
-4.773432e-15 7.572912e-16 4.185325e-15 1.251943e-15 1.481854e-15
5.740653e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-5.044026e-15 -2.801342e-15 -3.857039e-15 -7.683199e-15 4.525669e-15
-9.003944e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
1.116844e-15 -2.862491e-15 1.113581e-16 -4.537394e-16 4.063365e-15
2.612854e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
3.758227e-15 -6.329343e-15 -3.5316034e-15 -7.905129e-16 9.275631e-16
-1.083136e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad88a223e4b4c668e.final.pdb
1.114547e-16 -3.464335e-15 -5.945278e-16 -1.381087e-15 3.837065e-16
2.579816e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
-3.877159e-15 3.487891e-15 7.431662e-15 4.053269e-15 3.740352e-15
1.626502e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
4.980488e-15 -3.366946e-15 3.538994e-15 -6.667188e-15 1.184990e-14
1.134848e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e4f6fa27a165.final.pdb
1.697222e-15 -4.364413e-15 -3.014531e-15 -2.770007e-15 4.180453e-15
2.553193e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd9a5b.final.pdb
1.875766e-15 -6.021506e-15 4.507524e-16 1.811707e-15 7.355246e-16
-5.379472e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
1.697222e-15 -4.364413e-15 -3.014531e-15 -2.770007e-15 4.180453e-15
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| Filename                        | Distance          | Binding Energy   | qG   | qH   | qS   |
|--------------------------------|-------------------|------------------|------|------|------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | 3.718304e-15      | 2.773279e-15     | 1.648653e-15 | -8.140266e-16 | -3.584627e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb  | 5.094069e-15      | -3.709593e-15    | -1.837496e-15 | -6.558085e-15 | -8.622820e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb  | 1.713413e-15      | -3.889830e-15    | 3.746408e-16  | -3.652698e-16 | -2.441602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb  | 7.284896e-15      | -8.185511e-15    | -2.153342e-15 | 9.472142e-17   | -9.504828e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb  | 2.674613e-15      | -3.082996e-15    | 2.841081e-15  | 2.329906e-15   | -1.700828e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb  | 3.718304e-15      | -3.889830e-15    | 3.746408e-16  | -3.652698e-16 | -2.441602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb  | 2.153413e-15      | -3.889830e-15    | 3.746408e-16  | -3.652698e-16 | -2.441602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb  | 6.352989e-15      | 2.517865e-15     | -8.133873e-16 | -4.453716e-15 | -8.699702e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb  | 2.628031e-15      | -2.597967e-15    | 1.930546e-15  | 9.136495e-16   | -3.532175e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc4.final.pdb | 9.095197e-15      | -1.629938e-15    | -1.247496e-14 | -7.877076e-15 | -1.444058e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7bb7b8f7ebfc4.final.pdb   | 8.018943e-15      | -1.412190e-15    | -9.623936e-16 | 5.936782e-16   | -8.773201e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb  | 2.674613e-15      | -3.082996e-15    | 2.841081e-15  | 2.329906e-15   | -1.246850e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb  | 1.623942e-15      | -2.180698e-15    | 1.599561e-15  | -2.046200e-16 | -1.832323e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb  | 1.021265e-15      | -2.934483e-15    | 4.984304e-15  | 3.527760e-16   | 3.171570e-17  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb  | 1.713413e-15      | -3.889830e-15    | 3.746408e-16  | -3.652698e-16 | -2.441602e-15 |
| File Path                                      | Values                                    |
|------------------------------------------------|-------------------------------------------|
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\804b89c94a633196.final.pdb | -4.077942e-16 1.297601e-15 2.986417e-15 2.817633e-15 -3.347321e-15 -1.544255e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\813cc65a2298feba.final.pdb | -4.077942e-16 1.297601e-15 2.986417e-15 2.817633e-15 -3.347321e-15 -1.544255e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\83c0eefcfe12d3f9.final.pdb | 4.094681e-15 -1.834767e-15 8.310231e-16 3.480406e-15 -4.384686e-15 -5.445456e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\86d50469ef569760.final.pdb | 3.718304e-15 2.773279e-15 1.648653e-15 -8.140266e-16 -3.584627e-15 -4.336003e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\89d0666e1402203d.final.pdb | 2.674613e-15 -3.082996e-15 2.841081e-15 2.329906e-15 -1.246850e-17 1.700828e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b34852716dadc62.final.pdb | 3.102897e-15 -6.970479e-16 6.434583e-16 -1.121673e-15 3.202696e-16 -3.615260e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b6ef9ac3fe74395.final.pdb | 2.153413e-15 -3.889380e-15 3.746408e-16 -3.652698e-16 -2.441602e-15 -6.190609e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\98bbe0d5986c138f.final.pdb | -2.147485e-15 -7.072128e-15 -3.264279e-15 -1.275622e-14 -1.133674e-14 -1.645763e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\9dda8ed0d81fb3ef.final.pdb | 3.102897e-15 -6.970479e-16 6.434583e-16 -1.121673e-15 3.202696e-16 -3.615260e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\9d8a6ed0d81fb3ef.final.pdb | 4.243867e-15 -3.032865e-15 7.395164e-16 -4.796014e-15 2.956664e-16 -1.008462e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | 2.036237e-15 -2.514524e-15 1.184456e-15 -2.031554e-17 -1.266290e-15 -4.427382e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | -4.077942e-16 1.297601e-15 2.986417e-15 2.817633e-15 -3.347321e-15 -1.544255e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | 2.297110e-15 -2.362789e-15 2.091906e-15 -2.418653e-16 -5.659313e-16 -4.327897e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | 4.243867e-15 -3.032865e-15 7.395164e-16 -4.796014e-15 2.956664e-16 -1.008462e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | 2.036237e-15 -2.514524e-15 1.184456e-15 -2.031554e-17 -1.266290e-15 -4.427382e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a02c70083816d6ba.final.pdb | 4.243867e-15 -3.032865e-15 7.395164e-16 -4.796014e-15 2.956664e-16 -1.008462e-14 |
Supplementary Text 10

5.820100e-15  -6.367979e-15  2.628478e-16  3.341196e-15  1.804654e-15
-1.400532e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb

-1.021265e-15  -2.934483e-15  4.984304e-15  3.527760e-15  3.171570e-17
-3.170825e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb

2.168074e-15  -1.384652e-16  3.961278e-15  6.952185e-15  1.044845e-15
-1.383808e-15

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-1.021265e-15  -2.934483e-15  4.984304e-15  3.527760e-15  3.171570e-17
-3.170825e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb

8.027299e-15  -3.134617e-15  1.029649e-15  -4.645147e-15  2.359168e-16
-5.801267e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb

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-3.170825e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb

2.346267e-15  -2.728200e-15  9.415314e-16  8.433297e-16  -1.450503e-15
-4.185937e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb

8.027299e-15  -3.134617e-15  1.029649e-15  -4.645147e-15  2.591686e-16
-5.801267e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb

-1.021265e-15  -2.934483e-15  4.984304e-15  3.527760e-15  3.171570e-17
-3.170825e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb

8.027299e-15  -3.134617e-15  1.029649e-15  -4.645147e-15  2.359168e-16
-5.801267e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb

6.397280e-15  -2.446314e-16  3.605633e-15  6.681379e-15  6.451600e-15
5.708655e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249a61.final.pdb

6.397280e-15  -2.446314e-16  3.605633e-15  6.681379e-15  6.451600e-15
5.708655e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb

6.805505e-16  -1.426147e-15  2.171800e-15  -6.915451e-16  -2.171815e-15
-5.239585e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d7140af0f0efe39.final.pdb

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-1.256053e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d7b40af0f0efe39.final.pdb

5.878933e-15  6.144080e-16  1.193371e-17  2.420523e-16  3.319455e-15
-1.256053e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb

-1.80135e-15  -3.349600e-15  6.329744e-15  6.145745e-15  5.939580e-15
3.688146e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb

6.02699e-15  5.172391e-15  3.261652e-16  6.522841e-15  -4.394308e-15
-7.410238e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb

3.231163e-15  -5.665828e-15  4.949755e-16  -4.067036e-15  -1.452419e-15
-1.114712e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb

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| Path                                                                 | Values                                      |
|----------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -2.496650e-15 5.414671e-16 2.368087e-18 -3.096841e-16 5.043833e-15 8.898299e-16 -1.171052e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb | 4.006402e-16 -5.942305e-15 2.840036e-15 5.472564e-15 1.874676e-15 -4.065572e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f33068258e.final.pdb | 4.490623e-15 -2.988646e-15 -1.227476e-15 -1.113248e-15 4.919164e-15 -1.795822e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | -5.518572e-15 7.560641e-15 -3.047635e-15 -1.117314e-15 -2.871696e-15 -1.690302e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | 1.121231e-16 -1.047511e-16 -1.006356e-15 4.697159e-15 1.978693e-15 -1.622676e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -7.729016e-15 3.995096e-15 -5.070242e-15 9.661993e-15 -1.038674e-16 -9.397402e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -2.329606e-17 5.237044e-16 -1.999192e-16 4.470507e-16 1.472986e-15 -1.400766e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -7.729016e-15 3.995096e-15 -5.070242e-15 9.661993e-15 -1.038674e-16 -9.397402e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | -2.584819e-15 2.023545e-15 -5.070242e-15 9.661993e-15 -1.038674e-16 1.389228e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -3.587923e-15 6.656991e-15 2.977946e-15 -6.158161e-15 4.216553e-15 5.104881e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb | 3.316849e-16 -4.063689e-16 -2.512416e-16 4.772007e-15 1.424516e-15 -1.870605e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 2.891039e-15 -4.826183e-15 -1.71437e-15 9.055381e-15 5.749947e-15 -1.759853e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 9.612712e-15 -2.300126e-14 3.426654e-15 1.219121e-14 -3.736914e-15 4.183232e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287179b7ab.final.pdb | -7.68760e-15 -1.020256e-14 3.928348e-15 2.125317e-14 -1.112506e-15 -1.127313e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 5.158572e-15 7.560641e-15 -3.047635e-15 -1.117314e-15 -2.871696e-15 -1.690302e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 4.075422e-15 -6.545727e-15 -2.983789e-15 1.071264e-14 2.745189e-15 7.858481e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | -6.985510e-15 -2.087749e-14 5.946627e-15 1.774486e-14 -3.159227e-17 7.585433e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | -2.171067e-15 9.305690e-16 -9.774844e-15 5.130388e-15 4.378544e-15 |
| File Path                                                                 | Numbers                                                                 |
|--------------------------------------------------------------------------|-------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb     | -1.400828e-14                                                          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb     | 4.499023e-15 -2.988646e-15 -1.227476e-15 -1.113248e-15 4.919164e-15 -1.795822e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb     | 5.280851e-15 -1.740371e-15 -1.122684e-14 9.335630e-15 1.212446e-15 -3.356396e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb      | -3.811604e-15 8.469636e-15 3.603295e-14 2.413332e-14 -9.244687e-16 -1.038300e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb      | 1.398257e-16 1.126204e-14 -2.747735e-15 -9.158867e-16 1.390386e-15 -2.531698e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d8ac96.final.pdb       | -5.518572e-15 7.560641e-15 -3.047635e-15 -1.117314e-15 -2.871696e-15 -1.690302e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5e60752431cf2db.final.pdb       | 8.407347e-17 2.570750e-15 -1.475927e-15 5.603100e-15 2.104105e-15 8.348779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091fe385e05fc.final.pdb       | 4.006400e-16 -5.942305e-15 2.840036e-15 5.472564e-15 1.874762e-15 -4.065572e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb      | 1.398257e-16 1.126204e-14 -2.747735e-15 -9.158867e-16 1.390386e-15 -2.531698e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2db.final.pdb       | -3.463576e-15 4.088076e-15 -5.026577e-15 4.496887e-16 2.581076e-15 -5.597497e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb       | 4.499023e-15 -2.988646e-15 -1.227476e-15 -1.113248e-15 4.919164e-15 -1.795822e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6683d53ff3c8f7ef.final.pdb      | 8.407347e-17 2.570750e-15 -1.475927e-15 5.603100e-15 2.104105e-15 8.348779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea98affcc4.final.pdb      | 8.287874e-15 1.898565e-15 -5.861339e-15 1.388443e-15 -3.309325e-15 8.375052e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d41c2.final.pdb      | 3.306616e-15 4.271523e-15 4.125824e-15 1.031045e-14 -3.433644e-15 -9.272962e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb       | 8.407347e-17 2.570750e-15 -1.475927e-15 5.603100e-15 2.104105e-15 8.348779e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\76fa910fffb22872.final.pdb       | 1.332312e-15 4.705721e-16 -3.197015e-16 4.950376e-15 1.387987e-15 |

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| File Path                                                                 | Lines                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                               | -3.046569e-16 5.712765e-15 -1.285741e-15 -3.018118e-15 2.506568e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb     | -8.010021e-15 1.048691e-14 1.731394e-15 -7.118517e-15 3.251762e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb     | -1.266627e-15 5.764920e-15 -8.045184e-16 -6.737978e-16 2.057571e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb     | -1.619344e-15 4.791082e-15 -1.31831e-15 -2.730852e-16 1.356033e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb      | -3.405450e-15 6.329177e-15 2.514573e-16 2.118843e-15 4.539348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0f305f306825e8.final.pdb        | -3.405450e-15 6.329177e-15 2.514573e-16 2.118843e-15 4.539348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12626a78b57339c.final.pdb       | 8.304895e-18 -2.996028e-16 -6.003998e-16 3.923215e-15 6.181820e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | -6.423438e-16 5.182921e-16 -6.975461e-17 -1.004913e-15 1.778497e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb       | -3.405450e-15 6.329177e-15 2.514573e-16 2.118843e-15 4.539348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb      | -3.405450e-15 6.329177e-15 2.514573e-16 2.118843e-15 4.539348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d4759a.final.pdb       | 2.015769e-14 1.417767e-14 7.737354e-15 -7.364418e-15 4.285062e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e5436d.final.pdb       | 2.087327e-15 7.170255e-15 4.829795e-15 1.522570e-15 8.301655e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb       | -1.608270e-15 8.362964e-15 1.001888e-15 -4.051820e-15 -1.444661e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb32825184206.final.pdb       | -5.873728e-14 1.456573e-14 7.222219e-15 -5.512570e-15 -3.243299e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb      | -1.077015e-14 5.597901e-15 1.403926e-15 2.429128e-15 7.008293e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb      | 8.304895e-18 -2.996028e-16 -6.003998e-16 3.923215e-15 6.181820e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3d6edd.final.pdb       | -3.745883e-15 6.015883e-15 4.469925e-15 2.778328e-16 -3.365216e-15 |
Supplementary Text 10
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
4.413464e-15  9.652911e-15 -1.044181e-14 -1.549025e-15  2.645849e-15
5.020481e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f100ffbf22872.final.pdb
-9.306504e-16  4.185059e-15 -5.359987e-16 -7.391142e-16  2.905022e-15
4.030961e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\770f8c800dd5c3135.final.pdb
-1.619344e-15  4.791082e-15 -1.311831e-15 -2.730852e-15  1.356033e-16
1.695450e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\781f8c86a3f6099.final.pdb
-6.715934e-15  8.467394e-15  1.531655e-14 -3.556166e-15  3.269935e-15
6.026943e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\792f8c800dd5c3135.final.pdb
-1.608270e-15  8.362964e-15  1.001888e-15 -4.051820e-15 -1.444661e-15
6.945420e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7a3cc65a2298feba.final.pdb
-1.608270e-15  8.362964e-15  1.001888e-15 -4.051820e-15 -1.444661e-15
6.945420e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7b30eefcfe12d3f9.final.pdb
-3.745883e-15  6.015883e-15  4.469925e-15  2.778328e-16 -3.365216e-15
1.695450e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7c650469ef569760.final.pdb
1.342741e-15  4.810893e-15 -2.778878e-15 -9.402990e-16  1.817038e-15
1.277809e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7d90666e1402203d.final.pdb
4.413464e-15  9.652911e-15 -1.044181e-14 -1.549025e-15  2.645849e-15
5.020481e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7e83452716dadc62.final.pdb
5.495423e-15  3.381332e-16  2.697312e-17 -1.478192e-15  2.055349e-15
7.973871e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f8d98e66a3f6099.final.pdb
1.259780e-15  5.599666e-15 -1.738585e-15 -2.717823e-16  5.353046e-15
5.100612e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\80650469ef569760.final.pdb
-1.619344e-15  4.791082e-15 -1.311831e-15 -2.730852e-15  1.356033e-16
1.695450e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8183c0eefcfe12d3f9.final.pdb
3.925916e-16  6.106644e-16  8.689630e-16  8.299190e-16 -6.073076e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\82a97e70ad0f1be4.final.pdb
5.642607e-18  7.509072e-15 4.570361e-16 1.800952e-16 6.508804e-16
5.117719e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\839c70083816d6ba.final.pdb
2.304029e-15  2.652406e-15 -3.349921e-15 -2.727394e-15 5.758296e-15
4.287175e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\84a0c997d891e4082.final.pdb
2.041915e-15  7.034029e-15 3.321550e-15 1.638889e-15 -4.897857e-17
3.689832e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\85ab839ea2d23c616.final.pdb
-1.342964e-15  5.522217e-15 6.791319e-17 -1.478192e-15 2.055349e-15
3.693736e-15
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-8.815142e-16  2.348266e-15  3.357352e-15 -3.882974e-15 -4.068253e-15
-8.131627e-16

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
1.439680e-15  3.349631e-15  4.708953e-15 -3.674572e-15 -4.624067e-15
5.519804e-16

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
1.030574e-15  3.683724e-15  4.509764e-15 -3.003130e-15 -3.944233e-15
6.167109e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\03d855ad26c877c.final.pdb
4.771051e-15  7.083161e-15  1.674003e-15 -5.030047e-15  2.836272e-15
8.989695e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\02a705342ca0ds4.final.pdb
2.993922e-18  3.507957e-15  3.940731e-15 -3.911600e-15 -3.532313e-15
9.919553e-16

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-2.717750e-15  8.728507e-16  1.798903e-15 -6.603441e-15 -8.146262e-15
2.115878e-15

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1.627585e-16  2.795753e-16  5.862818e-16  5.133481e-16 -3.562472e-16
-7.624619e-16

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-4.471668e-16  3.216957e-15  3.943333e-15 -3.638056e-15 -3.444999e-15
8.505753e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
3.631453e-15  2.903880e-15  7.495157e-15 -2.987903e-15 -2.035924e-15
3.044108e-15

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1.300596e-16  2.570049e-15  3.659743e-15 -3.911952e-15 -3.369440e-15
7.934928e-16

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3.631453e-15  2.903880e-15  7.495157e-15 -2.987903e-15 -2.035924e-15
3.044108e-15

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-6.134273e-15

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-7.278806e-16 -2.583568e-15  8.445069e-15  5.754707e-15 -8.168675e-15
-3.801937e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
-3.831043e-16  2.421109e-15  4.177107e-15 -3.655409e-15 -3.834143e-15
1.123810e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354a32871797ab.final.pdb
-4.171470e-15  1.188190e-14  5.778525e-15 -1.333111e-14  2.117018e-15
5.203532e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb
| File Path                          | Lines 1-3  | Lines 4-6  | Lines 7-9  | Lines 10-12 | Lines 13-15 |
|-----------------------------------|------------|------------|------------|-------------|-------------|
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\716d9624611d1c42.final.pdb | 8.472731e-15 | 4.249716e-15 | 4.984101e-15 | -3.287286e-15 | -8.237400e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\75f27e70ad0f1be4.final.pdb | -9.216137e-16 | 1.293531e-14 | 3.559525e-15 | -8.515482e-16 | -7.316017e-16 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\769f910fffb22872.final.pdb | 8.437745e-17 | 2.598569e-15 | 4.056176e-15 | -3.832605e-15 | -2.972133e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\791f8c80dd5c3135.final.pdb | -1.736948e-15 | 4.262518e-15 | 3.776169e-15 | -5.628440e-15 | 3.299587e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\804b89c94a633196.final.pdb | -7.303632e-16 | 3.123426e-15 | 2.405104e-15 | -8.600910e-15 | 8.325240e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\813cc65a2298f8eaba.final.pdb | -7.303632e-16 | 3.123426e-15 | 2.405104e-15 | -8.600910e-15 | 8.325240e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\83c0eefcfe12d3f9.final.pdb | -1.053889e-15 | 5.029887e-15 | 2.060436e-15 | -4.758281e-15 | -1.328321e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\86d50469ef569760.final.pdb | -2.717750e-15 | 3.123426e-15 | 2.405104e-15 | -8.600910e-15 | 8.325240e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\89d0666e1402203d.final.pdb | -2.594651e-15 | -1.707542e-15 | 7.631436e-16 | -2.659610e-15 | -4.822939e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b34852716dadc62.final.pdb | -4.074910e-15 | -1.627982e-15 | 7.363377e-15 | -9.542489e-16 | -1.058242e-14 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8b6ef9ac3fe74395.final.pdb | -2.060436e-15 | -4.758281e-15 | -1.328321e-15 | -1.736948e-15 | 4.262518e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\8f752b361ee6033b.final.pdb | -5.051526e-15 | -5.777861e-15 | -3.638938e-15 | 1.994914e-15 | 3.09587e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\92b0e0d9986c138f.final.pdb | -1.736948e-15 | 4.262518e-15 | 3.776169e-15 | -5.628440e-15 | -3.761068e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\93c0eefcfe12d3f9.final.pdb | -2.312439e-15 | 3.306251e-15 | 5.951470e-15 | -6.165142e-15 | 1.307997e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\942c7008381ed6ba.final.pdb | 2.296989e-15 | -2.830290e-15 | 2.270589e-15 | 1.990075e-15 | -3.772693e-15 |
| E:\\R-3.1.2\\scripts\\mPDBS\\summary_pdb_93\\a0c997d891e4e082.final.pdb | 3.09587e-15 | 8.441780e-16 | -2.204876e-15 | -4.608358e-15 | 3.660557e-15 |
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-3.225297e-15 3.745105e-16 9.610230e-15 -4.166575e-17 -2.851001e-17
-2.409360e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb

9.615621e-17 3.080679e-15 3.171153e-15 -3.525966e-15 -3.372732e-15
4.412240e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb

-7.303632e-16 3.123426e-15 2.405104e-15 -8.600910e-15 -1.603491e-15
8.325240e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb

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1.014939e-15

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-2.211374e-15

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2.092801e-15

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-4.314678e-16 6.027353e-15 8.441780e-16 -2.204876e-15 -4.608358e-15
3.660557e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb

-7.341180e-15 4.046536e-15 4.413978e-15 -6.020529e-15 4.958314e-16
3.037466e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb

-1.736948e-15 4.262518e-15 3.776169e-15 -5.628440e-15 -3.761068e-15
3.299587e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb

-5.644954e-15 2.232891e-15 6.216383e-15 -6.804691e-15 -1.392412e-15
-5.653754e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb

-2.550600e-16 2.455803e-15 4.012308e-15 -3.500693e-15 -4.186394e-15
1.276032e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb

-1.553389e-15 6.401907e-15 -1.992915e-15 -9.275414e-15
7.564118e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb

-4.074910e-15 -1.627982e-15 7.363377e-15 -9.542489e-16 -1.058242e-14
2.092801e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb

-3.912444e-16 3.318770e-16 3.400533e-15 2.192639e-15 -2.949004e-15
2.818621e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb

-5.644954e-15 2.232891e-15 6.216383e-15 -6.804691e-15 -1.392412e-15
-5.653754e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb

1.236412e-15 2.788378e-15 1.011206e-15 -3.714943e-15 -5.208394e-15
2.508581e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
| Path                                                                 | Coordinates   |
|----------------------------------------------------------------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.840701e-15  |
|                                                                      | 1.681203e-14  |
|                                                                      | 4.634548e-15  |
|                                                                      | -5.816678e-15 |
|                                                                      | -5.184835e-15 |
|                                                                      | -3.354889e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | -2.564505e-15 |
|                                                                      | 1.371107e-14  |
|                                                                      | 9.976702e-16  |
|                                                                      | -1.118892e-14 |
|                                                                      | -7.662438e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -8.584631e-15 |
|                                                                      | -2.457088e-15 |
|                                                                      | -3.615074e-15 |
|                                                                      | -1.666271e-15 |
|                                                                      | -5.198944e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | -3.103251e-15 |
|                                                                      | 1.510800e-14  |
|                                                                      | 7.464164e-15  |
|                                                                      | -1.371750e-14 |
|                                                                      | 5.379078e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb | -3.103251e-15 |
|                                                                      | 1.510800e-14  |
|                                                                      | 7.464164e-15  |
|                                                                      | -1.371750e-14 |
|                                                                      | 5.379078e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | -7.303632e-16 |
|                                                                      | 3.123426e-15  |
|                                                                      | 2.405104e-15  |
|                                                                      | -8.600910e-15 |
|                                                                      | -1.603491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e589d9960a960.final.pdb    | 3.629781e-15  |
|                                                                      | -6.299814e-15 |
|                                                                      | 5.707125e-15  |
|                                                                      | -9.696799e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb  | 2.296989e-15  |
|                                                                      | -2.803290e-15 |
|                                                                      | 2.270589e-15  |
|                                                                      | 1.990075e-15  |
|                                                                      | -3.772693e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb  | -7.303632e-16 |
|                                                                      | 3.123426e-15  |
|                                                                      | 2.405104e-15  |
|                                                                      | -8.600910e-15 |
|                                                                      | -1.603491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ebadbe32db650e.final.pdb    | -1.736948e-15 |
|                                                                      | 4.262518e-15  |
|                                                                      | 3.776169e-15  |
|                                                                      | -5.628440e-15 |
|                                                                      | -3.761068e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ed589d9960a960.final.pdb    | 3.629781e-15  |
|                                                                      | -6.299814e-15 |
|                                                                      | 5.707125e-15  |
|                                                                      | -9.696799e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbbcad52078.final.pdb | 2.816045e-15  |
|                                                                      | 3.764866e-15  |
|                                                                      | -4.252954e-15 |
|                                                                      | -3.719221e-15 |
|                                                                      | 1.075493e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb  | -1.730944e-16 |
|                                                                      | 2.611928e-15  |
|                                                                      | 4.094274e-15  |
|                                                                      | -3.446158e-15 |
|                                                                      | -4.081992e-15 |
|                                                                      | 8.445198e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fca8e42003f09e.final.pdb | -3.998054e-17 |
|                                                                      | 3.197048e-15  |
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|                                                                      | -3.975612e-15 |
|                                                                      | -3.606933e-15 |
|                                                                      | 1.211373e-15  |
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|                                                                      | 1.011206e-15  |
|                                                                      | -3.714943e-15 |
|                                                                      | -5.208394e-15 |
|                                                                      | 2.508581e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb  | -2.312439e-15 |
|                                                                      | 3.306251e-15  |
|                                                                      | 5.951470e-15  |
|                                                                      | -6.165142e-15 |
|                                                                      | -4.013451e-15 |
|                                                                      | 1.307997e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb  | 4.771051e-15  |
|                                                                      | 7.083161e-15  |
|                                                                      | 1.674003e-15  |
|                                                                      | -5.030047e-15 |
|                                                                      | 2.836272e-15  |
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E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
8.204892e-16 1.661357e-15 8.178827e-16 -3.119249e-15 2.375306e-15
4.352905e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
1.522864e-15 1.308703e-15 -2.442542e-15 -4.787092e-15 -9.842770e-16
3.587162e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
6.324499e-16 2.383103e-15 8.954546e-16 -4.041555e-15 -1.172003e-15
4.738142e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
1.778841e-15 9.770576e-16 -2.756143e-15 -3.881096e-15 1.160053e-15
4.612059e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
1.667210e-15 3.947890e-16 -1.903573e-16 -7.102138e-15 2.666266e-15
-2.682058e-15

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8.259068e-16 1.646371e-15 3.456590e-17 -4.241864e-15 -1.333186e-16
3.649442e-15

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7.246149e-15

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4.659292e-15

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6.724480e-15

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9.022346e-15 1.994637e-15 -1.251371e-16 -4.086552e-15 -5.774078e-16
4.083774e-15

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9.168127e-16

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1.556722e-15 2.215749e-15 -3.037626e-16 -4.281639e-15 -8.972253e-16
4.040106e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f800b551be0a39.final.pdb
2.133946e-15 4.717639e-16 1.283298e-15 1.227748e-15 -1.275744e-15
9.168127e-16

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-1.162786e-14

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1.994057e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2f42.final.pdb
2.100215e-15 1.667340e-15 -1.363916e-15 -4.337059e-15 1.365388e-16
3.977280e-15

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3.511755e-15 1.384816e-15 2.911547e-15 -5.846625e-15 -1.892957e-15
2.603847e-15

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3.816342e-15 8.078268e-15 2.205245e-15 -9.936599e-15 -5.422362e-16

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| File Path                                                                 | Values                        |
|--------------------------------------------------------------------------|-------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb      | 2.925603e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb      | 1.607898e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb       | 1.545231e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb        | 3.511755e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668.e.final.pdb       | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb        | 6.115143e-16                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb         | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb         | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb         | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb         | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b88c8a505f3a288.final.pdb          | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e.final.pdb          | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb          | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb         | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2af55fc9d0681.final.pdb          | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce3428de3e81a3c.final.pdb          | 2.418970e-15                 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb         | 2.418970e-15                 |
| Path                                                                 | Score          | Score          | Score          | Score          | Score          |
|----------------------------------------------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | -1.022810e-15  | 4.606087e-15   | -3.709273e-15  | -9.816796e-16  | 3.573082e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 8.710658e-16   | 7.801104e-15   | 5.382478e-15   | -4.655622e-15  | -5.438020e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f6eefe39.final.pdb | 4.424477e-15   | 1.841532e-15   | 5.266131e-15   | -1.170674e-14  | -8.821883e-15  |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
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-2.682058e-15

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
2.393472e-15  2.294814e-15 -4.093609e-15 -1.155675e-16  1.206354e-15
-7.921900e-15

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-6.817945e-15

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-7.430639e-15

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-1.069612e-14

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-6.001502e-15

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-3.922824e-15

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-6.596505e-15

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-5.120689e-15

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-6.248486e-15

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-5.866279e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb
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-7.845095e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
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-5.866279e-15

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-2.843694e-15 -1.537583e-15  2.031875e-15 -4.819482e-15 -1.035716e-14
-6.223934e-15

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-1.201566e-15  2.305239e-15 -1.158899e-15  6.634463e-15  5.969830e-15
-1.313984e-14

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1.748743e-15  2.213822e-15 -3.115375e-15 -1.488840e-15  1.709023e-15
-4.760261e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
5.331042e-15  3.362447e-15 -3.976978e-15  5.635877e-15 -1.734054e-15
-1.076715e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-3.565067e-16 -2.962159e-15 -2.905256e-15 -1.532540e-14  1.738951e-14
-1.076715e-15
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2.098095e-15  3.228075e-15 -4.544373e-15  1.407475e-15  1.438780e-15
-4.517115e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
-1.050061e-16  5.028419e-15 -1.081915e-14 -5.128739e-16  1.474566e-14
-1.315121e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
2.098095e-15  3.228075e-15 -4.544373e-15  1.407475e-15  1.438780e-15
-4.517115e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
-2.76371e-15  1.655547e-15 -5.736615e-15  5.580810e-15  1.196471e-15
3.363966e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb
7.69775e-15 -7.367587e-16  1.468153e-15  1.909303e-15 -2.716556e-15
-4.099782e-15
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2.534293e-15 -7.776594e-16 -1.310778e-14  1.038914e-16 -4.875903e-15
-9.777323e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
5.735302e-16  8.097750e-15 -3.121951e-15  2.164546e-15  5.407097e-15
-5.866279e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e52e19ad281fea2.final.pdb
-1.585050e-15  8.195050e-15 -7.436719e-15 -4.536761e-15  2.662255e-15
-5.284425e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
2.501267e-15  3.719919e-15 -3.514289e-15 -2.009362e-15 -3.069528e-15
-4.897294e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
-8.100329e-15  1.270927e-15  6.802938e-15  2.414934e-15 -9.379786e-15
1.191489e-14
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1.361748e-15  1.582073e-15 -1.434977e-15  4.607697e-15 -1.683245e-15
-2.130760e-15
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-4.897294e-15
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5.089143e-16  6.110459e-16 -4.702213e-15  2.295486e-15 -2.042641e-15
-3.922824e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
2.122594e-15  2.516255e-15 -3.289241e-15  1.105261e-15  1.449549e-15
-7.236387e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
2.221807e-15  2.255889e-15 -3.043492e-15  1.396032e-15  1.442418e-15
-5.466728e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
2.117244e-15  2.880569e-15 -3.406988e-15  5.772735e-16  1.233009e-15
-5.907479e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
2.098095e-15  3.228075e-15 -4.544373e-15  1.407475e-15  1.438780e-15
-4.517115e-15
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| File Path | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|-----------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 1.573821e-14 | -9.157454e-16 | 5.682050e-15 | 1.006978e-14 | 4.845217e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 2.089132e-15 | 2.595297e-16 | -7.199475e-16 | -1.292655e-15 | -4.235720e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -2.265282e-15 | 2.307370e-15 | -4.740743e-15 | -1.458498e-15 | -4.991261e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 2.049849e-15 | 5.083761e-15 | -1.368383e-14 | -1.113832e-14 | -1.697167e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 9.081609e-15 | -2.079205e-15 | 9.547409e-15 | 4.850608e-16 | 8.64258e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 2.373043e-15 | 4.762871e-15 | -3.254519e-15 | 1.414204e-15 | 2.421213e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 9.027933e-15 | 6.842282e-15 | -1.176034e-14 | -8.151931e-15 | 5.703825e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4432d1f75a7fcfc.final.pdb | -3.63995e-15 | 3.865119e-15 | -1.786282e-15 | -1.988629e-15 | -8.901692e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cfdb.final.pdb | 2.033123e-14 | 7.438682e-15 | -1.090855e-14 | -8.137141e-15 | 6.47192e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -1.332262e-15 | -2.520692e-15 | 3.662360e-15 | 1.498139e-15 | -1.661469e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -3.633938e-15 | 1.850785e-15 | -5.690364e-15 | 5.084189e-15 | -2.822695e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -5.866504e-14 | 3.606351e-15 | -1.330150e-14 | -4.052976e-15 | -1.22247e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 8.764172e-16 | -4.327548e-15 | 8.302926e-15 | 2.850488e-15 | 3.668879e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 9.081609e-15 | -2.079205e-15 | 9.547409e-15 | 4.850608e-16 | 8.64258e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5a647f04822d30a.final.pdb | 2.237058e-16 | -1.687731e-15 | -1.787150e-15 | 8.216225e-16 | 1.937294e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091fe385e05fc.final.pdb | -8.046581e-16 | 1.151611e-15 | -2.197665e-15 | -5.504564e-15 | -2.711239e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 8.764172e-16 | -4.327548e-15 | 8.302926e-15 | 2.850488e-15 | 3.668879e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 3.599472e-15 | 3.599472e-15 | 3.599472e-15 | 3.599472e-15 | 3.599472e-15 |
## Supplementary Text 10

1.490098e-15 -4.006995e-16 -3.055425e-16 -1.049590e-15 -4.277846e-16
6.312744e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
6.284916e-17 7.956449e-16 -3.055425e-16 -1.049590e-15 7.078601e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
4.088243e-15 2.189692e-16 -4.131893e-15 -3.100674e-15 4.941397e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-3.633938e-15 1.850705e-15 -5.690364e-15 5.084189e-15 2.706559e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
2.940416e-16 4.231719e-15 -1.067797e-15 -4.275020e-15 -2.696876e-16

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
2.986533e-15 -9.343543e-16 1.083120e-15 3.572086e-15 2.291289e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.638837e-15 -3.037850e-15 1.255229e-15 2.97521e-15 2.857688e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
4.016679e-15 -1.155050e-15 1.335277e-15 2.826555e-15 3.524409e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
4.747305e-15 -1.241150e-15 -7.870123e-16 3.544662e-15 2.496475e-15

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4.960464e-15 3.955908e-15 4.034733e-15 1.479101e-15 -1.086541e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
3.844928e-15 -8.744298e-16 3.566575e-15 -1.230201e-15 -1.67644e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
2.006270e-15 5.322634e-15 4.363756e-15 -1.842096e-16 3.034805e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
3.352021e-15 -1.128455e-15 1.094153e-15 2.754810e-15 -8.202520e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
3.352021e-15 -1.128455e-15 1.094153e-15 2.754810e-15 -8.202520e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
2.006270e-15 5.322634e-15 4.363756e-15 -1.842096e-16 3.034805e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
2.006270e-15 -1.265827e-15 1.356811e-15 2.815699e-15 -4.413380e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b51bea0a39.final.pdb
2.006270e-15 5.322634e-15 4.363756e-15 -1.842096e-16 6.534611e-16

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Supplementary Text 10

3.095631e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb  
3.862040e-15  1.580186e-15  7.633834e-15  2.557970e-15 -6.504737e-15  
7.436545e-14  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb  
1.745190e-15  9.158326e-15  5.722494e-15  2.956957e-15 -1.433273e-15  
1.136667e-14  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb  
3.257842e-15 -1.816836e-15  1.053811e-15  2.787821e-15 -3.956914e-16  
2.037651e-15  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb  
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9.266710e-16  
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb  
1.079429e-14 -6.629437e-15 -9.753411e-16  1.885203e-15 -4.024736e-15  
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9.187321e-15  
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3.755536e-15 -5.747486e-15 -3.070421e-15  4.520932e-15 -8.307834e-16  
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6.243587e-15 -1.370772e-15 -3.603711e-15  2.62903e-15  2.199224e-15  
9.896814e-15  
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-2.389548e-15  
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6.598149e-15  9.021083e-15  2.434941e-15  5.056528e-15 -7.414452e-16  
1.373436e-14  
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-1.020200e-16  
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1.541333e-15  2.316143e-15 -2.091026e-15  1.412164e-14  3.583331e-15  
4.674756e-15  
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-8.602580e-15 -2.732319e-15  1.208218e-15  8.804741e-15  6.814627e-15  
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-1.081699e-16  
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3.406705e-15  
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4.438836e-15 -5.090693e-15 -8.951511e-16  9.156208e-16 -1.352391e-15
| File Name                                      | Values                  |
|-----------------------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 5.094685e-16 4.676242e-15 -4.608880e-16 6.100791e-15 7.047664e-16 -2.915309e-16 -1.081699e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 2.146035e-15 -4.855942e-15 6.731354e-15 -2.640613e-15 1.528564e-15 -1.081699e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff286d.final.pdb | 6.041516e-15 4.355161e-16 4.640264e-15 9.075069e-15 4.414835e-15 3.406705e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 2.227407e-15 -4.053311e-15 -3.662684e-16 2.316442e-15 -3.232623e-17 -1.020800e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 3.086854e-15 -1.228313e-15 1.046889e-15 2.769204e-15 -1.620696e-16 2.291248e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 3.967946e-16 5.316918e-15 5.564539e-15 6.695207e-15 -8.218985e-16 -1.438907e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6b5347ea982fffc4.final.pdb | 3.086854e-15 4.355161e-16 4.640264e-15 9.075069e-15 4.414835e-15 3.406705e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | 4.242096e-15 1.073777e-15 3.967946e-16 5.858664e-15 -3.191402e-15 8.496992e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb | 6.041516e-15 4.355161e-16 4.640264e-15 9.075069e-15 4.414835e-15 3.406705e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb | 3.749694e-15 -9.947953e-16 1.415051e-15 2.876276e-15 -4.871445e-16 3.070152e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 4.438836e-15 -5.90693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 3.182632e-15 -7.603255e-15 -6.738787e-15 9.344012e-15 1.779687e-15 8.520819e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -7.099590e-17 -1.390728e-15 -1.293847e-15 6.012360e-15 1.527573e-15 2.086562e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298febaf.final.pdb | -7.099590e-17 -1.390728e-15 -1.293847e-15 6.012360e-15 1.527573e-15 2.086562e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb | -3.375536e-15 -5.747486e-15 -3.070421e-15 4.520932e-15 -8.307834e-16 2.958043e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d0469ef569760.final.pdb | 2.227407e-15 -4.053311e-15 -3.662684e-16 2.316442e-15 -3.232623e-17 -1.020800e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | 6.041516e-15 4.355161e-16 4.640264e-15 9.075069e-15 4.414835e-15 3.406705e-15 |
| File Path                                                                 | 1.827437e-15 | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb |
|----------------------------------------------------------------------------|---------------|---------------------------------------------------------------------|
| 7.502078e-15 -1.602239e-15 -1.146827e-15 1.601048e-15 4.307784e-15       | -6.862567e-15|                                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb      | 7.502078e-15 | -1.602239e-15 -1.146827e-15 1.601048e-15 4.307784e-15 -5.094685e-16 |
| 4.438836e-15 -5.090693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15      |               |                                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d7e62fa.final.pdb       | 1.406315e-14 | 5.128797e-15 7.257798e-15 -8.337259e-16 -5.588696e-15 3.783555e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb       | 4.449392e-15 | 1.250836e-15 7.545926e-15 -2.907967e-15 9.523272e-16 -3.956112e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb       | 3.448285e-15 | -5.203056e-16 -2.156810e-15 3.985484e-15 -1.365297e-15 1.762355e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6b.final.pdb        | 4.676242e-15 | -6.08880e-16 6.100791e-16 5.094685e-15 -1.081699e-15 1.406315e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb       | 3.448285e-15 | -5.203056e-16 -2.156810e-15 3.985484e-15 -1.365297e-15 1.762355e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb       | 3.221151e-15 | -5.520705e-16 1.399882e-15 2.956207e-15 -3.932139e-15 2.075355e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb       | 2.732151e-15 | -6.503378e-15 8.395858e-15 -1.003241e-15 -6.460363e-15 2.258101e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb       | 3.221151e-15 | -5.520705e-16 1.399882e-15 2.956207e-15 -3.932139e-15 2.075355e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb       | 4.438836e-15 | -5.00693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb       | 4.438836e-15 | -5.00693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1ae1.final.pdb       | 4.438836e-15 | -5.00693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb       | 4.438836e-15 | -5.00693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a.final.pdb        | 4.438836e-15 | -5.00693e-15 -8.951511e-16 9.156208e-16 -1.352391e-15 5.094685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 5.094685e-16 |
|---------------------------------------------------------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 3.103587e-15 -1.125549e-15 1.281385e-15 2.954788e-15 -4.472994e-16 2.133170e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55cf9d6681.final.pdb | 1.579278e-14 6.420299e-15 1.059432e-14 -7.114279e-16 -3.177390e-16 2.133170e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 1.030554e-15 -6.789187e-15 -1.137722e-15 1.778334e-15 -1.414518e-15 1.827437e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249a61.final.pdb | 3.553639e-15 1.294824e-15 3.583580e-15 1.232273e-14 3.838985e-15 8.765017e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 6.219737e-15 -5.994511e-15 4.891112e-15 2.109398e-15 4.847092e-15 1.246338e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 5.679742e-15 -2.829762e-15 -3.052427e-16 4.432457e-15 8.468966e-16 2.987603e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 1.311742e-15 -5.647191e-16 2.377474e-14 -1.819758e-15 -2.519689e-15 1.850236e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -1.503000e-15 -1.893183e-15 -4.736025e-15 -2.432105e-15 -3.152309e-15 9.159803e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8009eff10197e2.final.pdb | 5.682830e-15 -1.664163e-15 -1.416027e-15 -7.764728e-16 -1.528328e-15 -9.459166e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 1.311742e-15 -5.647191e-16 2.377474e-14 -1.819758e-15 -2.519689e-15 1.850236e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -1.503000e-15 -1.893183e-15 -4.736025e-15 -2.432105e-15 -3.152309e-15 9.159803e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 5.679742e-15 -2.829762e-15 -3.052427e-16 4.432457e-15 8.468966e-16 2.987603e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 1.311742e-15 -5.647191e-16 2.377474e-14 -1.819758e-15 -2.519689e-15 1.850236e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -1.503000e-15 -1.893183e-15 -4.736025e-15 -2.432105e-15 -3.152309e-15 9.159803e-15 |

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2.815924e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
3.266597e-15 -1.301189e-15 1.291468e-15 -6.712956e-16
2.260130e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
3.266597e-15 -1.301189e-15 1.291468e-15 -6.712956e-16
2.260130e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
5.679742e-15 -2.829762e-15 -3.052427e-16 4.324573e-15 8.468666e-16
2.987603e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
3.448285e-15 -5.203056e-16 -2.156810e-15 3.985484e-15 -1.365297e-15
1.762355e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
1.541333e-15 2.316143e-15 -2.091026e-15 1.412164e-14 3.583331e-15
4.674756e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
4.960464e-15 3.955908e-15 4.034733e-15 4.179101e-15 -1.086541e-16
2.970826e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-1.375418e-15 -9.803430e-16 3.988293e-15 -2.051355e-15 -2.662658e-15
-3.758579e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
8.763043e-16 -1.825536e-15 1.613698e-15 5.678939e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
-1.220526e-15 -2.460596e-15 1.613698e-15 5.603104e-15 -1.532368e-15
1.658939e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
4.749891e-15 8.998137e-17 -1.125646e-14 5.249283e-15 -8.518217e-15
-2.422625e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
5.865513e-16 -1.825536e-15 2.360240e-15 -4.067354e-15
1.898476e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
4.851797e-15 -5.298517e-15 -7.040155e-15 5.123931e-15 -5.057824e-15
-3.514732e-15

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| File Path                                                                 | Coordinates                                  |
|---------------------------------------------------------------------------|----------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | [-4.207928e-15, -2.623721e-15, -3.084322e-15, -4.063075e-15, -2.211300e-15, 4.709692e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb       | [-7.599752e-15, -2.686211e-15, -7.476288e-15, 1.142841e-14, -2.780477e-15, 2.982192e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb       | [-7.599752e-15, -2.686211e-15, -7.476288e-15, 1.142841e-14, -2.780477e-15, 2.982192e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb       | [-1.220526e-15, -2.460596e-15, 1.613698e-15, 5.603104e-15, -1.532368e-15, 1.658939e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f490d67e2fa.final.pdb        | [3.071231e-15, -1.251663e-14, -5.545407e-15, 4.426947e-15, -1.203626e-14, 6.196489e-16] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d9a8ed0db81fd3ef.final.pdb      | [4.002042e-15, -6.391541e-15, 4.280492e-16, 1.908722e-16, 6.877696e-17, 9.204054e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb       | [-1.409635e-15, -1.59101e-15, -1.430893e-15, 5.369201e-15, -3.023634e-15, 1.932463e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c7008381666ba.final.pdb       | [2.250558e-15, -5.871186e-15, -8.254655e-15, 1.276569e-15, -8.505586e-15, 5.948818e-16] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c9b979c971d4d4c.final.pdb      | [2.331888e-15, -2.132144e-15, 3.097853e-15, 9.544917e-16, -1.611005e-15, 2.702184e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad5a8233e4b4c668e.final.pdb       | [1.570364e-15, -1.465646e-15, -2.055344e-15, 2.420087e-15, -3.653939e-15, 2.169856e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb       | [3.071231e-15, -1.251663e-14, -5.545407e-15, 4.426947e-15, -1.203626e-14, 6.196489e-16] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc8d9236e97d3c63.final.pdb        | [-7.614546e-16, -1.578117e-15, -6.020758e-15, 1.146138e-14, -8.758580e-15, -2.312685e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b269236e97d3c63.final.pdb        | [-1.220526e-15, -2.460596e-15, 1.613698e-15, 5.603104e-15, -1.532368e-15, 1.658939e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1ae6.final.pdb        | [-2.040421e-15, -1.114566e-15, -2.993290e-15, -7.987496e-15, 3.659444e-16, 1.658939e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb        | [-1.220526e-15, -2.460596e-15, 1.613698e-15, 5.603104e-15, -1.532368e-15, 1.658939e-15] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb        | [4.096886e-15, 7.509660e-16, -1.051279e-14, 8.018286e-15, -7.04689e-15, 4.820282e-15] |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb      | -1.220526e-15 -2.460596e-15 1.613698e-15 5.603104e-15 -1.532368e-15 1.658939e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2c8f975403e7.final.pdb       | -2.980324e-16 -2.232046e-15 -1.907791e-15 4.020576e-15 -3.909156e-15 1.762372e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb      | -2.980324e-16 -2.232046e-15 -1.907791e-15 4.020576e-15 -3.909156e-15 1.762372e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | 1.717486e-16 -1.067696e-14 -1.879936e-15 2.444999e-15 -1.022954e-14 -5.424345e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | 4.096886e-15 7.509960e-16 -1.051279e-14 8.018286e-15 -7.040689e-15 4.820282e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | -1.309863e-14 -1.351265e-14 -1.829623e-15 1.870545e-15 -2.230123e-15 5.479704e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb        | 1.001232e-15 -1.456952e-15 -6.534844e-16 -5.317270e-16 -2.299479e-15 3.165663e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 6.764313e-15 3.142731e-15 5.942176e-15 -6.477936e-15 -4.250783e-15 3.158876e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d060803e-14 -1.351265e-14 -1.829623e-15 1.870545e-15 -2.230123e-15 5.479704e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1b40af0f0efe39.final.pdb        | 4.851797e-15 -5.298517e-15 -7.040155e-15 5.123931e-15 -5.057824e-15 -3.514732e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d529e19ad281fe2a.final.pdb       | -1.375418e-15 -9.803430e-16 3.988293e-15 -2.051355e-15 -2.662658e-15 -3.758575e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d5602082718ec3a1.final.pdb       | 3.180813e-15 5.028797e-15 -1.247260e-15 6.504370e-15 -6.440990e-15 3.474871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb       | 4.851797e-15 -5.298517e-15 -7.040155e-15 5.123931e-15 -5.057824e-15 -3.514732e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090caef7.final.pdb       | -3.233188e-15 -2.132144e-15 3.978783e-15 9.544917e-16 -1.611005e-15 2.702184e-15 |

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2.470683e-15 -3.648959e-15 -9.373203e-15 -2.089352e-15 5.634341e-16
-1.017274e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb

1.902818e-15 -5.801548e-15 -8.019873e-15 2.531742e-15 -1.058861e-15
4.723969e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb

-1.166414e-15 -6.704597e-15 -1.064665e-15 -3.829433e-15 3.619881e-15
-5.845127e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb

-1.718058e-15 3.572392e-15 -7.236052e-15 -9.214396e-15 8.612185e-16
1.842892e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb

-1.166414e-15 -6.704597e-15 -1.064665e-15 -3.829433e-15 3.619881e-15
-5.845127e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb

4.734132e-15 -4.347867e-15 -8.756280e-15 -7.026163e-15 -9.245936e-16
-8.958563e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb

3.370665e-15 1.681832e-15 -9.271910e-15 -3.595952e-15 -1.575375e-15
2.283448e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb

1.313224e-16 -7.044581e-15 -8.635802e-16 -8.881293e-16 3.027166e-15
7.575676e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc.final.pdb

-6.440263e-15 9.166475e-15 2.994273e-15 -5.808919e-15 -4.558933e-15
2.442795e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69f910ff828272.final.pdb

3.677007e-16 -1.133729e-15 -5.040510e-15 -3.752136e-15 1.220482e-15
4.736987e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb

-1.718058e-15 3.572392e-15 -7.236052e-15 -9.214396e-15 8.612185e-16
1.842892e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb

-1.166414e-15 -6.704597e-15 -1.064665e-15 -3.829433e-15 3.619881e-15
-5.845127e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb

1.830292e-15 -2.256364e-15 -1.324045e-15 6.946114e-15 -3.498665e-15
-4.726267e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb

-6.440263e-15 9.164475e-15 2.994273e-15 -5.808919e-15 -4.558933e-15
2.442795e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
-1.718058e-15  3.572392e-15 -7.236052e-15 -9.214396e-15  8.612185e-16
1.842892e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
-1.353590e-15 -2.971354e-15 -9.133818e-15 -7.436106e-16 -1.511966e-15
5.076355e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
-1.718058e-15  3.572392e-15 -7.236052e-15 -9.214396e-15  8.612185e-16
1.842892e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb
-1.718058e-15  3.572392e-15 -7.236052e-15 -9.214396e-15  8.612185e-16
1.842892e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
-2.030482e-16  3.267249e-16 -5.368622e-15 -5.015064e-15  9.744092e-16
4.065409e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
-3.310791e-15 -5.821721e-15 -8.436025e-15 -4.510563e-15  3.855702e-15
5.076355e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb
-1.535390e-15 -2.971354e-15 -9.133818e-15 -7.436106e-16 -1.511966e-15
5.076355e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
-2.670121e-15  7.477356e-16 -7.705574e-15 -8.517638e-16  5.420995e-15
-2.144168e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-3.442108e-15 -1.753030e-14  8.546245e-15 -5.649322e-15  3.548305e-15
-1.891751e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
7.491842e-16  1.171172e-15 -5.491960e-15 -3.207169e-15 -9.624146e-16
7.646158e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
5.254734e-15  3.402077e-15 -3.919390e-15  2.269964e-15 -8.614677e-15
5.330684e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
3.538739e-15  3.501152e-15 -1.043269e-14 -5.937332e-15 -1.013899e-14
1.131008e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc8009ef10197e2.final.pdb
4.594099e-15  8.695538e-16 -1.625227e-14 -2.581828e-15 -2.902238e-16
-2.542563e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
3.494083e-15  3.767712e-15 -6.777760e-15 -2.480035e-15 -4.894142e-15
4.898658e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
8.505614e-15 -6.950257e-15 -9.083500e-15 -4.438870e-15  1.371403e-15
-2.052059e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f0e2.final.pdb
-2.636683e-15  2.639399e-15  1.025359e-16 -1.064934e-16  6.213533e-15
-3.854003e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d09a60.final.pdb
-8.920934e-16 -2.083449e-15 -7.519838e-15  5.612794e-15  1.923678e-15
4.501460e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fd.final.pdb
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| File Path                                                                 | Values                                                                 | Page 418 |
|-------------------------------------------------------------------------|------------------------------------------------------------------------|----------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb     | -3.979246e-15                                                         |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa4562cb6a25f.final.pdb       | -3.979246e-15                                                         |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5a647f04822d30a.final.pdb     | -3.979246e-15                                                         |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091f3e385e05fc.final.pdb     | -3.979246e-15                                                         |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac0f930d2db.final.pdb      | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\624566d66f2868d.final.pdb      | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d96246111d42.final.pdb      | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910ff82b2872.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f01be4.final.pdb     | 3.697142e-15                                                          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb     | 3.697142e-15                                                          |          |
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-9.154055e-15
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-9.154055e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfe12d3f9.final.pdb
4.049372e-15 8.936262e-15 4.879248e-15 -3.786082e-15 2.009207e-15
-4.289890e-15
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4.166325e-15 1.082293e-14 -8.561610e-16 5.895585e-15 6.607124e-15
-5.771029e-15
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-3.594227e-16 7.674406e-15 -3.347937e-15 5.271713e-15 -1.199311e-15
-4.353232e-15
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1.404340e-15
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2.447218e-15
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5.619594e-15 5.307889e-15 -2.388776e-15 6.835437e-15 8.611761e-16
-7.458571e-15
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-6.086196e-15
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-3.57004e-15
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-6.016420e-15
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-3.71993e-15
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-9.154055e-15
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-9.154055e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
5.619594e-15 5.307889e-15 -2.388776e-15 6.835437e-15 8.611761e-16
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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb     | 4.605032e-15 -1.407280e-15 5.352627e-15 1.230533e-15 1.115365e-15 2.208860e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dbaf9f3306825e8.final.pdb     | 1.187230e-14 -1.040247e-15 1.982062e-15 -1.977381e-15 2.837756e-15 4.108981e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb      | -1.932198e-15 -3.545979e-16 -5.176709e-15 -6.618363e-15 1.795621e-15 -2.369864e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | 2.060543e-15 9.745928e-16 3.006113e-15 -3.351625e-15 3.80932e-16 1.219767e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb     | -2.366915e-15 2.099847e-15 -2.722136e-15 -1.078421e-14 5.065422e-15 -5.856505e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb       | 1.975334e-15 4.631920e-15 2.609605e-15 -2.657995e-15 -3.485805e-16 2.236134e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb      | -2.366915e-15 2.099847e-15 -2.722136e-15 -1.078421e-14 5.065422e-15 -5.856505e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb      | 2.566732e-15 8.751478e-15 9.759192e-16 -2.32156e-15 -6.926813e-15 1.124937e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb       | -2.857531e-15 4.793056e-15 -4.962699e-15 -1.632818e-14 -2.964488e-15 7.791200e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb       | 1.890623e-15 7.413923e-16 3.390221e-15 -3.617315e-15 1.187661e-16 1.449918e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb       | 4.882730e-15 1.214515e-15 7.452953e-15 1.361360e-15 -1.167370e-15 8.205993e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb       | -3.031519e-15 6.113151e-15 6.588870e-15 6.285113e-16 -3.790712e-15 1.429796e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871979b7ab.final.pdb       | -7.080242e-15 2.715785e-15 5.644800e-15 4.197839e-15 -1.906652e-15 8.150323e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb       | -1.932198e-15 -3.545979e-16 -5.176709e-15 -6.618363e-15 1.795621e-15 -2.369864e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb       | 4.122488e-15 1.834057e-15 1.257822e-15 -7.439983e-16 -3.504476e-15 -5.12740e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb       | -4.059351e-15 6.992629e-15 2.492287e-15 -4.143500e-16 -1.189098e-15 1.087292e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb        | -5.237977e-16 -4.066206e-15 9.374287e-15 -1.198529e-15 -4.079288e-16 -3.855983e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb      | -3.013093e-14 1.127919e-14 -1.990881e-15 -1.163345e-14 -7.323904e-15 3.627382e-15 |
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**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb**

1.187230e-14 -1.040247e-15 1.982062e-15 -1.977381e-15 2.837756e-15
4.108981e-16

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb**

-4.640610e-15 2.405860e-15 5.601993e-15 -1.069889e-14 -1.633738e-15
-1.500846e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb**

-9.689881e-15 5.193048e-15 3.032003e-15 9.226602e-15 -1.139532e-15
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**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb**

4.247285e-15 -2.724091e-15 3.47209e-15 -5.880200e-15 2.030954e-15
-3.055123e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb**

-1.932198e-15 -3.545979e-16 -5.176709e-15 -6.618363e-15 1.795621e-15
-2.369864e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb**

4.459128e-16 1.216244e-15 3.665312e-15 -4.471519e-15 -1.169472e-15
7.870828e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb**

-4.605032e-15 -1.407280e-15 5.352627e-15 1.230533e-15 1.115365e-15
2.208860e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb**

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**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb**

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-6.516666e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb**

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4.108981e-16

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb**

4.459128e-16 1.216244e-15 3.665312e-15 -4.471519e-15 -1.169472e-15
7.870828e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\661353ff3c8f7ef.final.pdb**

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-9.026860e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb**

3.803672e-15 -4.829592e-15 1.103182e-15 -9.441155e-15 -1.228822e-15
-9.026860e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb**

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1.810820e-16

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc4.final.pdb**

-1.517000e-15 3.748035e-15 -2.847039e-15 -1.249803e-14 5.838065e-16
-1.265237e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb**

-2.34415e-15 9.731477e-15 7.539379e-15 -2.310862e-15 -2.539996e-15
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**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb**

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7.870828e-15

**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb2872.final.pdb**

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**E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb**

4.605032e-15 -1.407280e-15 5.352627e-15 1.230533e-15 1.115365e-15
2.208860e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feda2.final.pdb
-2.915828e-16  5.851886e-16  1.507922e-14 -6.229188e-15 -9.491457e-16
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8.205993e-16

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1.626057e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
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-3.055123e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
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7.557409e-15

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2.208860e-15

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2.072515e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682bc0ad52078.final.pdb
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-1.500846e-15

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Supplementary Text 10
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3.393686e-15

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4.347083e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
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5.184995e-15

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-1.783502e-15

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2.540954e-15

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| File Path                                                                 | Value 1                | Value 2                | Value 3                | Value 4                | Value 5                |
|--------------------------------------------------------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb      | 1.299716e-15           | -9.080616e-16          | 5.818452e-15           | 4.058538e-16           | 4.801155e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\76f910fffb22872.final.pdb       | 4.535114e-15           | -2.919184e-15          | 6.709085e-15           | 2.333758e-15           | 1.941348e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb      | 3.866248e-15           | 8.456022e-15           | -1.395441e-15          | -8.017257e-16          | 5.682836e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb       | 1.658007e-15           | -2.341140e-15          | 3.164448e-15           | 3.377025e-15           | 2.307387e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633916.final.pdb       | 9.501803e-15           | -3.041634e-15          | 5.167480e-15           | 4.535296e-15           | 9.011617e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | 9.501803e-15           | -3.041634e-15          | 5.167480e-15           | 4.535296e-15           | 9.011617e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12d3f9.final.pdb        | 5.815949e-15           | -7.921411e-15          | 6.093389e-15           | 4.629111e-15           | 4.028868e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d04696f569760.final.pdb        | 6.345943e-15           | -9.173442e-16          | 1.207494e-14           | 3.375531e-15           | -4.954677e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | 5.177892e-15           | -9.080616e-16          | 5.818452e-15           | 4.058538e-16           | 4.801155e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb       | 5.815949e-15           | -7.921411e-15          | 6.093389e-15           | 4.629111e-15           | 4.028868e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8f750404e569760.final.pdb        | 6.345943e-15           | -9.173442e-16          | 1.207494e-14           | 3.375531e-15           | -4.954677e-15          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98b00469ef569760.final.pdb       | 3.866248e-15           | -3.419953e-15          | 8.456022e-15           | 1.395441e-15           | -8.017257e-16          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9ac2f4909d67e2fa.final.pdb       | 4.535181e-15           | -1.321222e-15          | 7.472949e-15           | 1.076094e-15           | 1.213412e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f750404e569760.final.pdb        | 3.866248e-15           | -3.419953e-15          | 8.456022e-15           | 1.395441e-15           | -8.017257e-16          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | 4.535114e-15           | -2.919184e-15          | 6.709085e-15           | 2.333758e-15           | 1.941348e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb       | 4.442147e-15           | -3.451336e-15          | 8.064250e-15           | 4.224171e-15           | 4.041986e-16           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a188d0d0d81fb3ef.final.pdb       | 7.499935e-15           | -6.642728e-15          | 5.146728e-15           | 6.080432e-15           | -1.567108e-16          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | 4.535114e-15           | -2.919184e-15          | 6.709085e-15           | 2.333758e-15           | 1.941348e-15           |

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4.696093e-15 -2.885936e-15  7.056164e-15  2.427771e-15  1.404301e-15
4.347755e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
3.866248e-15 -3.419953e-15  8.456022e-15  1.395441e-15  -8.017257e-16
5.682836e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
3.660551e-15 -3.448693e-15 -9.389468e-16 -6.660562e-15 -1.468136e-15
6.282887e-15
| PDB File Path                                           | RMSD (A) | Quality Score | Sharpley Score | Annotations |
|-------------------------------------------------------|----------|---------------|----------------|-------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a960.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\edf9e72307a2fbd.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6862cbbcad52078.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6a0f8694090cae7.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6a517be32db050e.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e84b9545899c29d.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb | 0.000000 | 100.00         | 100.00         |             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e14fca8deec4fa3.final.pdb | 0.000000 | 100.00         | 100.00         |             |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
3.655286e-15  2.647980e-15  4.958696e-15  8.340734e-15 -8.201132e-15
-1.914905e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b4a0af0f0efe39.final.pdb
6.441242e-15 -2.086743e-16 -1.450401e-15  6.819189e-15  6.819189e-15
-1.914905e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb
2.523456e-15 -8.291545e-15 -3.319302e-15 -7.281936e-15  6.086008e-15
8.051450e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
1.098595e-14 -1.065026e-14 -4.072764e-15  3.246803e-15 -9.494292e-15
-3.335547e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
-1.762495e-16 -9.877366e-15  3.250942e-15  1.184130e-14 -7.190708e-15
1.777415e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb
9.131821e-16 -1.929138e-15 -2.305312e-15 -1.092548e-15 -6.253215e-15
6.235171e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
7.415042e-16 -2.832309e-15 -4.628028e-15  1.278228e-14  1.752004e-14
-7.627906e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e589d9960a960.final.pdb
3.085912e-15 -1.523109e-14  7.911061e-16  3.850975e-15 -1.141141e-14
-6.463190e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
2.629893e-15 -8.642469e-15  2.109265e-15  5.219976e-15  5.219976e-15
-3.621938e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
7.415042e-16 -2.832309e-15 -4.628028e-15  1.278228e-14  1.752004e-14
-7.627906e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb0517be32db050e.final.pdb
2.484178e-15 -1.374528e-16 -3.042087e-15 -2.230720e-15  2.016745e-15
4.504225e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
1.825742e-15 -2.700889e-15  2.111358e-16  2.430940e-15 -3.717229e-15
-5.606402e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
2.070663e-15 -1.811461e-15  2.269949e-16  9.334155e-16 -2.699101e-15
6.551199e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
2.022512e-15 -2.577650e-15  1.024192e-16  2.208593e-15 -3.789782e-15
-4.597282e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
2.163816e-15 -3.023845e-15 -1.413422e-16  6.044539e-16 -3.448988e-15
3.882197e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
8.625904e-16 -2.238549e-15 -2.631151e-15  1.609830e-15 -1.571499e-15
-6.148651e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8358e422003fb92.final.pdb
9.719327e-16 -4.660311e-15 -1.529050e-16  5.809555e-15 -4.510153e-15
1.533974e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
9.131821e-16 -1.929138e-15 -2.305312e-15 -1.092548e-15 -6.253215e-15
6.235171e-15

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| Path                                   | Values                                      |
|----------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb | 4.703212e-16  2.531191e-15 6.799759e-15  2.251188e-15 -7.018234e-15 -4.330471e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb | 1.266440e-15  6.498693e-15 6.665861e-15  1.826047e-15 -8.294560e-15 -5.726055e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | 9.516732e-16  3.493727e-15 6.396429e-15  3.159667e-16 -7.246210e-15 -1.704945e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | 9.658125e-16  2.505216e-15 7.363350e-15  1.059072e-15 -5.875841e-15 -3.829383e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 2.306067e-15  7.588664e-15 6.113568e-15  2.960493e-15 -6.733000e-15 -5.416049e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 1.116414e-15  5.000557e-15 7.109770e-15  8.416845e-16 -7.196333e-15 -4.367595e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcede4194d9.final.pdb | -6.598962e-16  4.487759e-15 6.445482e-15  4.339948e-15 -6.202377e-15 -4.795255e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -6.63816e-16  3.487778e-15 6.407684e-15  4.504397e-15 -6.521364e-15 -2.961415e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b53739c.final.pdb | 3.960993e-15  5.297962e-15 4.934399e-15 -6.437371e-15 -1.098394e-14 -5.571307e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | 1.261263e-15  5.122855e-15 6.928274e-15  6.543344e-16 -7.172915e-15 -4.482954e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | 7.533646e-15  2.161462e-15 7.763653e-15 -3.632529e-15 -8.438628e-15 -9.535260e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | 1.430196e-15  4.945306e-15 6.947269e-15  9.964399e-16 -7.796484e-15 -5.164026e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | 7.533646e-15  2.161462e-15 7.763653e-15 -3.632529e-15 -8.438628e-15 -9.535260e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | -4.543942e-15  7.204336e-15 5.717332e-15 -8.273226e-15 -1.032148e-14 9.005338e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | 9.887656e-15  1.110516e-16 2.156595e-15 -1.770182e-15 -1.959965e-14 -7.628906e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 1.249781e-15  4.966543e-15 6.945082e-15  1.339744e-15 -8.251085e-15 -3.686767e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -1.645469e-15  5.902873e-15 7.502381e-15  5.905707e-15 -1.691993e-15 -5.635871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | Page 442
| File Path                                                                 |
|--------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb       |
| 9.555849e-16 5.696949e-15 6.928455e-15 1.224902e-15 -8.685431e-15         |
| -3.590253e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb       |
| -2.981317e-15 7.395078e-15 2.686931e-15 -2.848719e-15 -1.395604e-14         |
| -4.783264e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb       |
| 1.454685e-15 4.344832e-15 5.680791e-15 -3.753598e-15 -2.296840e-16          |
| -9.888353e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       |
| 4.593719e-15 7.813001e-15 8.090431e-15 1.739831e-15 -1.371740e-14           |
| -5.800153e-16                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fff2b2872.final.pdb       |
| 1.551886e-15 5.126104e-15 7.138936e-15 1.257223e-15 -8.410005e-15           |
| -4.098637e-17                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80d5c3135.final.pdb        |
| -6.598962e-16 4.487759e-15 6.445482e-15 4.339948e-15 -6.202377e-15          |
| -4.795255e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6009.final.pdb        |
| -3.396706e-15 7.450438e-15 7.914388e-15 4.443581e-15 2.661785e-15          |
| -6.140411e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       |
| -1.645469e-15 5.902873e-15 7.502381e-15 5.905707e-15 -1.691993e-15           |
| -5.635871e-16                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       |
| -1.645469e-15 5.902873e-15 7.502381e-15 5.905707e-15 -1.691993e-15           |
| -5.635871e-16                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c00efcfe12d3f9.final.pdb        |
| -2.788651e-15 6.375585e-15 7.248077e-15 2.067632e-15 -3.790141e-15          |
| -1.472149e-14                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb        |
| -6.663816e-16 3.487778e-15 6.407684e-15 4.504397e-15 -6.521364e-15           |
| -2.961415e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb        |
| 4.593719e-15 7.813001e-15 8.090431e-15 1.739831e-15 -1.371740e-14           |
| -5.800153e-16                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb        |
| -2.741814e-15 3.571405e-15 7.871877e-15 -2.146879e-15 -7.831179e-15          |
| 1.067101e-15                                                             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb        |
| -3.827341e-15 -2.030693e-15 1.741382e-15 8.941757e-16 -1.107388e-14          |
| -1.846360e-14                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bee0d5986c138f.final.pdb        |
| -6.598962e-16 4.487759e-15 6.445482e-15 4.339948e-15 -6.202377e-15           |
| -4.795255e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb        |
| 8.638406e-15 3.125581e-15 4.621656e-15 -7.950958e-16 -1.366202e-14           |
| 4.316238e-15                                                             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9da8ed0d81fb3ef.final.pdb         |
| 3.414541e-15 7.937034e-15 8.147243e-15 8.753318e-15 -4.758211e-16           |
| -8.432792e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb        |
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8.033138e-16  3.641354e-15  7.326332e-15  2.288597e-16 -1.015953e-14
-1.479421e-15

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb

1.770241e-15  2.819440e-15  5.159436e-15  6.575130e-16 -5.875610e-15
-7.677538e-16

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb

-3.582584e-16  8.124685e-15  4.849659e-15 -7.456225e-16 -5.317469e-16
-1.569241e-16

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb

1.215136e-15  4.353396e-15  6.038161e-15  1.421481e-15 -7.319286e-15
-4.118165e-15

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb

-1.645469e-15  5.902873e-15  7.502381e-15  5.905707e-15 -1.691993e-15
-5.635871e-15

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb

4.028044e-15  1.025289e-14  8.590526e-15  3.510897e-15 -2.879046e-15
-7.520194e-15

e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb

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| File Path                                                                 | Distance | Charge 1 | Charge 2 | Charge 3 | Charge 4 | Charge 5 | Charge 6 |
|---------------------------------------------------------------------------|----------|----------|----------|----------|----------|----------|----------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | 3.283841e-15 | -2.878580e-15 | -2.642604e-15 | 2.530340e-15 | 6.965663e-15 | 4.619224e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | 2.716881e-15 | -5.924711e-15 | 1.775941e-14 | 1.140305e-14 | -8.687721e-15 | 8.910004e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb       | 1.251013e-16 | -5.462606e-15 | 3.203734e-15 | 1.589343e-15 | 1.163632e-15 | 3.714920e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fff4.final.pdb       | 1.281789e-15 | -3.437029e-15 | 1.318609e-14 | -2.906599e-15 | -4.30332e-15 | 1.771668e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d962461d1c42.final.pdb        | -7.239938e-16 | 7.878628e-15 | 6.528907e-15 | 4.870384e-15 | -5.391369e-15 | 4.619224e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb        | 2.716881e-15 | -2.878580e-15 | -2.642604e-15 | 2.530340e-15 | 6.965663e-15 | 4.619224e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | 3.010957e-17 | -4.604727e-15 | 3.283874e-15 | 1.710329e-15 | 1.479506e-15 | 3.581232e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | 1.390547e-15 | -3.715823e-15 | 3.555509e-17 | 4.973182e-16 | 6.095338e-15 | 2.32195e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f0699.final.pdb       | 5.497039e-16 | -1.120011e-14 | 2.599982e-15 | 4.621798e-15 | 9.977246e-15 | -5.162925e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | 7.601020e-16 | -6.388615e-15 | 3.171381e-15 | 4.274249e-15 | 3.481152e-15 | -1.915263e-16 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298f6ba.final.pdb       | 7.601020e-16 | -6.388615e-15 | 3.171381e-15 | 4.274249e-15 | 3.481152e-15 | -1.915263e-16 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfe12d3f9.final.pdb        | 1.390547e-15 | -3.715823e-15 | 3.555509e-17 | 4.973182e-16 | 6.095338e-15 | 2.32195e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | 5.177994e-16 | -2.956690e-15 | 4.358627e-15 | -2.248129e-15 | 4.931018e-15 | 3.283841e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | 2.716881e-15 | -2.878580e-15 | -2.642604e-15 | 2.530340e-15 | 6.965663e-15 | 4.619224e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb       | 5.302512e-16 | 2.299097e-15 | 9.700167e-16 | -4.025536e-15 | -1.346584e-15 | 6.081813e-16 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be6d5986c138f.final.pdb        | 3.581035e-16 | 3.549978e-16 | 2.206872e-15 | 1.039797e-15 | 1.256972e-14 | 8.286167e-14 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb       | 1.390547e-15 | -3.715823e-15 | 3.555509e-17 | 4.973182e-16 | 6.095338e-15 | 2.32195e-15 | |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9e22f4909d67e2fa.final.pdb       | -5.912476e-16 | -8.949717e-15 | 1.999792e-15 | 6.056982e-15 | 2.442486e-15 | |
Supplementary Text 10

6.081813e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
-2.879717e-15 -5.773270e-15 -1.623215e-15 -4.048911e-15 2.881261e-15 1.937695e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-2.487662e-16 -2.136791e-15 -8.362024e-16 5.803099e-15 6.281387e-15 7.148818e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
-1.209372e-16 -6.558010e-15 1.678518e-15 7.728136e-16 1.993294e-15 2.275238e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
-4.656280e-15 -6.957805e-15 3.600587e-15 -8.295848e-15 -6.406288e-15 -7.583939e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
-7.319565e-15 -1.336982e-14 3.224770e-15 7.725555e-15 1.316431e-15 4.725012e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d809eff10197e2.final.pdb
2.944480e-15 -3.279893e-15 5.995983e-15 6.281771e-15 1.410003e-14 1.093161e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1163918d3707839.final.pdb
1.215044e-15 -5.755402e-15 5.679081e-15 -5.931580e-16 -2.081353e-15 -4.567872e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d4b06824ef848.final.pdb
-2.968143e-15 -8.311831e-15 3.046999e-15 2.003881e-16 1.876938e-14 8.695197e-15
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-3.481726e-15 -1.417374e-14 5.247672e-15 8.827213e-15 3.026292e-15 6.557264e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d60282718ec3a.final.pdb
7.601020e-16 -6.388615e-15 3.171381e-15 4.274249e-15 3.481152e-15 -1.915263e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d589996d0a960.final.pdb
-4.439550e-15 -2.389871e-15 1.613761e-14 5.814603e-15 -3.456552e-15 8.486048e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d7df972370a2fbd.final.pdb
-2.229086e-15 -6.409839e-15 9.436158e-15 -5.120929e-16 -1.666642e-15 7.071509e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d40f816909eac7.final.pdb
7.601020e-16 -6.388615e-15 3.171381e-15 4.274249e-15 3.481152e-15 -1.915263e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b5d8996d0a960.final.pdb
1.390547e-15 -3.715823e-15 3.555509e-17 4.973182e-16 6.095338e-15 2.321950e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
8.790728e-17 -4.918940e-15 2.459652e-15 1.868977e-15 9.930105e-16 3.509001e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbbcad52078.final.pdb
1.970577e-16 -5.280218e-15 3.894881e-15 1.873388e-15 1.707355e-15 3.747892e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
2.738382e-16 -4.843034e-15 3.146831e-15 1.916199e-15 1.105239e-15 3.164898e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-1.209372e-16 -6.558010e-15 1.678518e-15 7.728136e-16 1.993294e-15
Supplementary Text 10

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-5.129925e-15 -6.474147e-15 -2.129400e-15  4.251329 e-15 -1.385405e-15
-8.535037e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-3.025818e-15 -5.881946e-15 -1.109731e-15  6.400040 e-15 -2.801335e-15
-1.052917e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
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-1.052917e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-6.119320e-15 -6.063510e-15 -9.131636e-15  7.306347 e-15  9.885146e-15
-9.578335e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-6.23542e-15 -7.235117e-15 -3.232859e-15  2.452273 e-15  3.154861e-15
-6.078888e-15

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.303975e-15  2.664924e-15  7.472808e-16  3.008532e-15
-9.429505e-16

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-6.329294e-16  2.203602e-15  3.717277e-16  4.641153e-16  4.524951e-15
-9.413043e-17

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-9.338604e-16  2.684626e-15  1.085207e-15  1.087635e-15  3.069812e-15
-6.005848e-16

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-5.906440e-16  3.006542e-15  1.309293e-15  3.565232e-16  3.670334e-15
-1.210599e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-4.698110e-15  2.173804e-15  9.691367e-16  4.733391e-15  4.457776e-15
7.371180e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
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-5.503058e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a5fceedb041945d.final.pdb
5.971158e-17  3.883651e-15  3.727336e-15  9.981011e-16  4.013922e-15
1.468859e-16

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-3.070909e-16 -9.747193e-16  3.561094e-16  3.578932e-15  6.76693e-15
-2.857630e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
3.849144e-15  1.714721e-16  4.295252e-15  7.790885e-16  5.571035e-15
-5.352412e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
-1.077851e-15  2.816935e-15  4.233236e-16  1.747648e-16  3.227152e-15
-4.091698e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
-4.998953e-16 -2.016455e-15  1.417671e-15  4.593674e-15  6.431419e-15
-4.428449e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb
-1.478164e-16  2.955436e-15  3.794773e-16  8.659548e-16  3.919692e-15
-7.805414e-16
Supplementary Text 10
-4.998953e-16 -2.016455e-15 1.417671e-15 4.593674e-15 6.431419e-15
-4.428449e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-3.772184e-15 1.868166e-14 -4.206039e-15 -8.291990e-15 3.169756e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
-3.087402e-15 3.572037e-15 7.167919e-15 1.237090e-14 4.332894e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
-2.801943e-15 3.926881e-15 -2.640689e-15 2.171334e-14 3.300830e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
-1.273284e-15 8.768417e-15 -4.234519e-15 -7.051793e-15 -4.762333e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-5.159930e-15 9.638211e-15 4.680295e-15 -1.060042e-14 -4.273863e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
5.349144e-15 1.714721e-16 4.295252e-15 7.790885e-15 5.571035e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\379368adbc32d5de.final.pdb
-5.352412e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
8.125157e-16 2.494460e-15 -6.932454e-16 1.077591e-15 2.768703e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb
-1.592596e-15 1.760580e-14 2.608675e-15 -2.890273e-15 -9.239405e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb
-8.313266e-15 -4.161883e-15 -7.494933e-15 2.382168e-15 4.664927e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cfd8.final.pdb
6.142725e-15 1.114680e-14 6.896820e-15 -1.099348e-14 4.049797e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb
-3.070909e-16 -9.747193e-16 -3.561994e-16 3.578932e-15 6.76693e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
-4.153986e-15 -1.812341e-15 -4.995419e-15 5.785969e-15 7.690885e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
4.265044e-15 8.040178e-15 -3.356613e-15 -5.936893e-15 -1.731284e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
3.223946e-15 7.479847e-15 4.567033e-15 1.968501e-16 4.490371e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091fe385e05fc.final.pdb
### Supplementary Text 10

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 5.971158e-17 | 3.883651e-15 | -3.727336e-15 | -9.981011e-16 | 4.013922e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dc.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff286d.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef0.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c4.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c313.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a63319.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f.final.pdb | 8.125157e-16 | 2.494460e-15 | -6.932454e-16 | 1.077591e-15 | 2.768703e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef56976.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc6.final.pdb | 3.855702e-15 | -1.184610e-15 | -3.493465e-15 | 5.494312e-15 | 1.410907e-14 |
**Supplementary Text 10**

```
-7.902039e-16  2.843798e-15 -3.331269e-16  3.213165e-16  4.020911e-15
-2.603200e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
-5.146987e-16  2.352757e-15 -3.077625e-16  9.096610e-16  4.140773e-15
-3.924988e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-7.782643e-16  2.684673e-15 -1.873821e-16  7.022554e-16  3.922358e-15
-4.830646e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-1.315780e-16  1.556927e-15 -1.479089e-15  7.164883e-16  4.515480e-15
1.893100e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-2.803848e-15  3.158996e-15 -5.345329e-16 -6.892490e-16  3.641636e-15
9.371196e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-4.153986e-15 -1.812341e-15 -4.995419e-15  5.785969e-15  7.690885e-15
2.949690e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-4.698110e-15  2.173804e-15  9.691367e-16  4.733391e-15  4.457776e-15
7.371180e-16

[,553]  [,554]  [,555]  [,556]  [,557]  [,558]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
1.783181e-15  2.324833e-15  4.198824e-15  3.456071e-15  3.759209e-15
9.999428e-16
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.177262e-16  1.814972e-15  2.529672e-15  2.426461e-15  4.358801e-15
1.852256e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
1.053028e-15  1.375240e-15  4.328539e-15  3.790954e-15  5.978728e-15
-2.323927e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
3.458719e-17  1.970729e-15  4.000716e-15  2.231746e-15  5.471897e-15
9.561468e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-3.810586e-16  2.915038e-15 -1.344613e-15  5.060719e-15  3.711611e-15
7.543661e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-1.306744e-15  1.273247e-15  3.607514e-15  2.906355e-15  2.544261e-15
3.348546e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcedeab4194d9.final.pdb
6.262265e-16  4.914433e-15  4.524121e-15  3.580135e-15  6.643957e-15
-7.322475e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59fcedeab4194d9.final.pdb
9.774641e-17  3.631045e-15  2.411714e-15  2.833767e-15  1.359326e-15
-1.443291e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
3.875107e-15 -2.765964e-15  4.116723e-16  7.399560e-16  1.237028e-15
2.343176e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
-7.065298e-16  1.669848e-15  4.164578e-15  2.638340e-15  3.004397e-15
1.454011e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
3.102145e-16  5.373005e-15 -1.869094e-15  4.715538e-15 -2.488922e-16
```
| Path                                         | Data       |
|----------------------------------------------|------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | 2.328009e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | 3.102145e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 7.553862e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -1.164008e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | -5.993022e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 7.627379e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\36342813cd3df6edd.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 3.875107e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 1.200533e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd2c9f3975403e7.final.pdb | 6.262265e-16 4.914433e-15 4.524121e-15 3.580135e-15 6.643957e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 7.051738e-16 1.321387e-15 3.510677e-15 2.847214e-15 3.034431e-15 1.146675e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 1.112696e-14 4.269590e-15 1.577821e-14 -2.736704e-15 1.180784e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.112696e-14 4.269590e-15 1.577821e-14 -2.736704e-15 1.180784e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 2.161913e-15 7.868071e-16 6.870432e-15 3.589103e-16 2.260216e-15 1.200533e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | -4.211917e-15 4.601894e-15 1.122371e-14 3.394286e-16 8.998317e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | 2.552069e-15 6.986533e-15 9.801291e-15 1.139302e-15 1.845791e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | -6.482482e-15 -6.049658e-15 2.501292e-15 9.875471e-15 1.014756e-14 1.196311e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -4.211917e-15 4.601894e-15 1.122371e-14 3.394286e-16 8.998317e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 2.552069e-15 6.986533e-15 9.801291e-15 1.139302e-15 1.845791e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e2089e10f0197e2.final.pdb | -2.545626e-15 2.075429e-15 3.772530e-15 1.447037e-15 1.912279e-15 7.507438e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 3.102145e-16 -5.373005e-15 -1.869094e-15 4.715538e-15 -2.488922e-16 2.328009e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | -3.810586e-15 2.915038e-15 -1.344613e-15 5.060719e-15 3.711611e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 7.543661e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6502082718ec3a1.final.pdb | -4.685040e-15 3.634789e-15 1.112668e-15 3.30925e-15 2.680019e-15 5.172685e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a960.final.pdb | -1.314885e-15 1.809912e-15 -5.244597e-15 4.192104e-16 -3.966285e-15 -1.989214e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | 3.804593e-15 -1.254945e-15 -8.804711e-18 2.456092e-15 5.905613e-16 4.259039e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | -4.685040e-15 3.634789e-15 1.112668e-15 3.30925e-15 2.680019e-15 |
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5.172685e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
6.262265e-16 4.914433e-15 4.524121e-15 3.580135e-15 6.643957e-15
-7.322475e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-1.050212e-15 1.150428e-15 3.321279e-15 2.479021e-15 3.251481e-15
1.173533e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
-1.142324e-15 1.445095e-15 3.536304e-15 2.815555e-15 2.246433e-15
6.446893e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-8.390398e-16 1.332677e-15 3.594431e-15 2.430907e-15 2.938662e-15
4.542908e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-2.254626e-15 2.075429e-15 3.772530e-15 1.955022e-15 3.805894e-15
7.587048e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-8.622562e-16 2.052399e-15 6.304469e-15 1.922979e-15 3.08571e-15
-1.254577e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-6.126185e-15 -2.71266e-15 -3.928658e-15 4.016418e-15 -3.286468e-15
6.309212e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa0.final.pdb
-3.810586e-15 2.915038e-15 -1.344613e-15 5.068729e-15 3.711611e-15
7.543661e-15

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E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.035561e-15 3.123533e-15 1.944256e-16 1.035845e-16 5.596453e-15
-2.817761e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-3.943712e-16 2.120548e-15 2.426646e-15 -1.246164e-15 5.987679e-15
-2.927114e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
3.173699e-16 1.478752e-15 2.553134e-15 -1.110047e-15 4.371671e-15
-3.669137e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-3.411479e-16 1.924482e-16 3.866822e-16 3.870466e-16 4.948230e-16
-3.357563e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-2.434581e-15 2.298554e-15 2.75103e-15 3.903053e-15 4.149069e-15
-9.373538e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-6.097528e-16 1.270055e-15 1.27808e-15 2.784577e-17 5.311294e-15
-2.583262e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
-1.651661e-16 -2.492474e-16 5.866262e-15 -3.858347e-15 2.581759e-15
-3.466347e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
-1.946256e-15 1.775101e-15 2.275717e-15 -2.990738e-15 -1.817512e-15
-4.722582e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-3.471837e-15 5.709020e-15 -3.515216e-15 5.633331e-15 1.264878e-14
-4.013000e-15

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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | -5.945740e-16 1.619819e-15 2.590259e-15 6.177060e-16 4.644293e-15 -2.553569e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb      | -5.078335e-15 4.970338e-15 -1.480273e-15 4.687718e-15 9.718433e-15 -1.112561e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b51be0a39.final.pdb        | -5.015120e-16 1.663772e-15 2.246740e-15 4.634853e-15 -2.381174e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\21945328d47579a.final.pdb       | 1.117814e-14 4.092846e-16 -6.488872e-15 -7.086667e-15 3.090033e-15 -4.698000e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd391854336d.final.pdb       | 3.928781e-15 6.719558e-15 -7.153271e-15 6.703029e-15 8.092108e-15 -7.879455e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb       | 1.823074e-15 1.506931e-15 2.111887e-15 -3.941583e-16 4.288293e-15 -2.122980e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcbb46e33793b0.final.pdb        | -1.03461e-15 8.007472e-16 2.370772e-15 -4.519601e-15 -6.959522e-16 -2.183416e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb      | 7.688404e-15 -8.190957e-15 7.533221e-15 -6.246181e-15 3.400531e-15 -4.739522e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb      | 7.992653e-16 -7.198235e-15 -2.246249e-15 -1.200308e-14 -2.078960e-16 -5.987638e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc3d2d5e.final.pdb       | -3.471837e-15 5.709020e-15 -3.515216e-16 5.633331e-15 1.264878e-14 -4.013000e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3d6edd.final.pdb        | -2.197313e-15 2.892824e-15 1.664740e-15 -2.579205e-15 4.290077e-15 -5.418675e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357ee6642bf12.final.pdb       | 7.931495e-15 -1.141255e-14 -3.939654e-15 -1.019323e-14 3.526370e-15 -1.334623e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb        | -9.835942e-15 1.576854e-15 4.387810e-15 4.615366e-15 8.481095e-15 -7.695378e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6bf.final.pdb       | -3.046351e-15 1.115166e-15 6.943503e-15 7.269580e-15 2.789142e-14 6.854493e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8ff113c7.final.pdb      | -1.946256e-15 1.775101e-15 2.275717e-15 -2.900738e-15 -1.817512e-15 -7.722502e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb       | -5.616697e-15 7.720710e-15 3.541299e-15 7.641081e-15 2.723573e-15 -3.406792e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb        | -6.992025e-15 -1.736413e-15 9.764092e-16 -4.282348e-15 9.398776e-15 3.723805e-16 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb  |
|---------------------------------------------------------------|
| -2.197313e-15  2.892824e-15  1.664740e-15 -2.579205e-15  4.290077e-15 |
| -5.418675e-15                                              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb  |
| -1.946256e-15  1.775101e-15  2.275717e-15 -2.990738e-15 -1.817512e-15 |
| -4.722502e-15                                              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb  |
| 5.430709e-15 -2.346312e-16  2.275717e-15 -2.990738e-15  3.542338e-15 |
| -4.859106e-15                                              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb  |
| 5.430709e-15 -2.346312e-16  2.275717e-15 -2.990738e-15  3.542338e-15 |
| -4.859106e-15                                              |

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4.851114e-15 -3.704523e-15  3.156911e-15 -5.890108e-15 -6.084350e-15 3.069157e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
8.423589e-15  5.617742e-15  1.494634e-15 -5.117482e-16 -7.484117e-15 2.747515e-15
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4.851114e-15 -3.704523e-15  3.156911e-15 -5.890108e-15 -6.084350e-15 3.069157e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
8.451560e-15 -7.103310e-15  2.044079e-15  3.718455e-16 -6.964802e-15 -1.78664e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
5.442221e-15 -1.079833e-15  2.299145e-15 -5.924857e-15 -4.090610e-15 8.944640e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
8.645118e-15  4.811746e-15 -2.656372e-15 -4.864580e-15 -9.272310e-15 -3.158077e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb
4.065695e-15 -6.885688e-15  6.435413e-15 -8.033986e-15 -5.867444e-15 -2.666274e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb
5.442221e-15 -1.079833e-15  2.299145e-15 -5.924857e-15 -4.090610e-15 8.944640e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
1.212259e-15  4.425100e-15  1.259505e-15 -1.075138e-14 -2.773844e-16 5.161886e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d07f60282718ec3a.final.pdb
| Path                                       | Data                                                                 |
|--------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceed419d9.final.pdb | 1.938672e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -6.632422e-15 -1.068861e-15 1.776834e-15 -4.300048e-15 1.648772e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 6.488444e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -7.440728e-16 4.269814e-15 3.208704e-15 2.539315e-15 1.912608e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a51b867b.final.pdb | 4.863556e-15 -1.878859e-15 3.089071e-15 -2.674446e-15 6.423983e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\19618a2a51b867b.final.pdb | -7.280383e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -2.110532e-15 -3.599138e-16 1.622379e-15 -1.419099e-15 2.568717e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551bea39.final.pdb | 1.783755e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 4.863556e-15 -1.878859e-15 3.089071e-15 -2.674446e-15 6.423983e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -7.280383e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2f4c42.final.pdb | -1.723263e-15 -1.431255e-15 6.904636e-16 -1.126588e-15 2.234241e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 1.986931e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb32871797b7ab.final.pdb | -2.007190e-15 9.528829e-16 -2.700805e-15 -1.362971e-14 3.287319e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | -2.107830e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 8.355537e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 4.266040e-15 5.342820e-16 4.920955e-15 -2.631454e-15 5.943908e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb | -2.482470e-15                                                         |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb     | -7.392932e-15 4.269814e-15 3.208704e-15 2.539315e-15 1.912608e-15 4.343667e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb     | -8.094977e-16 -6.203154e-15 1.213916e-15 8.580924e-15 5.852875e-15 -3.822861e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb      | -7.76288e-16 -1.934587e-15 9.049085e-15 3.290607e-16 2.092152e-15 -4.845163e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb      | 3.012137e-15 2.447945e-15 7.890193e-16 2.429650e-15 2.994077e-15 2.159405e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb      | -3.387438e-16 -6.091635e-15 -7.268592e-15 -3.896726e-15 5.290892e-15 -2.482470e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb      | 4.298248e-15 1.690397e-16 2.932085e-15 -2.701328e-16 1.109648e-15 -3.744587e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b9091fe385e05fe.final.pdb      | -6.632422e-15 -1.068861e-15 1.776834e-15 -4.300048e-15 1.648772e-15 6.488444e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb      | 3.012137e-15 2.447945e-15 7.890193e-16 2.429650e-15 2.994077e-15 2.159405e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb      | -2.058181e-15 5.941396e-15 2.040806e-15 -1.295576e-15 5.085125e-16 4.629120e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb       | -7.440728e-16 4.269814e-15 3.208704e-15 2.539315e-15 1.912608e-15 4.343667e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | 4.298248e-15 1.690397e-16 2.932085e-15 -2.701328e-16 1.109648e-15 -3.744587e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6b3547ea982fffc4.final.pdb      | 9.238754e-15 -2.606816e-16 -9.784486e-16 1.919544e-16 2.385852e-15 6.152410e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb      | 3.950206e-16 -4.027355e-15 2.739466e-15 -4.969524e-16 6.511523e-15 -5.054865e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e7ad0f1be4.final.pdb       | 4.298248e-15 1.690397e-16 2.932085e-15 -2.701328e-16 1.109648e-15 -3.744587e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb      | -1.179949e-15 -5.914235e-16 1.729047e-15 -1.207954e-15 2.371235e-15 1.998216e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb      | -6.632422e-15 -1.068861e-15 1.776834e-15 -4.300048e-15 1.648772e-15 1.998216e-15 |
| Path                                                                 | 9.191892e-15 | 1.608288e-15 | -1.727609e-15 | 4.108661e-15 | -1.066199e-14 | -1.153733e-15 | -2.212398e-15 | 6.488444e-15 | -1.235396e-14 | 5.108335e-18 | 4.139019e-15 | -1.375802e-15 | -3.426221e-15 | 6.103107e-15 |
|----------------------------------------------------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef27e.final.pdb  |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\be34248de3e81a3c.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb  |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d042212450d15047.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb  |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc8090eff10197e.final.pdb  |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb  |              |              |              |              |              |              |              |              |              |              |              |              |              |              |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb     | -7.284683e-16  6.718917e-15  4.103759e-16  -4.518199e-16  2.190875e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb     | -9.552062e-16  2.816582e-15  8.492317e-15  2.485330e-15  -9.146082e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a960.final.pdb      | -1.053330e-14  -1.411632e-15  1.157390e-14  -3.219652e-15  -7.685647e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb     | -1.053330e-14  -4.111632e-15  1.157390e-14  -3.219652e-15  -7.685647e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb     | -9.552062e-16  2.816582e-15  8.492317e-15  2.485330e-15  -9.146082e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a960.final.pdb      | -1.053330e-14  -1.411632e-15  1.157390e-14  -3.219652e-15  -7.685647e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb     | -1.053330e-14  -4.111632e-15  1.157390e-14  -3.219652e-15  -7.685647e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb     | -1.053330e-14  -4.111632e-15  1.157390e-14  -3.219652e-15  -7.685647e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb                                | -3.924499e-15  -6.760715e-15  2.869765e-15  -6.248980e-16  2.190875e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb                                | -4.826478e-15  -7.216106e-15  5.668369e-15  -1.240912e-15  2.190875e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                                | -4.741611e-15  -7.531237e-15  6.358379e-15  -1.33826e-15  -1.927305e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                                | -4.933986e-15  -6.291904e-15  2.470607e-15  -5.646285e-16  -1.927305e-15 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb       | 7.965842e-15 -1.333571e-14 1.333867e-15 -1.229409e-14 -2.457773e-15 -5.885455e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb       | 7.369207e-16 -1.568439e-14 -6.359161e-15 -4.755804e-16 6.937510e-15 6.167096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb       | 6.580071e-15 -3.814526e-15 -5.614235e-15 1.296167e-14 -4.052107e-15 -2.594001e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb       | 4.992296e-15 -8.291906e-15 4.436861e-15 -1.098473e-15 -2.820621e-15 -5.153915e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb       | -3.280423e-15 -5.655068e-15 6.360778e-15 -6.558309e-15 -2.442284e-15 -2.433106e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb       | 4.139239e-15 -5.701652e-15 -1.623323e-15 1.373519e-14 8.877462e-16 -4.514520e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb       | 3.592118e-15 -1.126083e-14 -2.240849e-15 -1.187606e-15 1.932255e-15 -5.204275e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f048222d30a.final.pdb      | 4.924222e-15 -3.555341e-15 -3.435343e-16 -2.325554e-16 1.454462e-15 -3.93635e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b0091fe38b505fc.final.pdb      | 6.125504e-15 -3.814526e-15 -5.614235e-15 1.296167e-14 -4.052107e-15 -2.594001e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac0f3903d2db.final.pdb       | 4.139239e-15 -5.701652e-15 -1.623323e-15 1.373519e-14 8.877462e-16 -4.514520e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb       | 5.039360e-15 -4.230172e-15 6.760937e-16 8.425387e-16 -6.798542e-15 1.966949e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\62465dd6df286d.final.pdb         | 6.580071e-15 -3.814526e-15 -5.614235e-15 1.296167e-14 -4.052107e-15 -2.594001e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ffcc87ef.final.pdb        | 5.924222e-15 -3.555341e-15 -3.435343e-16 -2.325554e-16 1.454462e-15 -3.93635e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\669760178986bef01.final.pdb      | -7.900819e-16 -1.341191e-14 -5.412585e-16 9.626142e-15 4.319144e-15 3.515953e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69a9d87d47926b1c8.final.pdb      | 4.638590e-15 -6.709780e-15 -3.006076e-15 3.565537e-15 -1.525049e-15 -1.801666e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4.final.pdb         | 2.480132e-15 -1.047948e-14 -4.516682e-15 -6.421335e-15 -7.852911e-15 7.242465e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611dc42.final.pdb        | 3.829824e-15 -1.229409e-14 -3.849149e-15 -3.676592e-15 5.331295e-15 -1.003734e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb         | 4.924222e-15 -3.555341e-15 -3.435343e-16 -2.325554e-16 1.454462e-15 -2.393635e-16 |
| File Path                                                                 | Numbers                                      |
|--------------------------------------------------------------------------|----------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | 5.233613e-15 -6.040253e-15 -4.14896e-15 2.239238e-15 -1.174023e-15 -2.042315e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | 6.125504e-15 -6.373302e-15 -5.577047e-15 6.590797e-15 -2.788962e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fa9e6e6a3f6099.final.pdb         | 9.108707e-15 -7.32273e-15 -6.449153e-16 8.264004e-16 3.373461e-19 -2.844890e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb        | 4.675177e-15 -5.136400e-15 -3.158596e-15 4.548179e-15 -4.270972e-15 -2.065902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb        | 4.675177e-15 -5.136400e-15 -3.158596e-15 4.548179e-15 -4.270972e-15 -2.065902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb        | 6.616657e-15 -1.073956e-14 -4.618583e-15 6.908270e-15 -6.947867e-15 -1.935364e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb         | 6.580071e-15 -3.814526e-15 -5.614235e-15 1.296167e-14 -4.052107e-15 -2.594001e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb        | 4.924222e-15 -3.555341e-15 -3.453533e-16 -2.325554e-16 1.454462e-15 -2.393635e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb        | 4.323895e-15 -6.119989e-15 -3.852486e-15 3.139583e-15 -1.626169e-15 -1.492576e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb         | 3.512173e-16 -1.626515e-16 -7.470702e-15 1.346389e-16 -2.529855e-15 4.175298e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b9be0d5986c1388f.final.pdb        | 6.125504e-15 -6.373302e-15 -5.577047e-15 6.590797e-15 -2.788962e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb         | 9.382782e-15 -4.180134e-15 -6.950485e-15 5.851390e-15 5.475138e-15 -3.984506e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9da8ed0d81fb3ef.final.pdb          | 1.012471e-14 -1.514850e-14 -3.928334e-16 -5.752717e-16 -7.786844e-15 -8.742978e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616ed0633b.final.pdb        | 5.082294e-15 -5.221371e-15 -6.903309e-15 7.234986e-15 -1.678124e-15 1.796473e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb         | 4.139239e-15 -5.701652e-15 -1.623323e-15 1.373519e-15 8.877462e-16 -4.514520e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb         | 9.495872e-15 -1.714252e-14 -2.768856e-15 4.203451e-15 -2.482457e-15 -1.027752e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a8039a2d823c616.final.pdb          | 4.694483e-15 -6.110978e-15 -4.324469e-15 -2.101194e-16 -4.430729e-16 -1.783447e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb          | 4.675177e-15 -5.136400e-15 -3.158596e-15 4.548179e-15 -4.270972e-15 -2.065902e-15 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb       | 4.936875e-15 -6.577254e-15 -4.168841e-15 4.522693e-15 -8.937528e-16 -1.930400e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababdb03b7b857.final.pdb      | 9.382782e-15 -4.180134e-15 -6.950485e-15 5.851390e-15 5.475138e-15 -3.984506e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb       | 1.072197e-16 -1.347579e-14 -1.028466e-14 5.95573e-15 -1.607325e-15 -3.099055e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb        | 6.125504e-15 -6.373302e-15 -5.77047e-15 6.590797e-15 -2.789626e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | 2.404644e-15 -2.128965e-15 -1.201179e-14 1.735055e-15 7.018087e-16 -5.151667e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb       | 6.125504e-15 -6.373302e-15 -5.77047e-15 6.590797e-15 -2.788962e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb        | 4.323895e-15 -6.11989e-15 -3.852486e-15 3.139583e-15 -1.621699e-15 -1.492576e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb        | 6.125504e-15 -6.373302e-15 -5.77047e-15 6.590797e-15 -2.788962e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb        | 6.125504e-15 -6.373302e-15 -5.77047e-15 6.590797e-15 -2.788962e-15 -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb        | 4.575745e-15 -6.814356e-15 -3.252951e-15 2.792186e-15 -1.375813e-15 -1.852737e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac066e4f4ef427e.final.pdb       | 1.747180e-15 1.396135e-15 -4.685803e-15 4.399199e-16 9.860953e-15 -1.554592e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ba21f55fc9d0681.final.pdb         | 4.323895e-15 -6.119989e-15 -3.852486e-15 3.139583e-15 -1.621699e-15 -1.492576e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b92cb2f3975403e7.final.pdb        | 4.323895e-15 -6.119989e-15 -3.852486e-15 3.139583e-15 -1.621699e-15 -1.492576e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb        | 2.444809e-15 -6.00639e-15 2.701734e-15 -4.532223e-15 1.917034e-15 -1.347150e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249461.final.pdb         | 1.454219e-15 -2.279789e-15 4.515506e-16 4.369917e-15 3.609349e-15 8.213430e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb        | 6.066690e-15 -4.152090e-15 -2.161793e-15 1.781777e-15 -1.091209e-15 -1.095629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb        | 8.175079e-15 -1.037141e-14 -7.640267e-15 3.193952e-15 -7.595925e-15 4.251026e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40afef0e9e39.final.pdb        | 9.049500e-15 -6.098871e-15 -9.248123e-15 1.143032e-14 -3.472905e-15 4.279293e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb        | 9.321179e-15 9.737226e-16 -3.823934e-15 1.367960e-14 1.851909e-15 -4.802763e-15 |
| Supplementary Text 10 |
|-----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb |
| 5.475972e-15 3.636389e-15 -1.770516e-14 2.278419e-14 1.493059e-15 |
| 2.008226e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb |
| -4.756869e-16 -9.370055e-15 -4.703157e-15 -2.298152e-16 -2.114460e-15 |
| -1.048752e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb |
| 3.958470e-15 -7.817401e-15 -1.748404e-15 -3.486982e-15 -9.762256e-16 |
| -2.756198e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb |
| 4.675177e-15 -5.136400e-15 -3.158956e-15 4.548179e-15 -4.270972e-15 |
| -2.065902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb |
| 5.073192e-16 -5.459770e-15 3.104821e-15 6.478948e-15 -3.574865e-15 |
| -3.678180e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb |
| 4.139239e-15 -5.701652e-15 -1.623323e-15 1.373519e-15 8.877462e-16 |
| -4.514520e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb |
| 4.675177e-15 -5.136400e-15 -3.158956e-15 4.548179e-15 -4.270972e-15 |
| -2.065902e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb |
| 6.125504e-15 -6.373302e-15 -5.770477e-15 6.590797e-15 -2.788962e-15 |
| -3.121687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb |
| 4.557436e-15 -5.963137e-15 -4.139186e-15 4.841511e-15 -9.962687e-16 |
| -1.751609e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb |
| 4.692839e-15 -6.558050e-15 -3.410378e-15 3.322578e-15 -1.379933e-15 |
| -1.776842e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb |
| 4.773912e-15 -6.113111e-15 -4.246274e-15 1.163706e-15 -1.069506e-15 |
| -1.870143e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb |
| 6.606690e-15 -4.152909e-15 -2.161703e-15 1.781777e-15 -1.091209e-15 |
| -1.095629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb |
| 5.082294e-15 -5.221371e-15 -6.903309e-15 7.234986e-15 -1.678124e-15 |
| 1.796473e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb |
| 4.992296e-15 -8.291906e-15 4.436861e-15 -1.098473e-15 -2.820621e-15 |
| -5.153915e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb |
| 3.958470e-15 -7.817401e-15 -1.748404e-15 -3.486982e-15 -9.762256e-16 |
| -2.756198e-15 |

| ,583 | ,584 | ,585 | ,586 | ,587 | ,588 |
|------|------|------|------|------|------|
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb |
| -2.771174e-15 1.731720e-15 7.630072e-16 6.153774e-16 5.016277e-16 1.977820e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb |
| -1.069997e-15 2.979317e-15 -7.796672e-17 6.549207e-15 -1.344255e-15 1.312452e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb |

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The table below contains information related to some pdb files. The values are statistical measures, possibly representing distances or other metrics in a biological context.

| PDB File                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | 5.405586e-15                                                          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fff622872.final.pdb       | -9.224266e-15 -1.407986e-15 5.818553e-16 6.776309e-16 5.419725e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | -3.880478e-15 6.036260e-16 2.432381e-15 9.005341e-15 2.009651e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -5.329967e-15 5.351605e-15 8.204381e-15 1.720125e-14 4.246014e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | -3.659739e-15 3.743530e-15 1.233690e-15 1.036209e-14 8.693127e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12df39.final.pdb       | -7.176481e-16 9.161749e-15 2.716784e-15 9.660397e-15 2.717444e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | 4.195185e-16 1.341105e-15 7.160026e-16 7.482661e-15 1.83514e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb       | 2.139441e-15 -1.052465e-15 7.005887e-15 1.452875e-15 5.550899e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb       | 1.234783e-15 -6.515817e-16 -6.302978e-15 8.631706e-16 3.617332e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb       | 6.426453e-16 -7.101721e-16 -3.350456e-15 1.041697e-14 3.539622e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb       | 2.661027e-15 3.848993e-16 2.755325e-15 4.650996e-15 -7.083481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac088ed0d81fb3ef.final.pdb       | 8.533926e-15 8.715210e-15 5.915064e-15 4.023045e-15 5.369824e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\af752b3616e6033b.final.pdb       | -3.039525e-15 3.222619e-15 1.883103e-15 6.710711e-15 3.685007e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | 2.661027e-15 3.848993e-16 -2.755325e-15 4.650996e-15 -7.083481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb       | 2.661027e-15 3.848993e-16 2.755325e-15 4.650996e-15 -7.083481e-15 |
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```
-2.210692e-15  1.588587e-14  7.313110e-15  1.660678e-14 -1.457913e-15
-1.013177e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb

1.353418e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb

-3.188640e-15 -8.476652e-15 -3.090070e-15  1.279905e-14 -3.117324e-15
-1.013177e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb

6.525288e-15  7.882217e-15  7.089792e-15  1.475968e-14 -2.899285e-16
6.040090e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb

2.089108e-15  9.465749e-15 -2.222278e-15 -2.260900e-15 -5.077357e-15
6.339524e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb

-5.806404e-15  2.641172e-15 -4.562002e-15  1.075088e-14 -6.559533e-15
2.537136e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb

3.565968e-15  2.636555e-16 -2.911656e-15  1.148562e-14  6.139175e-15
2.537136e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6163918d3707839.final.pdb

3.848993e-16 -2.755325e-15  4.650996e-15 -7.083481e-15
2.515269e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e659739e-15  3.743530e-15  1.233690e-15  1.036209e-14 -8.693127e-16
2.399639e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e804b9545899c29d.final.pdb

-3.023959e-15  3.576942e-15  9.657809e-16  6.066720e-15 -7.147327e-16
1.835662e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e893584e22003fb92.final.pdb

-1.517324e-15  3.095302e-15  5.666494e-16  6.254767e-15  2.710377e-16
1.187390e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb

-3.023959e-15  3.576942e-15  9.657809e-16  6.066720e-15 -7.147327e-16
1.835662e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb

-3.023959e-15  3.576942e-15  9.657809e-16  6.066720e-15 -7.147327e-16
1.835662e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb

-2.398325e-15  3.685617e-15  8.579834e-16  7.030791e-15  8.525349e-16
3.358681e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e2bf87e52caa29.final.pdb

-3.023959e-15  3.576942e-15  9.657809e-16  6.066720e-15 -7.147327e-16
1.187390e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb

-3.023959e-15  3.576942e-15  9.657809e-16  6.066720e-15 -7.147327e-16
1.187390e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb

-2.927681e-15  1.863060e-14  2.533110e-16  1.217300e-15  3.014489e-15
1.266259e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb

-5.806404e-15  2.641172e-15 -4.562002e-15  1.075088e-14 -6.559533e-15
2.527223e-15

[,589]      [,590]      [,591]      [,592]      [,593]      [,594]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.536767e-15 -3.137635e-15  9.744995e-16 -2.473478e-15  1.014024e-15
```

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-4.252926e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-2.826937e-15 -2.942851e-15 1.765914e-15 -4.224957e-15 3.121494e-16
-4.645546e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-2.474076e-15 -3.511157e-15 -1.575482e-15 -3.782453e-15 -1.440360e-15
-6.878457e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
1.178947e-16 -4.837187e-15 -2.406787e-16 -3.698656e-15 1.084301e-15
-4.063157e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
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-1.176686e-14
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-3.037718e-15 -3.691858e-15 1.150731e-15 -3.598690e-15 -1.514956e-16
-7.642385e-15
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-6.770266e-15 -2.645935e-15 -3.308072e-15 -2.963108e-15 3.230069e-15
-7.642385e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
-3.801253e-15 -5.305514e-15 3.666880e-15 -4.226969e-15 -4.586947e-15
-2.676913e-15
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-1.733462e-15 -8.439726e-15 2.096467e-15 -4.926657e-15 -3.913468e-15
1.460403e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
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-4.396069e-15
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9.555663e-16
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-4.734319e-15
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9.555663e-16
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-6.079399e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
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7.961772e-16
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-4.713305e-15
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-8.418871e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb32871977b7ab.final.pdb
-8.780107e-15 -3.564927e-16 -2.124596e-16 -6.832803e-15 8.078386e-15
-7.187898e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871977b7ab.final.pdb
-1.004690e-14 -8.932337e-15 1.844297e-15 2.122581e-15 5.969868e-15

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-1.176686e-14

[,595] [,596] [,597] [,598] [,599] [,600]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
1.908812e-15 -1.712480e-15 3.283681e-15 1.495863e-15 6.629299e-16
7.982959e-16
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
7.593686e-16 -1.522591e-15 3.079099e-15 1.038022e-15 4.900375e-16
5.480986e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
1.021517e-15 -3.512149e-15 3.889682e-15 8.102555e-16 6.405374e-16
1.951216e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
9.077931e-16 -2.952804e-15 3.856814e-15 8.207561e-16 1.073902e-15
6.564357e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
1.577290e-15 7.398482e-16 6.199192e-15 3.621939e-16 3.933626e-15
3.303541e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
5.749830e-16 -2.313435e-15 3.261967e-15 1.429965e-15 5.800679e-16
7.498758e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
1.503743e-15 -4.415744e-15 7.299234e-15 3.941409e-15 9.843088e-16
2.635823e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e.final.pdb
1.657521e-15 -8.037853e-15 1.107778e-15 4.607496e-16 -9.880489e-16
1.751838e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a708b57339c.final.pdb
-4.470513e-16 -5.892000e-15 -6.730136e-15 -2.342257e-15 -2.372358e-15
3.079328e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
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1.104577e-15 5.777882e-15 -6.090570e-15 -3.655476e-15 -2.257563e-15
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1.225800e-15 -3.455397e-15 2.640402e-15 1.127466e-15 5.631410e-16
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-5.558642e-15 -3.284704e-15 5.764438e-15 2.015216e-15 3.641471e-15
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8.284748e-16 -2.925616e-15 3.183169e-15 1.422916e-15 3.765050e-16
7.718563e-16
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5.220125e-16 -6.659621e-16 6.682308e-15 -7.556517e-17 1.272643e-15
-8.468517e-16

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-4.907443e-15 2.527487e-15 1.014852e-14 2.664002e-15 1.903929e-15
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-1.648542e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d0678141e4018054a.final.pdb
-2.392713e-15 6.182588e-15 6.930152e-15 -3.791003e-15 -2.834208e-15
6.680266e-15

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1.844126e-15

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-8.468517e-16

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6.345963e-16

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7.003962e-16

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-1.648542e-16

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-2.414434e-17

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2.627856e-15 -1.336847e-15 -2.279578e-15 -4.428780e-15 -2.546729e-15
2.424711e-15

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-3.018774e-15

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-1.911999e-15

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-2.143250e-15

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|-----------------------------------------------|---------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -2.267334e-15 -5.380324e-16 -1.759323e-15 3.327924e-16 -1.108190e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 1.785347e-15 -8.038821e-16 3.693234e-16 -7.295253e-15 4.536470e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -4.985835e-15 -4.411279e-15 -2.012214e-15 6.3690825e-15 7.187112e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4.final.pdb | -2.267334e-15 -5.380324e-16 -1.759323e-15 3.327924e-16 -1.108190e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 1.785347e-15 -8.038821e-16 3.693234e-16 -7.295253e-15 4.536470e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -4.985835e-15 -4.411279e-15 -2.012214e-15 6.3690825e-15 7.187112e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4.final.pdb | -2.267334e-15 -5.380324e-16 -1.759323e-15 3.327924e-16 -1.108190e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 1.785347e-15 -8.038821e-16 3.693234e-16 -7.295253e-15 4.536470e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -4.985835e-15 -4.411279e-15 -2.012214e-15 6.3690825e-15 7.187112e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4.final.pdb | -2.267334e-15 -5.380324e-16 -1.759323e-15 3.327924e-16 -1.108190e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 1.785347e-15 -8.038821e-16 3.693234e-16 -7.295253e-15 4.536470e-16 |

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Supplementary Text 10

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-2.440541e-15

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-2.384431e-15

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-2.945268e-15

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-2.067004e-16

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-4.367229e-15

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-2.206439e-15

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-1.761748e-15

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-2.502680e-15

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| File Path                                                                 | Values          |
|---------------------------------------------------------------------------|-----------------|
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb       | -1.900390e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4a3.final.pdb        | -6.504922e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb       | 2.682796e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb       | -8.679516e-16   |
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb                                 | 4.067712e-15    |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb                                 | 3.559076e-15    |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                                 | 2.826139e-15    |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                                 | 2.612926e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb      | 8.227777e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb      | 2.068406e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceaadb4194d9.final.pdb     | 4.401268e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb      | -4.389017e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a70b57339c.final.pdb      | 3.293764e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | 1.952667e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb      | 3.293764e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb      | 2.395951e-15    |

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[]
| File Path                                                                 | Numbers                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb      | 4.401268e-15 -7.174095e-16 -2.289258e-15 -3.523123e-15 -6.385574e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb      | 2.460546e-15 -1.929548e-15 -1.617486e-15 -3.629375e-15 -2.999177e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | -1.909199e-15 3.894499e-15 2.375153e-16 -6.545948e-16 -7.719204e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | -1.687588e-15 8.284855e-18 -6.167493e-15 -5.971170e-15 -6.659729e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 6.071608e-15 -4.199657e-16 -6.011277e-15 -4.109029e-15 -1.735263e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697722494a61.final.pdb       | 2.669881e-16 1.265813e-15 2.160741e-15 -1.266573e-15 -2.945184e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 1.953324e-15 -2.531781e-15 -1.157626e-15 -2.833361e-15 -3.132318e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | -1.675397e-15 -6.575163e-15 4.835826e-15 -8.427040e-15 -3.268463e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb       | 6.094829e-15 -5.165791e-16 4.954250e-15 -7.023425e-15 -4.159948e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb        | 8.980078e-16 3.498063e-15 -3.048563e-15 -3.781440e-15 -9.047020e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\de78141e4018054a.final.pdb       | -3.206852e-15 6.424892e-15 -7.212164e-15 -2.773767e-15 7.602471e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb       | 3.293764e-15 5.606486e-16 -1.440364e-15 -4.758764e-15 2.817576e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feaa2.final.pdb       | 8.227777e-15 -2.946128e-15 4.171061e-15 -1.949405e-15 -8.296747e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb        | 5.977287e-15 -1.459291e-15 -2.455185e-15 -3.614114e-15 -3.922552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996da0a960.final.pdb       | -3.206562e-15 -2.615219e-15 -1.841775e-16 -4.406704e-15 1.809010e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb        | 1.730917e-15 -4.680879e-16 -2.994847e-15 -5.416801e-15 1.010038e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb        | 5.977287e-15 -1.459291e-15 -2.455185e-15 -3.614114e-15 -3.922552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e517be32db050e.final.pdb         | 4.401268e-15 -7.174095e-16 -2.289258e-15 -3.523123e-15 -6.385574e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb       | 5.977287e-15 -1.459291e-15 -2.455185e-15 -3.614114e-15 -3.922552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996da0a960.final.pdb       | -3.206562e-15 -2.615219e-15 -1.841775e-16 -4.406704e-15 1.809010e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5b9e19ad281feaa2.final.pdb       | 8.227777e-15 -2.946128e-15 4.171061e-15 -1.949405e-15 -8.296747e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb        | 5.977287e-15 -1.459291e-15 -2.455185e-15 -3.614114e-15 -3.922552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996da0a960.final.pdb       | -3.206562e-15 -2.615219e-15 -1.841775e-16 -4.406704e-15 1.809010e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5b9e19ad281feaa2.final.pdb       | 8.227777e-15 -2.946128e-15 4.171061e-15 -1.949405e-15 -8.296747e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e517be32db050e.final.pdb         | 4.401268e-15 -7.174095e-16 -2.289258e-15 -3.523123e-15 -6.385574e-15 |

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-4.410820e-15  -5.954251e-15  4.824035e-15  2.286123e-15  3.501882e-15
-2.198154e-15

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-2.979942e-16  -2.189803e-15  6.249064e-16  -1.103173e-15  4.684642e-15
9.584484e-16

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7.744526e-15

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-2.198154e-15

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1.553840e-15

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-1.026075e-15

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-1.149326e-15

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7.242310e-15

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3.997231e-15

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-6.223875e-16  2.012347e-15  -4.359388e-15 -5.699214e-15  2.075835e-15
-3.816255e-15

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-1.037825e-14

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6.811405e-15

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-2.354459e-15

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7.003040e-15

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1.552851e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | \(4.441798\times 10^{-15} -7.685553\times 10^{-15} 5.180384\times 10^{-15} 5.183651\times 10^{-15} 9.192491\times 10^{-15} 5.914572\times 10^{-15}\) |
|---|---|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | \(-1.225384\times 10^{-15} 9.016669\times 10^{-16} -2.288276\times 10^{-15} -4.748564\times 10^{-15} 6.422113\times 10^{-15} -1.091288\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | \(2.321951\times 10^{-15} -4.704806\times 10^{-16} 4.456163\times 10^{-15} -2.521777\times 10^{-16} 2.693213\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | \(2.177590\times 10^{-15} -3.597711\times 10^{-15} 8.094514\times 10^{-15} 2.381914\times 10^{-16} 8.036308\times 10^{-16} -2.391950\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | \(-3.198093\times 10^{-15} -1.549461\times 10^{-15} -1.635327\times 10^{-15} -3.226764\times 10^{-15} 2.201530\times 10^{-15} -3.544599\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | \(4.441798\times 10^{-15} -7.605553\times 10^{-15} 5.180384\times 10^{-15} 5.183651\times 10^{-15} 9.192491\times 10^{-15} 5.914572\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | \(-3.399404\times 10^{-16} -9.188811\times 10^{-15} 7.329242\times 10^{-15} 7.683645\times 10^{-15} -1.14803\times 10^{-15} 2.166707\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | \(-5.430414\times 10^{-16} -2.217980\times 10^{-15} 1.071709\times 10^{-15} -2.830472\times 10^{-16} 4.218796\times 10^{-15} 1.919032\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | \(-3.393366\times 10^{-15} -4.827774\times 10^{-15} -7.711419\times 10^{-15} 3.00630\times 10^{-15} 4.125355\times 10^{-15} 7.239993\times 10^{-15}\) |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611dic42.final.pdb | \(-2.986816\times 10^{-15} 1.895470\times 10^{-15} -4.695470\times 10^{-15} -5.437379\times 10^{-15} 3.398345\times 10^{-15} -1.091288\times 10^{-15}\) |
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-2.986816e-15  1.895470e-15 -4.695491e-15 -5.437379e-15  3.398345e-15
-1.026075e-15

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1.590340e-15

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3.540972e-15

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-3.698859e-15

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-6.360341e-16 -4.839486e-15  2.963083e-15  5.421992e-15 -3.422015e-16
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| File Path                                      | Values                                      |
|-----------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -2.323074e-15                             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -2.406447e-15  -4.503416e-15  3.470426e-15  9.605013e-15  5.446634e-16  -1.020063e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -2.762188e-15  1.798076e-16  2.249412e-16  3.121370e-15  1.827825e-15  1.430641e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -2.406447e-15  -4.503416e-15  3.470426e-15  9.605013e-15  5.446634e-16  -1.020063e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | -4.422453e-15  1.001939e-14  -3.867918e-15  -5.955205e-15  -5.569813e-15  3.948058e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -1.144212e-14  -1.987498e-15  -2.588342e-15  2.120366e-15  4.352155e-15  1.957896e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | -2.887548e-15  5.582090e-16  1.193355e-15  3.048877e-15  1.408113e-15  1.661692e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fc3b46e33793b0.final.pdb | -1.923883e-15  2.287497e-15  2.506103e-15  4.140520e-15  3.264217e-16  5.466475e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -5.690659e-15  7.683960e-15  -7.449688e-15  -8.357026e-15  6.482185e-16  5.689662e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 5.546263e-15  7.567434e-15  2.561487e-15  5.655520e-16  -9.942783e-17  -4.041897e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -6.360341e-16  -4.839486e-16  2.963083e-15  5.421992e-15  -3.422015e-16  -2.323074e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 1.740070e-15  -1.568794e-15  5.207718e-15  6.214382e-15  -3.143459e-15  7.191224e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | -2.615419e-15  9.131771e-15  -7.189561e-15  -1.058650e-14  -1.519802e-15  6.007584e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 2.045177e-15  -1.859532e-14  4.825829e-15  8.904813e-15  -1.19538e-16  -1.615446e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdff.final.pdb | -9.637331e-15  -2.165539e-15  3.150552e-15  5.720853e-15  8.220281e-15  -3.144906e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -1.669712e-15  2.808910e-15  -5.326817e-16  2.714089e-15  1.458008e-15  3.158738e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -1.074112e-14  -1.189450e-14  1.542503e-14  1.378768e-14  -2.618614e-15  -5.205982e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 3.335264e-15  7.804914e-15  1.004596e-14  1.371413e-15  2.586879e-15 |
Supplementary Text 10

-2.230365e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
-5.790481e-15 -3.582502e-15  2.831029e-15  9.718387e-15  2.371252e-15
4.243576e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea0f8694090cae7.final.pdb
-1.923883e-15  2.287497e-15  2.506103e-15  4.140520e-15  3.264217e-16
5.466475e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
-1.619357e-15 -3.112446e-15 -6.183282e-16  3.411718e-15
2.885973e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-2.851513e-15 -1.621437e-16  2.886595e-16  3.195838e-15  1.702373e-15
2.365744e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee682cbcad52078.final.pdb
-3.038578e-15  6.406084e-16  1.054360e-15  3.313423e-15  1.459287e-15
1.913788e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-3.086567e-15 -6.09631e-16  3.537786e-16  3.118882e-15  1.695869e-15
1.913788e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fca8deec4fa3.final.pdb
-1.903227e-15  2.480457e-16 -1.117745e-15 -3.119201e-16  1.862642e-15
-6.768267e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-1.074112e-15 -1.189450e-14  1.542503e-14  1.378768e-14 -2.618614e-15
-5.205902e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-8.106838e-15 -3.630384e-15  3.517978e-15  1.059407e-14  3.907437e-15
1.021247e-14
[,631]        [,632]        [,633]        [,634]        [,635]        [,636]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
3.845779e-15  1.801813e-15  3.074905e-15 -1.032279e-15  1.859780e-15
-2.664911e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.138492e-15  8.814888e-16  1.908498e-15 -1.549908e-16 -3.397431e-16
-7.590069e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
1.869905e-15 -5.505726e-17  1.895698e-15 -2.137747e-15  2.062978e-15
-1.694605e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
3.503141e-15  1.204684e-15  2.930986e-15 -9.294519e-16  1.146189e-15
-1.957083e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-1.758093e-15 -3.928847e-15 -6.538384e-15 -1.056556e-15 -6.352853e-15
2.902716e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
2.299450e-15  1.462433e-15  1.741317e-15 -9.704817e-16  1.606868e-15
-5.963963e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
1.633243e-15  1.790269e-15  7.667822e-16  3.672184e-16 -6.464781e-16
-7.297213e-15
| File Path                                      | Supplementary Text 10 |
|-----------------------------------------------|------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcede0194d9.final.pdb | -4.750487e-15 1.483998e-15 -2.490598e-15 5.595815e-15 5.926157e-15 3.397810e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dbaf5903306825e8.final.pdb | -2.590820e-15 -1.662939e-16 -1.640719e-15 6.524964e-15 6.711515e-15 1.425315e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a785b73839c.final.pdb | -8.437705e-15 -2.067117e-15 -5.443016e-15 1.039253e-14 4.839965e-15 1.070825e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e3427b706.final.pdb | -5.096565e-15 1.755699e-15 -2.052580e-15 5.965311e-15 5.543109e-15 3.260984e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -1.151961e-14 7.437272e-15 -8.526448e-15 5.281628e-15 5.496133e-15 9.214410e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598964edeb2.final.pdb | -4.882933e-15 1.698879e-15 -2.954207e-15 5.698059e-15 5.157021e-15 3.136681e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551be0a39.final.pdb | -1.151961e-14 7.437272e-15 -8.526448e-15 5.281628e-15 5.496133e-15 9.214410e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | -6.609230e-15 -1.061833e-14 -1.711057e-14 5.293988e-15 6.921435e-15 1.609796e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -1.041782e-14 -1.370518e-15 -1.091218e-14 1.208196e-14 1.260992e-14 1.301415e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027899e2fdc42.final.pdb | -4.355824e-15 1.873198e-15 -1.805536e-15 5.966193e-15 6.316234e-15 3.357713e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -2.549730e-15 2.997320e-15 -1.955006e-15 2.596373e-15 5.683509e-15 1.040268e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\3eb328251842006.final.pdb | -7.108202e-15 3.512017e-15 4.506145e-15 2.647673e-15 1.540616e-14 5.294474e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797bac.final.pdb | 2.878609e-15 9.159736e-15 7.467533e-15 -1.360855e-15 1.879224e-15 1.054786e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | -8.437705e-15 -2.067117e-15 -5.443016e-15 1.039253e-14 4.839965e-15 1.070825e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6ed3.final.pdb | -5.956055e-15 -2.163049e-15 -6.680580e-16 4.083898e-15 7.957515e-15 1.103618e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf15.final.pdb | -4.269703e-15 -2.200099e-15 -6.187461e-15 1.160725e-14 5.305526e-15 2.738774e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7f6f8c.final.pdb | -1.127543e-14 2.104216e-14 -2.527968e-15 3.916174e-16 3.298100e-15 6.676187e-16 |
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-1.715652e-15 -3.022082e-15 -3.885234e-15  2.988730e-15  6.865689e-15 -7.544506e-15 
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-6.840179e-15 -4.172390e-16 -6.089548e-15  7.683993e-15  4.864358e-15 -8.910590e-16 
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-1.034171e-15 -4.082712e-15 -4.371111e-15  5.122208e-15  4.121226e-15  3.921960e-15 
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
-2.683117e-15  2.085051e-15  1.339952e-15  8.000157e-15  6.087846e-15 -8.910590e-16 
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-6.840179e-15 -4.172390e-16 -6.089548e-15  7.683993e-15  4.864358e-15 -8.910590e-16 
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-9.476308e-15  5.276754e-15 -2.595982e-15  3.612159e-15  7.626620e-15 -1.877484e-15 
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-5.727570e-15  1.545580e-15  2.822076e-17  3.763947e-15  5.401620e-15 -1.152472e-14 
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
-1.921718e-15 -2.553167e-15  7.855193e-16  3.484690e-15  3.434869e-15  1.034171e-15 
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | -5.903152e-15 |
|-------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb | -4.739369e-15 | -1.058516e-14 | -4.675065e-15 | 1.107940e-14 | 1.084724e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -1.677439e-15 | -6.284949e-15 | -1.417239e-15 | 4.322831e-15 | -6.664397e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -4.839087e-15 | -9.872978e-15 | 6.520790e-15 | 7.980672e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -5.348114e-15 | -1.218127e-14 | 1.288035e-14 | 7.160835e-15 | -1.239317e-14 | -1.342407e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | -8.224944e-16 | -2.396660e-15 | -6.118119e-15 | 9.675896e-15 | 1.944220e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 5.679524e-15 | -4.525072e-15 | 1.245702e-14 | 1.220975e-14 | -3.021477e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | -8.224944e-16 | -2.396660e-15 | -6.118119e-15 | 9.675896e-15 | 1.944220e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | -1.969513e-15 | -8.558325e-15 | -4.541914e-15 | 5.355257e-15 | 3.592639e-15 | 9.574218e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | -1.677439e-15 | -6.284949e-15 | -1.417239e-15 | 4.322831e-15 | -6.664397e-16 | 4.068879e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 1.161216e-16 | -8.827017e-15 | -1.424194e-15 | 7.100380e-15 | -3.870031e-15 | 3.394145e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -2.254751e-16 | -6.825749e-15 | -2.447665e-15 | 6.949419e-15 | -2.064627e-15 | 1.938639e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | 2.439024e-15 | -5.196769e-15 | -2.215259e-15 | 8.912017e-15 | 2.086362e-15 | 1.272108e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | 7.355789e-17 | -7.884988e-16 | 2.795967e-15 | 9.639265e-15 | -2.105927e-15 | 4.711620e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad6f1be4.final.pdb | 1.161216e-16 | -8.827017e-15 | -1.424194e-15 | 7.100380e-15 | -3.870031e-15 |
Supplementary Text 10

3.394145e-15
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1.815750e-17 -6.961512e-15 -2.063832e-15 6.692462e-15 -2.330431e-15
2.325120e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
-4.031140e-15 -9.201640e-15 -7.251496e-16 3.705589e-15 -1.160436e-15
-2.556605e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
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4.535292e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
-4.292662e-15 -5.648293e-15 6.405121e-15 4.103079e-15 -3.600684e-15
1.287940e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb
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1.287940e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
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4.080844e-15
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3.394145e-15
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1.738095e-15
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-4.031140e-15 -9.201640e-15 -7.251496e-16 3.705589e-15 -1.160436e-15
-2.556605e-15
Supplementary Text 10

1.287940e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
4.481940e-16 -6.680311e-15 -1.991375e-15 6.737231e-15 -2.358199e-15
2.189137e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
3.365274e-15 -5.056319e-15 -1.563107e-14 7.975850e-15 5.678352e-15
9.271137e-15
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3.463271e-15 7.41622e-17 -5.356812e-15 3.548750e-15 -4.742724e-15
4.990090e-15
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-2.556605e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
-3.474322e-15 -7.906746e-15 -3.870154e-15 9.886671e-15 3.509355e-15
2.374127e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
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-2.556605e-15
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-8.162766e-16 -8.782505e-15 -7.802264e-15 8.904577e-15 3.636583e-15
1.825704e-15
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-4.031140e-15 -9.201640e-15 -7.251496e-16 3.705589e-15 -1.160436e-15
-2.556605e-15
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4.727314e-15
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-7.415883e-15 -1.378863e-14 -7.258213e-15 1.325446e-14 -2.687345e-16
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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|                                                                      |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb      | -2.50306e-15, 7.772192e-16, 3.449154e-15, 1.181459e-16, 7.608149e-15, 1.376418e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | -1.129284e-15, -6.803594e-15, -1.856321e-15, 2.387736e-15, -4.805249e-15, -1.061657e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | -3.612908e-15, 7.626607e-16, 3.444180e-15, -4.238736e-15, 2.123531e-15, -6.618891e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | -3.073586e-15, 7.546107e-16, 7.906893e-15, -1.850723e-15, 7.061375e-16, -9.447714e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb        | 3.024298e-15, -2.964695e-16, 1.389958e-14, 2.089782e-15, 8.809560e-15, -3.146303e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -1.618049e-16, 2.566689e-15, 5.431862e-15, -4.039271e-16, 2.120373e-15, -1.037803e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | -1.618049e-16, 2.566689e-15, 5.431862e-15, -4.039271e-16, 2.120373e-15, -1.037803e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcefe123df9.final.pdb      | -2.684960e-15, 4.059852e-15, 5.365943e-15, -1.565347e-15, 1.023259e-14, -8.806636e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | -6.107010e-15, 3.725461e-15, 4.537203e-16, -1.949432e-16, -2.014208e-15, -8.695552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | -1.129284e-15, -6.003594e-15, -1.856321e-15, 2.387736e-15, -4.805249e-15, -1.061657e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb       | -6.871715e-15, -6.789788e-16, 1.057757e-15, -4.478793e-15, 1.045712e-15, -1.772064e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb        | -7.848726e-15, -3.782535e-15, 6.608198e-15, 1.562525e-15, -1.756629e-15, -1.372687e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb       | -3.073586e-15, 7.546107e-16, 7.906893e-15, -1.850723e-15, 7.061375e-16, -9.447714e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb       | -1.034593e-14, 8.662290e-15, 9.870668e-16, 2.350368e-15, -2.815565e-15, -8.334704e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb        | -4.857638e-15, -1.219227e-15, -2.466878e-15, -1.524007e-14, 8.677307e-16, -1.179434e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f572b36166033b.final.pdb        | -2.769403e-15, 6.859699e-16, 6.303326e-15, 1.575369e-15, 2.079372e-15, -5.694067e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | -4.284558e-15, 4.629760e-15, -3.743916e-15, -3.054581e-15, -3.195298e-16, -7.331291e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb       | 5.055702e-16, -2.267487e-15, -1.323749e-15, -1.100327e-15, -2.851643e-15, -6.144955e-15 |
Supplementary Text 10

1.240934e-15  1.458725e-15 -1.108922e-15  3.780482e -15 -4.308912e-16
-4.069836e-16 
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb

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-9.407860e-16 
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-1.592985e-15 
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb

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1.107162e-15 
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-1.273719e-15 
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-9.806513e-17 
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-1.467629e-15 
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Supplementary Text 10

-9.636212e-16  3.255586e-15 -4.777301e-16  2.978954e-15 -1.772684e-16
-1.705672e-15

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-1.729218e-15

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-8.247183e-16

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Page 557
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4.465301e-15
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1.824592e-15
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6.806091e-16
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3.976065e-15 1.346727e-15 -1.573066e-15 4.611497e-16 -1.330273e-15
4.948938e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
7.610814e-15 -4.185142e-15 -3.731956e-16 -3.784502e-15 1.026442e-15
6.806091e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
2.095702e-15 1.586212e-14 5.096813e-15 -2.163075e-15 -6.01646e-15
-5.946969e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
1.331416e-14 -7.931998e-15 3.757607e-15 1.018841e-15 -6.015159e-15
5.369283e-15
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -6.273961e-15 | -1.047227e-14 | 5.239904e-15 | 2.726373e-15 | 8.574760e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 1.721813e-15 | -4.967121e-15 | -2.070220e-15 | 2.222436e-15 | 1.088128e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 6.997431e-15 | -9.314742e-15 | -3.386593e-15 | 3.563965e-15 | 2.880021e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -3.382424e-15 | -1.022187e-14 | -3.877274e-15 | 4.212233e-15 | -4.425853e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | -8.744325e-15 | -6.879262e-15 | -3.950821e-15 | -8.647060e-16 | -4.550998e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | -7.919674e-15 | 1.398651e-15 | 5.702603e-16 | -2.049279e-15 | -1.304551e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -2.08886e-15 | -8.672894e-15 | -6.409589e-16 | -1.321883e-15 | -3.652879e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee66442bf12.final.pdb | 4.25144e-15 | -5.255451e-15 | -5.232239e-15 | 1.364795e-14 | -3.964697e-14 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 9.202597e-15 | -1.046229e-14 | -4.401551e-16 | -2.432000e-15 | -8.000348e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | -7.190437e-15 | 2.52662e-16 | 2.747974e-14 | -1.147494e-14 | -2.733034e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 5.068634e-15 | -6.858633e-15 | -6.335058e-15 | 5.129080e-16 | 6.519052e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 1.582918e-15 | -2.184232e-15 | -1.510715e-15 | 1.93704e-15 | 2.059166e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | -7.919674e-15 | 1.398651e-15 | 5.702603e-16 | -2.049279e-15 | -1.304551e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | -3.504360e-15 | 6.087196e-16 | -3.190559e-15 | 4.475235e-15 | 7.242667e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b091fe338e05fc.final.pdb | 5.675357e-15 | -7.613441e-15 | -5.246065e-15 | 5.903519e-15 | -1.734701e-15 |
|---------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | -1.218127e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | 7.797115e-16 -1.054195e-14 -2.139731e-15 8.252122e-15 9.788272e-15 -2.220348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 2.220348e-15 -1.218127e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | 3.350163e-16 -7.402233e-15 -1.019385e-14 -4.778647e-15 -5.916078e-15 -5.531019e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | 4.666800e-15 -5.638218e-15 -2.486968e-15 2.977007e-15 4.296613e-15 8.388528e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 1.582918e-15 -2.184232e-15 -1.510715e-15 1.934704e-15 2.059166e-15 4.517534e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 6.313698e-15 -8.233983e-15 -1.031990e-14 -2.293144e-15 -2.498109e-15 -2.196959e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 1.789582e-15 -5.055153e-15 -1.011926e-14 8.033587e-15 5.018752e-15 9.670384e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | 6.997431e-15 -9.314742e-15 -3.386593e-15 3.563965e-15 2.880021e-15 -2.827752e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 5.154512e-15 -9.250581e-15 4.452199e-15 5.275810e-15 -1.646490e-15 2.351565e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 1.7897067e-15 -2.093573e-15 3.011022e-15 -7.351428e-16 -3.796198e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 1.789582e-15 -5.055153e-15 -1.011926e-14 8.033587e-15 5.018752e-15 9.670384e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 5.154512e-15 -9.250581e-15 4.452199e-15 5.275810e-15 -1.646490e-15 2.351565e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 5.675357e-15 -7.613441e-15 -5.246065e-15 5.903519e-15 -1.734701e-15 -2.220348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 5.675357e-15 -7.613441e-15 -5.246065e-15 5.903519e-15 -1.734701e-15 -2.220348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 5.154512e-15 -9.250581e-15 4.452199e-15 5.275810e-15 -1.646490e-15 2.351565e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 5.675357e-15 -7.613441e-15 -5.246065e-15 5.903519e-15 -1.734701e-15 -2.220348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf39754b03f.final.pdb | 5.675357e-15 -7.613441e-15 -5.246065e-15 5.903519e-15 -1.734701e-15 -2.220348e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 5.675357e-15 -7.613441e-15 -5.246065e-15 5.903519e-15 -1.734701e-15 -2.220348e-15 |
| File Path                                                                 | Values                                |
|----------------------------------------------------------------------------|---------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb        | 1.589998e-15                          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb         | 1.187108e-14 -4.724660e-15 3.141149e-15 6.822132e-15 5.446495e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb          | 3.561786e-14 -5.049504e-16 5.982613e-15 -1.416736e-14 1.283564e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb          | 1.298571e-14 -2.852127e-15 1.408514e-15 -9.661170e-16 1.082273e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb          | 1.946703e-15 -3.544945e-15 1.480572e-15 -6.56743e-16 2.956823e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb           | -2.188030e-15 -4.236335e-16 -4.304511e-15 -2.825127e-15 1.140827e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb          | -1.207006e-14 -4.642154e-16 9.448641e-16 -5.438136e-15 2.776431e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb           | 1.589998e-15 -4.724660e-15 3.141149e-15 6.822132e-15 5.446495e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb           | 8.502864e-15 -7.026599e-15 3.112299e-15 3.985717e-15 5.902430e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb          | 8.774431e-16 -2.452338e-15 -3.840996e-15 1.495636e-15 3.064322e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb          | 8.502864e-15 -7.026599e-15 3.112299e-15 3.985717e-15 5.902430e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\43257eee6642bf12.final.pdb          | 2.772924e-15 -1.712955e-14 2.470778e-15 -1.022712e-15 2.816919e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb          | 2.899297e-16 -1.712955e-14 2.470778e-15 -1.022712e-15 2.816919e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6edd.final.pdb          | 5.789316e-15 1.445097e-15 1.292910e-14 9.168751e-15 1.408529e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb          | 3.324932e-15 -2.835453e-15 -8.917744e-16 -2.251048e-15 2.715092e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb          | 4.324932e-15 -2.835453e-15 -8.917744e-16 -2.251048e-15 2.715092e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb          | -1.886687e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb          | 6.942328e-16 -5.132108e-15 1.794557e-15 6.131341e-15 5.096171e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb          | -2.558762e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb          | 2.587457e-15 -1.580435e-15 -7.638548e-15 2.169461e-15 4.002691e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6edd.final.pdb          | 2.310276e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6edd.final.pdb          | 4.103996e-15 -4.699484e-15 -2.052765e-16 7.479988e-16 2.970080e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb          | -2.074838e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb          | 8.502864e-15 -7.026599e-15 3.112299e-15 3.985717e-15 5.902430e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb          | 4.333029e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb          | -5.642219e-15 -1.625892e-15 1.651989e-15 -3.306475e-15 1.071025e-16 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb     | -2.042930e-15 -4.974669e-17 -2.024460e-15 -7.515835e-16 -4.434795e-15 2.390653e-15 9.481173e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2d.final.pdb      | 4.103996e-15 -4.699484e-15 -2.052765e-16 7.479988e-16 2.297080e-15 -2.074838e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb      | 2.525527e-15 -7.576374e-16 1.382477e-15 2.146507e-16 3.798798e-15 -1.888180e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb      | 3.324932e-15 -2.834535e-15 -8.917744e-16 -2.251048e-15 2.715092e-15 -1.886837e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\668353ff3c87ef.final.pdb        | -5.642219e-15 -1.625892e-15 1.651989e-15 -3.304675e-15 1.071025e-16 -2.042930e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986ef01.final.pdb      | 1.118924e-14 -3.140886e-15 1.903500e-15 4.227757e-15 2.128314e-15 -3.299030e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6aa9d8747926b1c8.final.pdb      | 7.833450e-16 -3.578620e-15 1.466148e-15 -9.322242e-15 2.704467e-15 1.586094e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ff4c.final.pdb      | -3.647829e-15 -7.504973e-15 8.507370e-15 5.481433e-15 7.943525e-15 7.962932e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624111dc42.final.pdb        | 5.042828e-15 -1.966631e-15 6.265712e-16 -2.083000e-17 4.112123e-15 5.395392e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\72f27e0ad0f1be4.final.pdb        | -5.642219e-15 -1.625892e-15 1.651989e-15 -3.304675e-15 1.071025e-16 -2.042930e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb      | 9.512294e-17 -3.961869e-15 1.530290e-15 -3.512829e-16 3.415785e-15 1.086321e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\79f18c80dd53c3155.final.pdb      | -4.974669e-17 -2.024460e-15 -7.515835e-16 -4.434795e-15 2.390653e-15 9.481173e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fadd9866a3f099.final.pdb        | -1.266498e-14 -8.384855e-16 -1.057557e-15 -5.286862e-16 2.801678e-15 3.299489e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -2.188030e-15 -4.236335e-16 -4.304511e-15 -2.825257e-15 1.140514e-15 -9.661170e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | -2.188030e-15 -4.236335e-16 -4.304511e-15 -2.825257e-15 1.140514e-15 -9.661170e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0ecfece1234f9.final.pdb       | 8.774431e-16 -2.452338e-15 -3.840986e-15 1.495636e-15 3.064322e-15 5.316320e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8650469ef567960.final.pdb        | 3.324932e-15 -2.835453e-15 -8.917744e-16 -2.251048e-15 2.715092e-15 -1.886837e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e140203d.final.pdb        | -5.642219e-15 -1.625892e-15 1.651989e-15 -3.304675e-15 1.071025e-16 |
| FilePath                               | Score1   | Score2   | Score3   | Score4   | Score5   | Score6   |
|----------------------------------------|----------|----------|----------|----------|----------|----------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -2.042930e-15 | -1.13573e-14 | 2.189427e-15 | 1.110961e-15 | 5.721268e-15 | 1.831373e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -1.220755e-14 | 6.695245e-15 | 6.583948e-15 | 1.542793e-15 | 2.203020e-15 | -1.587232e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9bbee0d5986c138f.final.pdb | 1.831373e-16 | -2.024460e-15 | -7.515835e-16 | -4.434795e-15 | 2.390653e-15 | 9.481173e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 6.821256e-15 | -3.835997e-15 | 8.474330e-15 | 3.972213e-15 | 9.726851e-15 | 1.726851e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | 1.831373e-16 | -2.024460e-15 | -7.515835e-16 | -4.434795e-15 | 2.390653e-15 | 9.481173e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | -1.220755e-14 | 6.695245e-15 | 6.583948e-15 | 1.542793e-15 | 2.203020e-15 | -1.587232e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 4.103996e-15 | -4.699484e-15 | 7.479988e-15 | 2.297080e-15 | -2.074838e-15 | 1.831373e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 8.224632e-16 | -3.224959e-15 | 1.372350e-15 | 2.597992e-15 | 9.212998e-16 | 9.661170e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 1.059801e-15 | -3.603765e-15 | 1.128273e-15 | 2.941119e-15 | 1.071026e-15 | 2.941119e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 6.821256e-15 | -3.835997e-15 | 8.474330e-15 | 3.972213e-15 | 9.726851e-15 | 1.726851e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 5.039124e-15 | 6.025231e-15 | 3.387146e-15 | 4.370836e-15 | 8.497196e-15 | 8.497196e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -1.838838e-15 | -4.818813e-15 | 9.198936e-15 | 3.904770e-15 | 2.454834e-15 | 1.011843e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.920419e-16 | 1.668185e-15 | -2.579869e-15 | -2.995526e-15 | 2.203020e-15 | -1.530156e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 9.212998e-16 | -3.224959e-15 | 1.372350e-15 | 2.597992e-15 | 9.212998e-16 | 9.661170e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 5.930476e-15 | -1.135673e-14 | 2.189427e-15 | 1.110961e-15 | 5.721268e-15 | 1.831373e-16 |
| Path                                                                 | Value          |
|----------------------------------------------------------------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb  | -9.481173e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb  | -4.974669e-17  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb  | -2.024460e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb  | 1.097791e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb  | 1.034444e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb  | 3.568019e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb  | 9.293791e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb  | 9.827442e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0e39.final.pdb    | 1.548063e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb  | 9.053491e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b8b06824ef848.final.pdb    | 7.764844e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb  | 9.844414e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb    | 4.103996e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1a0f8694090cae7.final.pdb   | 2.188030e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e517be32db950e.final.pdb     | 9.74669e-17    |
Supplementary Text 10

-7.377408e-16 3.561819e-15 -2.921272e-15 -9.118975e-15 -9.120438e-15
6.132830e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
-3.122892e-15 4.699381e-15 1.439720e-15 -3.713908e-15 3.781976e-16
-3.930422e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
-3.134688e-16 1.745169e-15 -9.383338e-16 -7.561354e-15 -3.103755e-15
2.697921e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
-3.134688e-16 1.745169e-15 -9.383338e-16 -7.561354e-15 -3.103755e-15
2.697921e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
-3.164465e-15 -3.617624e-15 -8.440606e-15 -7.816356e-15 5.293391e-15
1.088180e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-9.762465e-15 -9.230698e-15 -9.949407e-15 1.00106e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
-3.617624e-15 -8.440606e-15 -7.816356e-15 5.293391e-15 1.088180e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
-3.164465e-15 -3.617624e-15 -8.440606e-15 -7.816356e-15 5.293391e-15 1.088180e-14
| Path                                                                 | Value                                                                 |
|----------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | -7.193449e-16 -4.297662e-15 4.114023e-15 -1.875294e-14 8.366747e-15 |
|                                                                      | 3.645005e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae.final.pdb | -3.769600e-15 5.539488e-15 3.036962e-15 4.013460e-16 5.319078e-15 |
|                                                                      | 3.765595e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db6500.final.pdb | -4.657076e-15 5.993829e-15 4.218105e-16 2.977048e-16 1.770819e-15 |
|                                                                      | -2.396980e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | -3.546647e-15 4.663127e-15 1.242844e-15 -3.859868e-16 1.857916e-16 |
|                                                                      | -6.239426e-17 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad50278.final.pdb | -3.802614e-15 4.377500e-15 1.437777e-15 -3.807952e-16 3.071457e-16 |
|                                                                      | 3.446523e-16 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | -3.592076e-15 4.757733e-15 7.066177e-16 -3.523189e-15 -1.375951e-16 |
|                                                                      | -2.892732e-17 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e2bf87e52ca29.final.pdb | -4.528584e-15 6.660658e-15 2.237196e-15 -2.136613e-15 -5.146235e-16 |
|                                                                      | -1.946324e-16 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | -6.610627e-15 3.321019e-15 -3.719135e-16 -2.756157e-15 2.920932e-15 |
|                                                                      | -1.058428e-17 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f38584e22003fb92.final.pdb | 1.566224e-15 5.642764e-15 3.947488e-15 -6.869902e-15 -7.707681e-16 |
|                                                                      | -1.327621e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | -4.156860e-15 9.194899e-15 3.799481e-15 -5.491993e-15 -2.814068e-15 |
|                                                                      | -1.396738e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 2.182215e-15 -4.212361e-15 -3.699029e-15 2.069373e-15 -1.702460e-15 |
|                                                                      | -2.141775e-15 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 2.509091e-16 6.892202e-16 -2.283593e-16 -3.425841e-16 2.131451e-15 |
|                                                                      | -3.290236e-16 E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb | 2.460495e-15 -2.142606e-15 2.113644e-15 1.992187e-16 2.566010e-15 |
| File Path                                      | Values                                      |
|-----------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -5.718835e-15 9.224205e-16 -1.740713e-16 7.188908e-16 5.925792e-16 -5.188730e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 5.341580e-15 7.814043e-15 -1.223170e-14 -1.847633e-15 3.046346e-15 5.319545e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -1.059024e-15 4.793186e-16 -2.087894e-15 1.817360e-16 1.153935e-15 -2.738593e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -6.528748e-16 -3.930925e-16 -1.281907e-14 9.476056e-16 1.595239e-15 1.047047e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | 4.413278e-16 9.122041e-16 -2.132657e-15 2.844300e-16 2.031328e-15 -3.322627e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551bea039.final.pdb | -6.528748e-16 -3.930925e-16 -1.281907e-14 9.476056e-16 1.595239e-15 1.047047e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f4532847579a.final.pdb | 2.277482e-15 4.050356e-15 1.057198e-15 7.448194e-15 -5.463158e-15 5.058785e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.ppb | 238dd3918e54336d.final.pdb 4.560798e-15 3.210317e-15 -1.096631e-14 -1.283536e-15 -2.210118e-15 3.604220e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | 1.849222e-15 1.507686e-15 -2.406611e-15 4.086866e-16 1.997021e-15 -2.831605e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 5.218492e-15 1.507686e-15 -2.406611e-15 4.086866e-16 1.997021e-15 -2.831605e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 34eb328251842006.final.pdb -1.351294e-14 2.109713e-15 3.754042e-15 2.277392e-15 7.737539e-15 -3.443215e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 354b32871797b7ab.final.pdb 2.184669e-15 -8.382015e-15 6.006661e-16 -3.188292e-15 1.452299e-14 -9.863415e-18 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\37368adbc32d5e.final.pdb | 5.341580e-15 7.814043e-15 -1.223170e-14 -1.847633e-15 3.046346e-15 5.319545e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 411ca13cd3df6edd.final.pdb 5.650269e-15 1.518056e-15 -6.754394e-15 1.034264e-15 -2.837173e-15 -2.117861e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357ee6642bf12.final.pdb | 42357ee6642bf12.final.pdb 5.437435e-15 -5.357367e-15 3.115562e-15 -1.084552e-15 1.195313e-15 -2.901966e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 44342d1f75a7fcfc.final.pdb 4.897428e-15 -5.96981e-15 -7.736736e-15 2.220059e-15 -5.363304e-15 -9.562465e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb | 448ef21dffe8cdefb.final.pdb 4.399967e-15 1.835077e-15 -1.00514e-14 -5.317859e-15 2.611103e-14 8.056075e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 472a40b3e8f113c7.final.pdb -6.245681e-16 9.224205e-16 -1.740713e-16 7.188908e-16 5.925792e-16 |
Supplementary Text 10

-9.184249e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04b89c94a633196.final.pdb
5.218756e-15 -2.446221e-15 1.784348e-15 2.238162e-15 -2.263847e-15
-5.820845e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
5.218756e-15 -2.446221e-15 1.784348e-15 2.238162e-15 -2.263847e-15
-5.820845e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcefe12d3f.final.pdb
5.650269e-15 1.518056e-15 -6.754394e-15 1.034264e-15 -2.837173e-15
-2.117861e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
-6.245681e-16 9.224205e-16 -1.740713e-16 7.188908e-16 5.925792e-16
-5.188730e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb
4.841917e-15 7.400434e-15 4.900725e-15 -4.120789e-15 4.040632e-15
-9.328662e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
2.186460e-15 3.633985e-15 -1.563668e-15 -2.67120e-16 2.947262e-15
-4.387747e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe7439f.final.pdb
-1.713718e-15 3.935524e-15 4.427075e-15 4.218249e-15 1.402315e-15
-5.438640e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
1.476621e-15 9.041775e-16 6.446171e-16 1.70821e-16 3.145194e-15
-2.809703e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
-6.882241e-15 2.180287e-15 -5.601454e-15 1.771522e-15 4.614765e-15
6.000169e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
5.137036e-15 7.913913e-15 -5.939887e-15 7.51225e-15 1.971975e-15
-1.035610e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6833b.final.pdb
2.698729e-15 1.449286e-15 -1.783600e-15 8.501510e-16 5.073482e-16
-2.964796e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb
3.982578e-15 -7.272724e-15 -5.139976e-16 -1.336558e-15 4.074026e-15
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| Path                                                                 | Values                                      |
|----------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb  | 2.460495e-15 -2.142606e-15 2.113644e-15 1.992187e-16 2.566010e-15 -5.718835e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb  | -6.481491e-15 -6.287835e-15 -5.965800e-15 1.759490e-15 -3.230277e-15 -4.528297e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb  | 2.460495e-15 -2.142606e-15 2.113644e-15 1.992187e-16 2.566010e-15 -5.718835e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb   | 2.186460e-15 3.633985e-15 -1.563668e-15 -2.672120e-16 2.947262e-15 -4.387747e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb   | 1.755981e-15 7.049422e-16 -2.055113e-15 4.737387e-16 1.572013e-15 -2.920075e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb   | -9.236261e-15 3.644652e-16 7.359966e-15 -1.121130e-15 9.512757e-15 -6.427131e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb   | 2.186460e-15 3.633985e-15 -1.563668e-15 -2.672120e-16 2.947262e-15 -4.387747e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb   | 7.497664e-15 2.467742e-15 -9.891983e-16 -4.156247e-15 -3.590957e-15 -7.880069e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb    | 4.584664e-15 9.465025e-16 6.205207e-15 -7.579715e-15 5.439146e-15 5.970382e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb  | -1.000568e-15 3.553940e-15 -2.942612e-15 9.420914e-16 4.921694e-16 -2.404481e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb   | 6.781228e-15 -1.064800e-14 -1.710481e-15 4.703053e-15 1.193639e-14 -1.593044e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d14603f29723397d.final.pdb   | 6.83811e-15 6.352255e-15 1.032937e-14 1.147967e-15 9.084973e-15 -4.831558e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d14603f29723397d.final.pdb   | -7.404364e-15 -3.675341e-15 -6.105445e-15 4.759424e-15 -4.465151e-15 7.077485e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d528748e-16 -3.930925e-16 -1.281907e-14 9.476056e-16 1.595239e-15 1.047047e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb   | 2.182215e-15 -4.212361e-15 -3.699029e-15 2.069373e-15 -1.702460e-15 |
Supplementary Text 10

-2.157517e-15
e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb 5.218756e-15 -2.446221e-15 1.784348e-15 2.238162e-15 -2.263847e-15 -5.820845e-15
e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb -5.898010e-15 1.009425e-14 -1.123661e-14 2.901069e-16 6.021432e-15 -7.882346e-15
e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb 5.676668e-15 4.136183e-15 -5.469348e-15 2.295471e-16 -3.735405e-15 -1.096776e-15
e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb 5.218756e-15 -2.446221e-15 1.784348e-15 2.238162e-15 -2.263847e-15 -5.820845e-15
e:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb 2.460495e-15 -2.142606e-15 2.113644e-15 1.992187e-16 2.566010e-15 -5.718835e-15
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 1.427821e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 7.605625e-15  4.724358e-15 -3.596960e-15  3.551206e-15 -1.132042e-14 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 4.655144e-15 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 3.024278e-15 -3.195414e-15  1.629747e-15 -4.745533e-15 -9.072545e-16 |
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2.374562e-15
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-9.245257e-16
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-4.100452e-15

-9.245257e-16
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9.318542e-16

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-1.590582e-15

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-4.950975e-15 -8.851018e-16 5.201142e-15 -7.494223e-15 -2.965632e-15
-6.718218e-16

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2.603601e-15 -2.953564e-15 7.524193e-15 -8.012368e-15 -2.403704e-15
9.318542e-16

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7.021443e-16

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-3.783504e-15

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-3.783504e-15

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-2.952241e-16

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-1.590582e-15

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-3.783504e-15

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-6.407579e-16

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-1.869548e-15

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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb      | 1.943732e-15                                                            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb      | 5.924873e-15 9.271692e-16 -1.948668e-15 3.255800e-16 -4.274603e-15 -3.783504e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | 1.666545e-15 4.318585e-16 -4.226705e-16 -1.349768e-15 -3.61905e-15 -2.316217e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | 1.398546e-15 -5.895482e-16 -2.40973e-16 -3.618634e-15 -3.247524e-15 -2.952241e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7ad998e66a3f6099.final.pdb       | 1.652897e-15 -9.046934e-16 6.154708e-15 -4.749575e-15 -5.522482e-15 -8.866744e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | 4.006115e-15 -2.837675e-15 -1.219310e-15 -3.529506e-15 -4.698011e-15 -4.947892e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb       | 4.006115e-15 -2.837675e-15 -1.219310e-15 -3.529506e-15 -4.698011e-15 -4.947892e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12d3f9.final.pdb        | -1.580996e-15 -2.257193e-15 -2.952190e-15 -4.542151e-15 -7.142183e-16 -9.245257e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | 1.131255e-15 -2.231702e-15 -1.966371e-15 -9.587126e-16 -3.731349e-15 -1.590582e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | 5.924873e-15 9.271692e-16 -1.948668e-15 3.255800e-16 -4.274603e-15 -3.783504e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb       | -1.749698e-15 1.625769e-15 3.035967e-15 -1.669089e-17 -4.868014e-15 2.508784e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8c0eeecfe12d3f9.final.pdb        | 8.142391e-15 -2.703499e-15 4.300119e-15 -9.952230e-16 -3.136862e-15 1.508740e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8d50469ef569760.final.pdb        | -1.38546e-15 -5.895482e-16 -2.40973e-16 -3.618634e-15 -3.247524e-15 -2.952241e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb       | 1.781765e-15 4.745019e-15 -4.276651e-15 2.786189e-15 -3.101198e-15 -6.684567e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d98e66a3f6099.final.pdb         | 1.943732e-15 7.400116e-15 -2.751257e-15 7.369875e-16 -8.908941e-15 -2.415924e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb       | 3.687863e-15 1.120787e-15 -3.829966e-16 -2.846781e-15 -3.935064e-15 -4.297826e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb       | 1.220458e-15 4.381268e-16 -4.437071e-16 2.741301e-15 -3.449092e-15 7.021443e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb       | 4.438061e-15 -5.918649e-15 -2.417454e-15 4.047605e-15 8.613159e-16 |
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3.083291e-15
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-2.952241e-16
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-6.916089e-15
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-2.952241e-16
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-5.408677e-15
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-2.952241e-16
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-5.408677e-15
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-1.269264e-14
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Page 603
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-2.161608e-15
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-2.073695e-15
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-2.279354e-15
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-3.873622e-15
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-4.297826e-15
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-6.718218e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52ca4a.final.pdb
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| File Path                                                                 | Values                                                                 |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0c97d891e4e082.final.pdb       | -9.218604e-15 1.529946e-14 1.185589e-15 -9.890105e-15 3.24535e-15 3.576892e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c61.final.pdb       | -3.631060e-15 6.249084e-15 -2.036660e-15 -1.433328e-15 -1.537198e-15 4.056979e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb      | -3.004181e-15 7.669526e-15 5.373649e-16 -1.723376e-17 -4.267168e-15 9.245253e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb      | -4.047706e-15 6.379884e-15 -1.752696e-15 -1.453294e-15 -1.553838e-15 4.072132e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb     | -7.166650e-15 -1.762708e-15 7.498685e-16 -7.371969e-16 3.905477e-16 -7.948390e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb      | -3.142858e-15 8.545638e-15 -7.945297e-15 -3.667854e-15 -3.099134e-15 1.277341e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb      | -7.292862e-16 1.253574e-15 -4.396798e-16 -1.238526e-16 -4.957666e-15 5.884665e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb      | -3.884662e-15 1.587445e-15 5.443299e-15 -4.821445e-15 -2.050927e-15 -8.693972e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb      | -7.292862e-16 1.253574e-15 -4.396798e-16 -1.238526e-16 -4.957666e-15 5.884665e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb      | -3.763318e-15 4.681279e-15 -1.845239e-15 -1.345098e-15 -1.998995e-15 3.706503e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb      | -3.763318e-15 4.681279e-15 -1.845239e-15 -1.345098e-15 -1.998995e-15 3.706503e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb      | -8.186948e-15 -7.601082e-15 3.997271e-15 -3.997557e-15 -9.105762e-15 -1.667676e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb      | -2.756116e-15 3.470628e-15 -3.187211e-15 -7.101019e-17 -4.408131e-15 2.159341e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81ac3.final.pdb      | 1.455412e-15 1.641861e-15 4.079154e-15 1.528900e-16 -4.024848e-15 1.654883e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb      | -1.898031e-14 3.769031e-15 -1.345835e-14 -1.773575e-15 -7.070459e-15 4.415354e-15 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb -1.429695e-15 3.966513e-15 5.402717e-16 -2.450422e-16 -5.640179e-16 4.680176e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb -2.366517e-15 1.273522e-14 -1.564666e-14 -2.290081e-15 2.401798e-15 1.779796e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feaa2.final.pdb -2.645998e-15 9.348003e-15 -2.181667e-15 2.273152e-15 1.243095e-15 5.944712e-15
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3.272040e-15  3.782638e-15  4.394238e-16 -1.530585e-15  4.885955e-15
-5.404860e-15

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-3.176376e-15

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-6.123804e-15

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1.537149e-15

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-1.394236e-14

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-1.783191e-14

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-4.522351e-15

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4.005813e-15  1.030588e-14  6.644117e-15  8.026415e-15  6.202825e-15
-3.970515e-15
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1.408700e-15
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 4.401954e-16 | 7.672384e-15 | -2.656685e-15 | 1.617730e-15 | 3.517557e-15 | -4.522351e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | -7.174605e-16 | 3.517027e-15 | -4.956937e-16 | -8.382217e-16 | 5.378571e-15 | 7.388504e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | -3.136789e-15 | 2.146842e-15 | 4.793012e-16 | 2.306492e-16 | 7.388504e-15 | -2.60867e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -2.159088e-15 | 4.383300e-15 | -2.146102e-15 | 1.472493e-15 | 1.030757e-15 | 3.312640e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb | -3.082869e-15 | 2.321014e-15 | 4.413117e-15 | 5.892516e-15 | 3.217867e-15 | 3.628871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0f305f598641eb2.final.pdb | -1.816277e-15 | -4.935244e-16 | -1.228136e-14 | -8.927779e-15 | 1.618508e-14 | -4.778599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -9.046658e-15 | -5.852113e-15 | 9.814785e-15 | -3.006084e-15 | 5.902868e-15 | 5.633137e-15 |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
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|-----------------------------------------------|----------------------------------|
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -3.082869e-15  2.321014e-15  4.413117e-15  5.892516e-15  3.321046e-15  3.628871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -1.004939e-15  3.633638e-15  5.345457e-15  -1.414722e-15  6.502593e-15  1.725672e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -1.819485e-14  -1.664827e-15  3.604340e-16  2.582970e-15  3.882220e-16  -1.061018e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | -1.048199e-14  -1.063784e-14  -3.408709e-15  -2.599444e-15  -4.255493e-15  4.055866e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611dc42.final.pdb | -8.250640e-15  3.130207e-15  -6.062926e-15  2.501871e-16  -2.570156e-15  3.374660e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb | -1.004939e-15  3.633638e-15  5.345457e-15  -1.414722e-15  6.502593e-15  1.725672e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffbb22872.final.pdb | -4.775094e-15  3.579283e-15  1.785710e-16  2.014395e-16  1.332362e-15  4.159659e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c70ad0f1be4.final.pdb | -9.929689e-15  6.678586e-15  -3.044876e-15  -1.758793e-15  -1.602024e-15  1.545945e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -2.520685e-15  6.058313e-15  1.207365e-15  3.202730e-16  1.876314e-15  1.183930e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298f001.final.pdb | -2.520685e-15  6.058313e-15  1.207365e-15  3.202730e-16  1.876314e-15  1.183930e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8300000000000000.final.pdb | -9.929689e-15  6.678586e-15  -3.044876e-15  -1.758793e-15  -1.602024e-15  1.545945e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef596760.final.pdb | -3.082869e-15  2.321014e-15  4.413117e-15  5.892516e-15  3.321046e-15  3.628871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88be0d5986c138f.final.pdb | -1.605508e-15  6.113576e-15  6.102334e-16  2.952691e-15  2.501794e-15  3.334269e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -2.765248e-15  6.151076e-15  -3.967772e-15  5.690817e-15  -6.714215e-16  5.389866e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 3.955006e-15  -4.274642e-15  1.069060e-14  9.051987e-16  1.991974e-15  -2.956408e-15 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-1.894787e-15  2.753399e-15 -7.607613e-16  2.230793e-16 -1.429286e-16
3.147106e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
-1.977281e-15  2.774290e-15  1.666598e-15  5.039507e-16  3.758524e-15
5.163638e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-1.136945e-14 -2.494985e-16 -8.106427e-15 -2.890725e-15 -9.773977e-15
9.640976e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-8.236733e-15  1.413343e-16 -6.921566e-15 -5.515476e-16 -7.087165e-16
1.252974e-14

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.460353e-15 -2.342355e-15  1.725937e-15 -1.926243e-15 -1.479574e-16
1.701267e-16

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-1.681464e-15 -3.296285e-15  7.345286e-16 -2.055643e-15  1.011909e-15
-6.601845e-17

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-2.930186e-15 -1.882008e-15  1.60358e-15 -1.513931e-15  5.817352e-16
-3.617568e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-1.394933e-15 -2.198712e-15  1.700383e-15 -8.315462e-15  5.139893e-16
-6.702486e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-3.821700e-15  3.093903e-15 -4.017278e-15 -2.454198e-15 -1.547745e-15
3.548319e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
-1.616978e-15 -2.203482e-15  1.384229e-15 -5.084540e-16  6.474546e-16
-4.620818e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
-3.026084e-15  3.201190e-15  1.790691e-15 -1.859534e-15 -1.184975e-15
1.321495e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
-3.041936e-15 -2.005309e-15  1.112739e-15 -8.392666e-16  2.333833e-17
2.434236e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
-3.826084e-15  3.201190e-15  1.790691e-15 -1.859534e-15 -1.184975e-15
1.321495e-15

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| File Path | PDB ID | X, Y, Z Coordinates |
|-----------|--------|---------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | -8.449207e-16 -2.599130e-15 -2.726318e-15 -9.895337e-16 9.937879e-16 1.662212e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | -8.021497e-18 2.603436e-15 -3.358721e-15 2.121387e-15 -1.058754e-15 1.642463e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 7.882572e-17 -3.475061e-15 2.463649e-15 7.585104e-16 1.172518e-15 1.050859e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -1.029923e-14 3.480087e-15 6.448299e-16 -3.443587e-16 2.062086e-15 -3.774590e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -5.627612e-15 -5.038922e-17 -3.965289e-15 -4.630381e-16 3.416022e-15 -2.640953e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -2.33195e-15 -2.261189e-15 1.260618e-15 -1.603735e-16 1.262048e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | -2.341646e-15 1.003316e-15 4.071759e-16 5.982861e-15 -5.330499e-15 -3.097851e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -2.828248e-15 -3.389599e-15 2.868936e-15 -6.300868e-15 8.153975e-16 -1.085932e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | -1.029923e-14 3.480087e-15 6.448299e-16 -3.443587e-16 2.062086e-15 -3.774590e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb2872.final.pdb | -1.673433e-15 -1.676418e-15 1.135941e-15 -1.048550e-15 2.952866e-16 -3.956098e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 1.305465e-15 -6.400169e-15 2.710021e-15 -1.949174e-14 -6.421426e-16 1.218452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 4.146824e-16 -3.642091e-15 7.057593e-16 5.783657e-16 3.353343e-15 -1.061061e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -1.054810e-15 -5.939662e-15 3.218476e-15 1.304438e-16 2.256795e-15 -2.005645e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | -1.054810e-15 -5.939662e-15 3.218476e-15 1.304438e-16 2.256795e-15 -2.005645e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c00eefcfe12d3f9.final.pdb | -1.769950e-15 -3.890520e-15 -1.870119e-15 -1.107281e-15 2.905365e-15 1.011798e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 7.882572e-17 -3.475061e-15 2.463649e-15 7.585104e-16 1.172518e-15 1.050859e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -1.029923e-14 3.480087e-15 6.448299e-16 -3.443587e-16 2.062086e-15 -3.774590e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -3.867664e-15 1.478015e-15 -3.838162e-15 1.17501e-15 2.448482e-15 2.741425e-15 |
| File Path                                                                 | Values                                      |
|--------------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | -1.512160e-15 -2.411173e-15 1.456466e-15 -1.139058e-15 1.532281e-16 -6.405215e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb       | -1.366387e-15 -2.124844e-15 1.683572e-15 -7.011720e-16 6.453755e-16 -4.274311e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb       | -1.125428e-15 -9.789938e-16 1.338902e-15 -4.391377e-15 4.546215e-16 -1.508212e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb       | -1.472225e-15 -4.171514e-15 2.693131e-15 2.064577e-16 8.502338e-16 -1.771978e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb       | -8.859581e-15 4.829997e-15 -4.234186e-15 -9.357744e-15 -5.799094e-16 -4.989148e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb       | -1.125428e-16 -8.037384e-15 3.901084e-15 -3.854987e-15 -4.053336e-15 -2.507276e-15 |

[,745] [,746] [,747] [,748] [,749] [,750]
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | 9.398671e-16 -5.326576e-15 -2.068207e-15 -1.319906e-15 -1.009657e-15 -9.244990e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 1.448193e-15 -1.919066e-15 5.933227e-15 -3.231895e-15 -4.755847e-15 1.944659e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | -2.078254e-15 -3.459059e-15 1.867395e-15 -4.354259e-15 -2.554084e-15 3.467266e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | -7.924865e-16 4.898168e-16 -4.718945e-15 -3.995770e-15 -2.955666e-15 1.314483e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -1.185642e-16 3.772811e-15 5.293067e-16 -7.571428e-15 4.397393e-15 5.107505e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -5.326576e-15 -2.068207e-15 -1.319906e-15 -1.009657e-15 -9.244990e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 4.788742e-16 -3.267218e-15 -1.485788e-15 -4.857194e-15 -2.606237e-15 3.220793e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | -2.078254e-15 -3.459059e-15 1.867395e-15 -4.354259e-15 -2.554084e-15 3.467266e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -7.924865e-16 4.898168e-16 -4.718945e-15 -3.995770e-15 -2.955666e-15 1.314483e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 1.448193e-15 -1.919066e-15 5.933227e-15 -3.231895e-15 -4.755847e-15 1.944659e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | -2.078254e-15 -3.459059e-15 1.867395e-15 -4.354259e-15 -2.554084e-15 3.467266e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | 1.605208e-15 -4.361866e-16 5.572274e-15 -7.660796e-15 -2.772110e-15 1.814579e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | 1.605208e-15 -4.361866e-16 5.572274e-15 -7.660796e-15 -2.772110e-15 1.814579e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb | -5.326576e-15 -2.068207e-15 -1.319906e-15 -1.009657e-15 -9.244990e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 4.788742e-16 -3.267218e-15 -1.485788e-15 -4.857194e-15 -2.606237e-15 3.220793e-15 |
| Path                                                                 | Score   | Score   | Score   | Score   | Score   |
|----------------------------------------------------------------------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 9.398671e-16 | -5.326576e-15 | -2.068207e-15 | -1.319906e-15 | -1.009657e-15 |
|                                                                      | -9.244990e-16 |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 1.532349e-15  | -1.313089e-15 | 2.944168e-15  | 1.203641e-15  | 2.161444e-15  |
|                                                                      | 4.346842e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9bbbe0d5986c138f.final.pdb | 1.448193e-15  | -1.919066e-15 | 5.933227e-15  | -3.231895e-15 | -4.755847e-15 |
|                                                                      | 1.944659e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | -3.209857e-16 | -5.621790e-15 | 3.523457e-15 | 4.062682e-15 | 3.616053e-15 |
|                                                                      | 2.284256e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | -1.121751e-14 | 4.145583e-15 | -1.288922e-14 | -1.693990e-14 | -5.020338e-15 |
|                                                                      | 4.432544e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | 3.282663e-15 | 8.856766e-16 | -1.189253e-16 | -6.705985e-16 | -1.263264e-15 |
|                                                                      | 3.405972e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c70083816d6ba.final.pdb | -2.078254e-15 | -3.459059e-15 | 1.867395e-15 | -4.354259e-15 | -2.554084e-15 |
|                                                                      | 3.467266e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4082.final.pdb | 5.286572e-15 | -9.677148e-15 | -5.914049e-15 | -5.548875e-15 | -5.149226e-15 |
|                                                                      | -5.051146e-16 |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d8236f6.final.pdb | 1.035415e-15 | -4.370546e-16 | -2.054549e-16 | -2.693845e-16 | -1.303344e-15 |
|                                                                      | 2.617605e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd74b9c71d4dc.final.pdb | 1.605208e-15 | -4.361866e-16 | 5.572274e-15 | -7.660796e-15 | -2.772110e-15 |
|                                                                      | 1.814579e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a8234e4b4c668.final.pdb | 1.046343e-15 | 1.090309e-15 | -5.283966e-16 | -2.623989e-15 | -1.270542e-15 |
|                                                                      | 3.061381e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | -3.209857e-16 | -5.621790e-15 | 3.523457e-15 | 4.062682e-15 | -3.616053e-15 |
|                                                                      | 2.284256e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b26923e697d3c63.final.pdb | 5.214876e-15 | 7.216187e-16 | 5.485307e-15 | -1.586511e-15 | -1.319555e-15 |
|                                                                      | -2.358138e-16 |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 1.448193e-15 | -1.919066e-15 | 5.933227e-15 | -3.231895e-15 | -4.755847e-15 |
|                                                                      | 1.944659e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 1.448193e-15 | -1.919066e-15 | 5.933227e-15 | -3.231895e-15 | -4.755847e-15 |
|                                                                      | 1.944659e-15  |       |       |       |       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87b107b.final.pdb | 1.532349e-15 | -1.313089e-15 | 2.944168e-15 | 1.203641e-15 | 2.161444e-15 |
|                                                                      | 4.346842e-15  |       |       |       |       |
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5.051452e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
-5.335083e-15 -8.237204e-15  3.254897e-15  2.807860e-15  3.117513e-15
-2.403810e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
-4.735492e-15 -2.405477e-15  2.122541e-16  2.397077e-15 -2.247235e-15
5.051452e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb
-4.753492e-15 -2.404577e-15  2.122541e-16  2.397077e-15 -2.247235e-15
5.051452e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
-4.745913e-15 -6.819968e-16 -1.637828e-15  3.509360e-15  1.309816e-15
-1.730470e-18
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e646f4ef427e.final.pdb
-1.447949e-14  8.305119e-15 -4.315111e-15  1.310214e-14 -1.740926e-14
-9.351226e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2af55fc9d681.final.pdb
-5.335083e-15 -8.237204e-15  3.254897e-15  2.807860e-15  3.117513e-15
-2.403810e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
-6.380598e-15  2.369542e-15  2.861520e-15 -2.589263e-16 -3.695394e-16
3.754788e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
-2.593535e-15  5.878727e-15  8.449945e-16  1.183105e-14 -3.746036e-15
8.454492e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
-5.622448e-15 -8.943102e-16 -1.417995e-15  2.395644e-15  3.481165e-16
2.906822e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054.final.pdb
-7.022973e-15  6.952181e-16 -1.043846e-14  3.524848e-14  5.492933e-15
-3.175543e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
-1.467685e-15 -1.374253e-14 -4.557808e-15  4.252479e-15 -6.740876e-15
-2.503962e-18
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8009eff10197e2.final.pdb
-5.766597e-15 -5.551643e-15  9.306369e-15  5.709910e-15 -2.722752e-15
-1.544048e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea163918d370789.final.pdb
2.202698e-15 -6.868659e-15  3.151311e-15  1.063467e-14 -1.153540e-14
3.001254e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b061824ef84.final.pdb
-4.280741e-15  2.285690e-16 -5.492047e-15  2.349380e-15  4.843890e-15
-7.868040e-17
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-3.809808e-15  5.838006e-15 -6.624265e-15  5.017601e-15 -1.160359e-15
3.375328e-15
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-3.043850e-16 -3.522225e-15 -5.096702e-16  1.242272e-15  1.658611e-15
3.384962e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6e89d97d00a960.final.pdb
3.831327e-16 -2.239027e-15 -5.907559e-15 -1.144941e-15  3.913785e-15
6.821717e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbb.final.pdb
-5.402688e-15 -2.021600e-15 -7.379223e-17  1.219490e-15  5.293368e-15
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| File Path | Values |
|----------|--------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -1.409550e-14, -2.690602e-15, 3.032075e-15, -7.076524e-15, 1.423608e-15, 2.747502e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 5.499866e-16, 1.900597e-15, -2.087044e-16, 1.806282e-15, -2.940807e-15, 7.216992e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | 6.297912e-15, 2.629795e-15, -1.093097e-15, -4.245456e-15, 1.635244e-15, 1.454459e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 1.393992e-15, -4.660342e-15, -3.405421e-15, -5.655125e-15, -6.296478e-15, 5.216223e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | 1.555164e-15, -2.568204e-15, -1.440976e-15, -1.079654e-15, -1.733208e-15, 1.561514e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 5.499866e-16, 1.900597e-15, -2.087044e-16, 1.806282e-15, -2.940807e-15, 7.216992e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 4.184795e-15, -1.800263e-15, -8.265184e-16, -1.853567e-15, 1.113215e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 9.527952e-16, 1.763300e-15, 2.730233e-15, 3.643199e-15, -6.478058e-15, -2.761329e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 1.393992e-15, -4.660342e-15, -3.405421e-15, -5.655125e-15, -6.296478e-15, 5.216223e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -4.860806e-15, 1.019587e-15, 1.088536e-15, 4.275731e-15, -2.557945e-15, 1.073196e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 1.256806e-15, -9.159800e-16, -5.186353e-16, -1.594798e-15, -2.777893e-15, 4.590742e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982f4c4.final.pdb | 9.177552e-15, 1.653800e-15, 2.913997e-15, -1.09572e-14, -7.709583e-15, 1.756842e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -6.89778e-16, 2.045511e-15, 6.709988e-15, -9.619193e-16, -6.568595e-16, 7.862845e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1e4.final.pdb | 1.393992e-15, -4.660342e-15, -3.405421e-15, -5.655125e-15, -6.296478e-15, 5.216223e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 1.424906e-15, -9.23983e-16, -1.546206e-15, -6.678361e-16, -3.187242e-15, 4.964144e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | 1.555164e-15, -2.568204e-15, -1.440976e-15, -1.079654e-15, -1.733208e-15, 1.561514e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 2.811024e-15, -1.017457e-14, -7.171862e-16, -3.664426e-16, -1.083346e-15, 3.897742e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -4.544501e-15, -2.252740e-15, 1.312980e-16, 9.986052e-16, 5.312126e-15, -3.478218e-15 |

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| File Path                                                                 | Values                                                                 |
|---------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | 4.176488e-15 4.140490e-16 -7.784730e-15 7.275504e-15 4.263651e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb      | 1.555164e-15 -2.568204e-15 -1.440976e-15 -1.079654e-15 -1.733208e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb      | 4.176488e-15 4.140490e-16 -7.784730e-15 7.275504e-15 4.263651e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb      | 1.555164e-15 -2.568204e-15 -1.440976e-15 -1.079654e-15 -1.733208e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb      | 1.555164e-15 -2.568204e-15 -1.440976e-15 -1.079654e-15 -1.733208e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb      | 9.280616e-16 -9.525257e-16 -4.183561e-16 -2.439777e-15 -2.646826e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb       | 3.317266e-15 4.275891e-15 -3.624378e-15 -2.623497e-15 3.930481e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | 1.555164e-15 -2.568204e-15 -1.440976e-15 -1.079654e-15 -1.733208e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\cbc88c8a505f3a288.final.pdb     | 6.528673e-15 -2.208071e-15 -9.217994e-15 9.973197e-15 -2.507945e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 3.317266e-15 4.275891e-15 -3.624378e-15 -2.623497e-15 3.930481e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb       | 8.987668e-15 3.920256e-16 1.096325e-14 -1.655712e-14 -3.758213e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 3.345399e-15 -3.023027e-15 -3.181771e-15 -1.157820e-14 -1.078933e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d22121245d015047.final.pdb       | 6.480011e-15 -1.251701e-15 1.207900e-15 -7.301807e-16 -2.843865e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d418256e-15 -2.623497e-15 3.930481e-15 | 3.242101e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | -3.231611e-15 -9.026143e-16 5.324219e-16 1.176789e-15 2.823896e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb       | -1.154043e-15 6.971096e-16 1.453792e-15 2.637078e-15 -4.274497e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb       | 1.480806e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d876468e-15 -8.257245e-15 6.978687e-15 -2.845523e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d9199900e-15 -7.301807e-16 -2.843865e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb       | 9.341194e-15 -9.824034e-16 5.324575e-15 4.268158e-16 -1.147029e-14    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb       | 5.103791e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb       | -1.101369e-15 5.006642e-15 5.207940e-15 -1.365195e-15 -2.130583e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb       | -4.544501e-15 -2.252740e-15 1.312980e-16 9.986052e-16 -5.312126e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e592208218ec3a1.final.pdb       | -3.478218e-15 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
2.545732e-15 -1.373401e-15 -5.657449e-15 4.900763e-15 1.675632e-15
8.636762e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
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5.587808e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93aad.final.pdb
2.648011e-15 -1.251701e-15 1.207900e-15 -7.301807e-15 -2.843865e-15
4.422450e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93aad.final.pdb
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1.340722e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f3WY9.pdb
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2.536390e-15
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4.364403e-15
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2.452433e-15 -1.884201e-18 4.228424e-17 -1.320003e-15 -4.905706e-16
2.963019e-15
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8.057480e-15 -2.613912e-15 -2.754749e-15 1.060266e-15 1.229226e-15
4.011337e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\02a2a75342ca0d54.final.pdb
9.423683e-16 -3.059844e-15 3.973774e-16 -1.766685e-15 -1.574148e-15
1.546645e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a5fcedeab4194d9.final.pdb
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2.533160e-15 -1.934182e-15 -7.543999e-17 -1.044311e-15 -1.523796e-15
2.560764e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb

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-6.533345e-16

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-1.415745e-15

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9.301792e-15

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7.921059e-16

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3.546936e-16

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-1.047691e-14

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-1.041736e-14

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-1.415745e-15

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-1.597738e-15

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6.592556e-15

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3.078994e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdefb.final.pdb

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4.210984e-15

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Supplementary Text 10

2.701657e-15 -2.353703e-15 1.308840e-15 -2.350200e-15 -2.140639e-16 -6.533345e-16
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6.338670e-16 -6.656685e-15 -4.128650e-15 5.469716e-15 -1.301546e-14 -5.667130e-15
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-6.693013e-15 -4.603959e-15 4.821663e-15 -4.496003e-15 -1.770020e-15 5.726845e-16
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-8.831652e-15 -3.985211e-15 4.549304e-15 -5.247405e-15 -1.025047e-15 -1.415745e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9f910fffb22872.final.pdb
-3.221616e-15 8.534290e-15 -3.174303e-17 8.534290e-15 -3.221616e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
Supplementary Text 10

-7.070848e-15 -2.533860e-15 -1.182804e-15 7.279257e-15 -8.818897e-15
6.407061e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb

2.533160e-15 -1.934182e-15 -7.543999e-17 -1.044311e-15 -1.523796e-15
2.560764e-16

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3.329662e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb

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-1.796012e-16

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2.560764e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb

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2.560764e-16

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1.798246e-16

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4.030573e-16

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-1.796012e-16

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-1.784164e-17 -3.180752e-16 2.754978e-15 -1.263035e-15 -1.794185e-15
-3.848231e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb

1.384529e-14 -1.240541e-14 -7.238764e-15 -3.645163e-16 -1.274876e-14
1.294308e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb

3.583032e-16 -3.116885e-15 8.645754e-16 -4.797219e-15 3.061546e-16
-3.836499e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb

-1.453958e-16 2.584733e-15 -4.152237e-15 3.128635e-15 -3.739357e-15
3.055837e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb

8.866490e-15 2.368026e-15 -7.171401e-15 -2.647740e-15 -1.381758e-14
8.744177e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb

1.899218e-15 -7.346723e-15 1.342968e-15 -4.354096e-15 -5.786956e-15
-2.066464e-15

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1.288411e-14 -3.745564e-15 -8.339493e-16 -1.681240e-15 4.451521e-15
-5.647924e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb

-9.454226e-15 -2.192096e-15 -1.893261e-15 4.833417e-16 1.989024e-16
3.393189e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fear finalized.pdb
Supplementary Text 10

5.218712e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
-6.590663e-15 -3.312632e-15 3.342060e-15 -2.109093e-15 1.894701e-15
5.470111e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
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2.921144e-15
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-1.317158e-15 -2.578827e-15 1.432212e-16 1.213103e-15 1.266555e-15
1.211776e-15
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6.417174e-16
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-1.317158e-15 -2.578827e-15 1.432212e-16 1.213103e-15 1.266555e-15
1.211776e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
-8.680544e-16 3.719937e-15 2.613476e-15 -2.660897e-15 6.996957e-15
2.779555e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
-1.317158e-15 -2.578827e-15 1.432212e-16 1.213103e-15 1.266555e-15
1.211776e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb
-9.533120e-15 -9.832834e-15 -1.808949e-15 -6.453904e-15 -2.816364e-15
Page 649
| Path                                                   | Coordinates                                      |
|--------------------------------------------------------|--------------------------------------------------|
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb              | -4.306104e-15 -4.202095e-15 -1.679366e-16 5.164702e-15 -3.953557e-15 1.653742e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | -7.079616e-15 -3.422422e-15 -3.398805e-15 5.417983e-16 7.766098e-16 -3.171893e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -4.926265e-15 -3.623622e-15 -4.155644e-16 1.287464e-16 -2.850724e-15 1.998457e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d49.final.pdb | -4.771899e-15 -7.301586e-15 -1.412839e-15 2.896383e-16 -6.747475e-15 6.761747e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -6.885432e-15 -3.135751e-15 -3.302731e-15 -2.138601e-15 -4.885770e-15 -1.014078e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | -9.147840e-15 -1.513792e-15 1.060518e-15 -6.620998e-16 -4.550241e-15 -5.045448e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -4.860345e-15 -3.901828e-15 -4.689716e-15 -6.970852e-16 -2.412489e-15 2.115442e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -6.885432e-15 -3.135751e-15 -3.302731e-15 -2.138601e-15 -4.885770e-15 -1.014078e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -5.063652e-15 -3.906578e-15 -4.537807e-16 1.064140e-15 -2.611044e-15 1.583377e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -6.885432e-15 -3.135751e-15 -3.302731e-15 -2.138601e-15 -4.885770e-15 -1.014078e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d4759a.final.pdb | 7.892473e-15 7.380841e-15 -7.604501e-15 -7.979495e-16 -5.601362e-16 4.464973e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | -4.721135e-15 3.216567e-16 -1.432382e-16 -5.478861e-15 -4.801427e-15 -6.691033e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2f42c.final.pdb | -5.005300e-15 -3.667123e-15 -8.458012e-16 -8.499463e-18 -2.158033e-15 1.804721e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -1.751197e-15 -5.897173e-15 -3.591895e-15 3.529035e-15 -3.537386e-15 4.133218e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -6.202778e-15 -1.826065e-15 3.489741e-15 6.402867e-15 -4.306476e-15 6.997294e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 6.443477e-15 -1.015253e-14 -1.480067e-15 8.190415e-15 -8.160589e-15 6.378546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368ad1b32d5e.final.pdb | -9.147840e-15 -1.513792e-15 1.060518e-15 -6.620998e-16 -4.550241e-15 -5.045448e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -4.134274e-15 -2.142798e-15 -6.331241e-15 3.147395e-16 -1.022171e-14 -1.206207e-15 |
| File Path                                      | X Coordinates | Y Coordinates | Z Coordinates | Temperature | Formula |
|-----------------------------------------------|---------------|---------------|---------------|-------------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | -3.421751e-15 | -1.204223e-14 | 2.065530e-15  | -6.287579e-16 | 5.193955e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb     | -5.197980e-15 | -1.845467e-15 | -1.595169e-15 | 1.802749e-16  | -7.790651e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb     | -6.885432e-15 | -3.135715e-15 | -3.302731e-15 | -2.138601e-15 | -4.885770e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb     | -7.079616e-15 | -3.422422e-15 | -3.99805e-15  | 5.417983e-16  | 7.766609e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb     | -1.751197e-15 | -5.897173e-15 | -3.591895e-15 | 3.529035e-16  | -3.537386e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb     | -6.516662e-15 | -8.247967e-15 | 6.742360e-15  | 3.112332e-15  | -5.781099e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb     | -8.969541e-15 | -3.101314e-15 | -1.537529e-15 | -1.550057e-15 | -2.535857e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb     | -1.751197e-15 | -5.897173e-15 | -3.591895e-15 | 3.529035e-16  | -3.537386e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea517be32db050e.final.pdb     | -4.77189e-15  | -7.301586e-15 | -1.412839e-15 | 2.896383e-15  | -6.747475e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | -5.042723e-15 | -4.228684e-15 | -3.13892e-15  | 6.607933e-16  | -2.839208e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb     | -5.006063e-15 | -3.893288e-15 | -2.48058e-16  | 5.076693e-16  | -2.468766e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb     | -4.764949e-15 | -4.819340e-15 | -5.05763e-16  | 2.778687e-16  | -2.748374e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb     | -6.769934e-15 | -2.980708e-15 | 2.602995e-15  | -1.045150e-15 | -2.531658e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb     | -3.447048e-15 | -3.638432e-15 | 4.059294e-16  | -1.728669e-15 | -7.080350e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb     | -5.79821e-14  | 2.408312e-15  | 1.110818e-14  | -6.736536e-15 | -6.995743e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb     | -7.079616e-15 | -3.422422e-15 | -3.99805e-15  | 5.417983e-16  | 7.766609e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb     | -3.171893e-15 | [-,781]       | [-,782]       | [-,783]       | [-,784] |

Supplementary Text 10

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\40.1ns_data\NAT0.pdb
-5.703916e-15 -9.660611e-16 3.608321e-15 -3.755028e-15 -8.343957e-16
-2.978764e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\40.1ns_data\LJP6.pdb
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Supplementary Text 10

-4.620258e-15  3.235559e-16  1.052770e-15 -4.906675e-15 -1.731131e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
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E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-6.927416e-15 -3.055892e-15  2.724080e-15 -3.007129e-15 -2.690170e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
-5.296235e-15 -8.320598e-17  1.844665e-15 -3.463627e-15 -2.836134e-16
Supplementary Text 10

6.294123e-15 -8.440918e-15 -4.162229e-15 -8.081689e-16 1.337666e-15
-6.823309e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb

-5.741822e-15 -5.803779e-15 2.950385e-15 -2.501348e-15 -1.975826e-15
-7.505456e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb

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3.350615e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb

-8.388577e-15 2.585183e-15 5.494194e-15 -6.050429e-15 -1.954618e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb

-9.536996e-15 -5.737342e-16 2.600781e-15 -5.135700e-15 -3.364113e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb

-9.350615e-15 2.585183e-15 5.494194e-15 -6.050429e-15 -1.954618e-15

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-8.388577e-15 2.585183e-15 5.494194e-15 -6.050429e-15 -1.954618e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb

-5.851409e-15 2.738391e-15 3.480629e-15 -7.962906e-15 -1.026947e-14
3.173936e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d66a.final.pdb

Page 658
-2.489489e-16 -5.463797e-15 -5.456659e-15 2.259090e-16 -4.123133e-16
-2.792407e-15 -2.266238e-15 -4.066734e-15 -6.705145e-15 -4.950312e-15
-7.273850e-15
-5.136996e-15 -5.737342e-16 2.600781e-15 -5.135700e-15 -3.364113e-15
-6.92187e-15
-6.635504e-15 4.488293e-15 1.068232e-14 5.113439e-15 4.557207e-15
-1.33152e-14
-2.847869e-15 -4.249285e-15 3.608123e-15 -2.256161e-15 -3.705893e-15
-2.805450e-15
-9.536996e-15 -5.737342e-16 2.600781e-15 -5.135700e-15 -3.364113e-15
-6.92187e-15
-6.221122e-15 -2.426748e-15 1.086702e-15 -4.080595e-15 -1.218121e-15
-3.158238e-15
-6.473876e-15 -3.101240e-15 7.095892e-16 -4.064837e-15 -9.431352e-16
-3.045274e-15
-7.583642e-15 -2.260343e-15 2.162289e-15 -2.400383e-15 -1.998782e-15
-2.855177e-15
-4.706643e-15 8.564272e-17 -4.671613e-16 -4.838628e-15 -1.179884e-16
-3.178691e-15
-8.822475e-15 -7.075925e-15 -1.015084e-14 -1.886225e-15 1.462353e-15
-3.796870e-16
-2.847869e-15 -4.249285e-15 3.608123e-15 -2.256161e-15 -3.705893e-15
-2.805450e-15
| File Path                                                                 | Data       |
|---------------------------------------------------------------------------|------------|
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb                               | 2.609602e-15 4.946202e-15 6.372577e-15 3.893019e-15 -7.224477e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb                               | 1.702599e-15 2.689352e-15 5.015356e-15 3.587576e-15 -6.473057e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                               | 2.581703e-15 3.923107e-15 4.987632e-15 2.750377e-15 -6.280643e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb    | 3.846526e-15 4.249584e-15 5.342010e-15 4.328670e-15 -5.489771e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb    | 2.418453e-15 3.955389e-15 4.495561e-15 3.752448e-15 -6.416651e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcede4b419d9.final.pdb     | 4.893281e-15 2.499442e-15 2.426018e-15 4.624824e-15 -7.434485e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb     | 4.165000e-15 3.358444e-15 6.527061e-15 3.888402e-15 -5.074286e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb     | 1.687347e-15 4.861799e-15 7.234395e-15 4.672930e-15 -1.358121e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb     | 1.913974e-15 3.720551e-15 4.892487e-15 4.355047e-15 -6.095023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eb2.final.pdb      | 2.653669e-15 4.148634e-15 4.892520e-15 3.870648e-15 -6.113772e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551be0a39.final.pdb      | 2.664426e-15 6.280061e-15 6.243407e-15 -8.26308e-15 -6.570978e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551be0a39.final.pdb      | 2.664426e-15 6.280061e-15 6.243407e-15 -8.26308e-15 -6.570978e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb     | 1.794198e-15 5.955444e-15 1.098341e-14 3.320312e-15 1.499983e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb      | 4.766924e-15 6.134423e-15 1.866912e-14 1.539579e-14 -3.16502e-15 -3.693420e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fcd42.final.pdb     | 2.222186e-15 3.656936e-15 5.156472e-15 3.938307e-15 -5.913783e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b.f0.final.pdb    | 3.396130e-15 4.018530e-15 2.862027e-15 5.213324e-15 -7.448028e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb     | 1.621716e-15 1.086675e-14 3.950725e-15 2.087317e-15 -4.758642e-15 |
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4.964555e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
2.565117e-15 3.866501e-15 4.993132e-15 4.010266e-15 -5.562448e-15
2.224829e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb
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2.224829e-15
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-1.923560e-15 1.230331e-14 7.566455e-15 2.295280e-15 -1.766725e-15
-1.495760e-15
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1.318137e-15 5.984630e-15 -1.390744e-15 -2.638532e-16 -4.140516e-15
3.987126e-15
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2.482725e-15 3.687310e-15 4.951805e-15 3.925600e-15 -5.747649e-15
2.855527e-15
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5.209452e-15
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-6.619070e-16 3.435141e-15 5.039066e-15 6.907729e-15 -4.571677e-15
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3.397382e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12d3f9.final.pdb
1.386020e-15 8.620534e-15 2.656462e-15 6.506994e-15 -5.608263e-15
3.954825e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
4.416501e-15 3.358444e-15 6.527061e-15 3.888402e-15 -5.074286e-15
2.552421e-15
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4.893281e-15 2.499442e-15 2.426018e-15 4.624824e-15 -7.434485e-15
5.209452e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8c0eefce12d3f9.final.pdb
1.860250e-15 5.414932e-16 1.427998e-14 3.065737e-15 -1.192336e-14
8.659666e-15
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1.005218e-14 -7.616099e-16 1.206073e-14 -3.029822e-15 -7.188882e-15
6.787238e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
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-5.508363e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9ddd8ed081fb3ef.final.pdb
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1.488874e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
2.979956e-15 2.073488e-15 6.028500e-15 2.520329e-15 -4.235523e-15
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| File | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 2.673990e-15 |
|------|-------------------------------------------------|----------------|
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 1.780690e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 5.468705e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\abf4d74b9c71d4dc.final.pdb | 2.327717e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac4f4d74b9c71d4dc.final.pdb | 3.396130e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\add8823e4b4c668e.final.pdb | 2.022469e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab16ababd03b7b857.final.pdb | 1.860250e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 2.416868e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 4.807379e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 4.893281e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 6.109238e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 4.148634e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 4.443795e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b2a1f55fc9d0681.final.pdb | 6.109238e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b3e34248de381a3c.final.pdb | 3.388208e-15 |
|      | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | 3.023401e-15 |
| Path                                                                 | Values                          |
|---------------------------------------------------------------------|---------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 3.126645e-15                    |
| 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -1.08874e-14 3.894058e-15 5.598100e-15 4.79238e-15 -1.071050e-15 |
| -1.879529e-15                                                 | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.195282e-15 2.645429e-15 5.864962e-15 4.964309e-15 -7.178673e-15 |
| -6.90457e-15                                                  | 2.702307e-15                    |
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-1.252935e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-1.099920e-15 3.367985e-15 8.706741e-15 -2.016872e-17 -3.561612e-15

[,793] [,794] [,795] [,796] [,797] [,798]

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
8.938063e-16 3.639432e-15 -5.631291e-16 -6.22396e-15 5.665151e-15 -4.751665e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-9.180723e-16 3.485332e-15 -1.601077e-15 -6.487697e-15 4.475694e-15 -5.008160e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-2.216881e-16 2.399800e-15 -1.664885e-15 -7.715358e-15 2.822874e-15 -3.533700e-15

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-3.950518e-16 3.389899e-15 -8.64333e-16 -5.085955e-15 6.099590e-15 -4.859823e-15

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4.449822e-16 2.465759e-15 -7.636360e-16 -5.675348e-15 5.070818e-15 -3.609378e-15

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-1.921564e-15 1.007832e-14 1.046943e-15 1.277517e-15 6.431940e-15 5.556692e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0ba5f93306825e8.final.pdb
-3.994934e-17 3.646377e-16 -4.373554e-15 -5.883720e-15 1.767700e-15 -5.603335e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
4.239613e-15 8.565293e-15 -2.639944e-16 -1.235710e-15 5.489007e-15 -3.687024e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
6.117467e-17 2.759093e-15 -1.423915e-15 -5.997031e-15 5.178912e-15 -4.102483e-15

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
4.220241e-16 2.780856e-15 -6.740293e-16 -6.362749e-15 5.072874e-15 -4.479997e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0f8a00b551bea0a9.final.pdb
-1.542626e-15 1.080737e-14 1.046943e-15 1.277517e-15 6.431940e-15 -6.540883e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\129f45328d47579a.final.pdb
1.117647e-14 -1.019068e-14 -3.361463e-15 -1.704108e-14 1.991093e-15 -8.081953e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
9.387098e-15 3.768809e-16 -7.014357e-15 1.084937e-14 1.001788e-14 -1.437239e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb
4.602111e-16 1.759076e-15 -8.114192e-16 -4.83707e-15 5.367624e-15 -3.537302e-15

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| File Path                                                                 | Value                                    |
|--------------------------------------------------------------------------|------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456ddf6ff2868d.final.pdb      | 6.663012e-15 -1.856309e-15 -3.577822e-15 -1.508400e-15 -4.793746e-15 -2.003991e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53f3c8f7ef.final.pdb        | -8.980900e-16 1.631557e-15 5.524422e-15 2.112411e-15 -1.515338e-16 2.908009e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | 5.139313e-15 4.594207e-15 -3.865663e-15 -2.019431e-17 -2.669893e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb      | -6.246759e-15 4.349773e-14 8.739121e-16 -6.326594e-16 -5.627559e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0a0df1be4.final.pdb        | -8.898090e-16 1.631557e-15 5.524422e-15 2.112411e-15 -1.515338e-16 2.908009e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\76f910ffbf22872d.final.pdb       | -2.098153e-15 1.257970e-15 -3.578969e-16 -4.256299e-15 -2.462633e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c67a50d3135.final.pdb       | -6.220626e-15 -3.801143e-17 -4.286344e-16 -5.168945e-15 -4.469439e-16 -1.681225e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb       | -8.400024e-15 -9.173663e-15 3.89692e-15 -1.038073e-14 4.135349e-15 -3.920797e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -4.128781e-15 3.04665e-15 -1.317382e-15 -7.761817e-15 -3.142883e-15 -3.101018e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb       | -4.128781e-15 3.04665e-15 -1.317382e-15 -7.761817e-15 -3.142883e-15 -3.101018e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb       | -4.059785e-15 1.256424e-16 2.860266e-15 -4.961106e-15 -6.251942e-15 -2.558917e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb       | -2.057552e-15 1.904171e-15 -3.559223e-15 -4.664735e-15 -2.466588e-15 -1.875389e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb       | -8.898090e-16 1.631557e-15 5.524422e-15 2.112411e-15 -1.515338e-16 2.908009e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb       | -2.938967e-15 9.024384e-16 3.210453e-14 -7.797760e-15 -1.784420e-15 3.110843e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb       | -5.133913e-15 4.594207e-15 -3.865663e-15 -2.019431e-17 -2.669893e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\998bbe0d5986c138f.final.pdb       | -4.059785e-15 1.256424e-16 2.860266e-15 -4.961106e-15 -6.251942e-15 -2.558917e-15 |
Supplementary Text 10

-6.220262e-15 -3.801143e-17 -4.288634e-16 -5.168945e-15 -4.469439e-16
-1.681225e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d7e2fa.final.pdb
3.796981e-15 2.990538e-15 -5.058747e-15 -3.268449e-15 4.201502e-15
-1.982121e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
3.759860e-15 -8.777760e-15 8.610062e-15 -3.526312e-16 -1.709566e-14
-6.021914e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b361666e033b.final.pdb
-3.856922e-15 1.361042e-15 9.590466e-15 -5.608876e-15 2.663138e-16
-2.156881e-15

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-1.234782e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb
-3.846333e-16 1.092652e-15 1.092652e-15 -3.824903e-16 2.835735e-15
-3.855550e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb
-1.892338e-15 1.165286e-15 5.503433e-15 -4.075136e-15 -1.033783e-15
-2.341456e-15

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-3.101018e-15

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-2.154571e-15 5.089142e-15 3.572125e-15 -4.396462e-15 -1.154936e-15
-2.788171e-15

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-1.982121e-15

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5.688495e-16 4.143436e-15 3.902022e-15 -1.171425e-15 -4.553611e-15
-8.593765e-16

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-1.681225e-15

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-7.777949e-15 4.446254e-15 -3.903800e-15 -9.953025e-15 7.910810e-15
1.471658e-15

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-1.681225e-15

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-2.351696e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
Supplementary Text 10

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb |
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| 1.799921e-15  3.269937e-15  6.154506e-15 -3.753305e-15  7.679189e-15  |
| -1.733189e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb |
|-----------------------------|
| 6.144324e-17 -2.506042e-15  1.555107e-14 -7.166807e-15 -2.419504e-15  |
| -4.013483e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb |
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| -4.063435e-16 -4.014548e-15 -6.163071e-16 -4.176194e-15 -9.721926e-16 |
| 1.409586e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb |
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| -1.089397e-15  6.058566e-15  5.887265e-15 -6.634344e-16  5.960908e-15 |
| -2.097559e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb |
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| -7.036440e-15  1.205983e-15  6.221197e-16 -2.015030e-15  5.298269e-16 |
| 2.375472e-16 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb |
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| 6.794754e-16  6.776387e-15 -2.243120e-14 -7.984269e-15  3.032967e-15 |
| -2.508072e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb |
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| -3.290003e-16 -1.516949e-16 -7.626511e-16 -7.784640e-15  3.829744e-15 |
| 4.050992e-15 |

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| -7.495189e-15  7.475081e-15 -1.064667e-14 -2.060076e-14  1.405130e-14 |
| 1.086983e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb |
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| 3.651344e-15  1.049804e-15 -4.450668e-16  1.942732e-14 -8.280352e-15 |
| -6.570827e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d529e19ad281fda2.final.pdb |
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| -3.45585e-15  2.143563e-15  2.824560e-15 -2.001935e-15 -7.110479e-16 |
| -1.308135e-16 |

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| -3.101018e-15 |

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| -1.681225e-15 |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef642fc83b81e5d.final.pdb |
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| -1.498995e-15  1.485076e-15  3.916619e-15 -1.750672e-15 -4.839117e-17 |
| -2.461851e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | -2.145845e-15  1.211241e-15  3.189613e-15 -3.373328e-15 -1.231303e-15 -1.745260e-15  9.804709e-15  1.811243e-15  3.607781e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | -1.745260e-15  1.361042e-15  9.590466e-15 -5.608876e-15  2.663138e-15 -2.474162e-15  4.098049e-15 -4.934848e-16  8.901781e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | -3.856922e-15  1.361042e-15  9.590466e-15 -5.608876e-15  2.663138e-15 -2.156881e-15  4.098049e-15 -4.934848e-16  8.901781e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | -2.408432e-15  2.704431e-15  2.164627e-15 -8.521624e-16  1.833984e-15 -1.788727e-15  4.098049e-15 -4.934848e-16  8.901781e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | -1.830169e-15  3.474800e-15  4.514924e-15 -1.997220e-15  2.754455e-15 -1.388500e-15  2.972295e-15 -4.24823e-15  8.308715e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -1.143950e-15  2.972295e-15  2.448423e-15 -1.242814e-15  4.304883e-15 -1.006685e-15  2.337373e-16  9.21539e-16  3.802871e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb | -1.96751e-15  2.21539e-15  2.939452e-15 -1.185723e-15  3.802871e-15 -1.814960e-15  5.21257e-16  1.899638e-16  2.857803e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | -3.378996e-15  1.599718e-15 -3.117867e-15 -2.069792e-15  6.454652e-15 -3.144357e-15  2.408432e-15  2.704431e-15  4.514924e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | -4.350491e-15  7.064351e-15  1.519809e-15 -5.914925e-15  2.950851e-15 -1.806251e-15  5.721257e-16  1.899638e-16  2.857803e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | -7.386731e-16  1.625877e-15  2.847245e-16 -1.007658e-15  3.374050e-15 -1.865616e-15  4.350491e-15  7.064351e-15  1.519809e-15 |
Supplementary Text 10

-1.806251e-15

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-9.473051e-17  5.009260e-15  6.003957e-15  8.776116e-16  -5.774498e-15

-3.573318e-15

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-5.092960e-15  5.600804e-15  6.603957e-15  8.776116e-16  -5.774498e-15

-3.553318e-15

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-7.891620e-16  2.823566e-15  1.460149e-16  -9.138157e-16  4.175659e-15

-1.903379e-15

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1.815977e-16  1.439935e-15  -4.593318e-15  1.819074e-15  6.869629e-16

-1.921127e-15

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-4.632883e-16  -5.863947e-15  -1.422542e-15  -6.783490e-15  4.512380e-15

-3.280390e-15

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-9.017516e-15  -4.519653e-15  5.269539e-15  -2.164778e-15  1.421712e-14

-8.824661e-15

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-4.664575e-15  3.137073e-15  3.743065e-15  -3.602814e-15  6.312897e-15

-2.912811e-15

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-4.885313e-16  -1.883190e-16  -7.164612e-15  -6.401134e-16  2.839755e-15

-3.291342e-15

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-8.824661e-15

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3.936743e-15  -5.350751e-15  -1.071043e-14  -1.847422e-14  2.116079e-15

-2.912765e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8cdff0.final.pdb
-1.116009e-14  -6.069790e-16  1.510273e-14  5.976339e-15  1.70143e-14

1.064000e-14

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4.045040e-16  6.268141e-15  -3.352388e-15  -1.712182e-15  1.821698e-15

-4.873566e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
2.901029e-15  7.964202e-15  -3.352922e-15  -9.611286e-15  3.539883e-15

-2.047795e-15

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-9.742110e-15  1.651283e-15  5.387583e-15  9.085821e-15  8.339054e-15

-3.640394e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62c6a25f.final.pdb
3.555281e-15  6.713437e-15  1.228022e-15  -1.811779e-16  7.637060e-16

-6.683567e-16

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-2.911811e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
2.402814e-15  -1.819781e-15  7.851111e-15  4.445815e-15  3.830854e-15

-4.791037e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
-3.378996e-15  1.599718e-15  -3.117867e-15  -2.069792e-15  6.454652e-15

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| File Path | Z Score 1 | Z Score 2 | Z Score 3 | Z Score 4 | Z Score 5 |
|-----------|-----------|-----------|-----------|-----------|-----------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 1.490455e-15 | 1.190790e-17 | 6.756986e-15 | -3.897887e-15 | 7.221445e-16 | 2.696219e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | -7.481482e-16 | -1.488682e-15 | -1.587444e-15 | 7.286525e-16 | -8.712242e-16 | -4.926954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 1.390813e-15 | 1.301229e-15 | 9.406073e-15 | -5.896982e-15 | -3.264689e-15 | 6.031734e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 3.630670e-15 | -2.049308e-15 | 6.879620e-15 | -6.138072e-15 | -6.902464e-15 | -7.947193e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 1.490455e-15 | 1.190790e-17 | 6.756986e-15 | -3.897887e-15 | 7.221445e-16 | 2.696219e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 1.490455e-15 | 1.190790e-17 | 6.756986e-15 | -3.897887e-15 | 7.221445e-16 | 2.696219e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -2.807486e-15 | 4.885393e-15 | 1.465444e-14 | -8.427723e-15 | -1.058408e-14 | 2.012349e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -1.116643e-15 | -1.288235e-15 | 3.764486e-15 | -1.697736e-15 | -1.735784e-15 | 7.416231e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffe4.final.pdb | -1.266696e-15 | -1.004490e-14 | 2.060356e-14 | -3.35608e-15 | -5.14835e-15 | -3.627459e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6f8f9178986bef01.final.pdb | -7.773402e-15 | -2.475400e-15 | 7.191464e-15 | -1.659016e-15 | 1.673141e-15 | 1.458253e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -2.852771e-16 | 6.636735e-17 | 2.678143e-15 | -5.168918e-15 | -3.604081e-15 | 6.243124e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 1.490455e-15 | 1.190790e-17 | 6.756986e-15 | -3.897887e-15 | 7.221445e-16 | 2.696219e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb | -2.346986e-16 | -1.837118e-15 | 4.404122e-15 | -1.795453e-15 | -1.152819e-15 | 1.275611e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | -7.481482e-16 | -1.488682e-15 | -1.587444e-15 | 7.286525e-16 | -8.712242e-16 | -4.926954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | -4.891404e-16 | -5.791196e-15 | 9.487374e-15 | -2.072943e-15 | 4.965031e-15 | -5.058122e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -2.445773e-15 | 7.434875e-17 | 1.644475e-15 | -2.591753e-15 | -2.267186e-15 | 1.080854e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feda.final.pdb | -2.445773e-15 | 7.434875e-17 | 1.644475e-15 | -2.591753e-15 | -2.267186e-15 | 1.080854e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12df9.final.pdb | -3.121882e-15 | -4.640847e-15 | 8.114014e-16 | -1.337548e-15 | -3.034046e-15 | 6.342577e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d0469ef569760.final.pdb | -2.852771e-16 | 6.636735e-17 | 2.678143e-15 | -5.168918e-15 | -3.604081e-15 | 6.243124e-16 |
| Path                                                                 | Values                                                                 |
|----------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -7.481482e-16 -1.488682e-15 -1.587444e-15 7.286525e-16 -8.712242e-16 -4.926954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -7.481482e-16 -1.488682e-15 -1.587444e-15 7.286525e-16 -8.712242e-16 -4.926954e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | -6.995760e-16 -1.339659e-15 3.794345e-15 -1.921138e-15 -1.986651e-15 7.365731e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 4.690879e-15 5.088242e-15 1.423363e-14 -2.937830e-15 2.831925e-15 2.671474e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 7.903534e-16 -1.106998e-15 3.117255e-15 -5.554661e-15 -1.561153e-15 5.512078e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | -1.354885e-15 3.758555e-15 2.754169e-16 -5.220446e-15 3.399173e-15 2.715708e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | -4.999955e-16 -4.304030e-15 8.864454e-15 3.453036e-15 1.069064e-15 -8.706482e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 5.456465e-19 -1.777795e-15 4.527870e-15 -1.895530e-15 -3.102296e-16 2.521204e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -2.706783e-15 -1.526107e-14 4.519387e-15 3.933678e-15 2.069944e-15 -4.15813e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -5.836828e-16 -8.234883e-16 -5.674060e-15 1.494741e-15 -4.070960e-15 6.878830e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | 3.741914e-15 4.856895e-15 2.990691e-15 -8.334634e-15 -5.232690e-15 4.378762e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 1.847080e-15 -1.269158e-14 -1.621051e-15 8.162778e-15 4.836201e-16 -2.214133e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | -2.120777e-15 -3.327120e-16 2.601961e-15 -1.765095e-15 -3.132572e-15 3.636786e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e52919ad281fe2a.final.pdb | -4.565707e-15 -9.623237e-16 7.826802e-15 1.211395e-15 -1.414860e-15 1.227129e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 2.946795e-15 4.993798e-15 1.618196e-14 -1.616964e-14 -5.042158e-15 6.202822e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5df9e72307a2fbd.final.pdb | 1.390813e-15 1.301229e-15 9.406073e-15 -5.896982e-15 -3.264689e-15 6.031734e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea0f8694090cae7.final.pdb | -2.445773e-15 7.434875e-17 1.644475e-15 -2.591753e-15 -2.267186e-15 1.108054e-15 |
| File Path                                                                 | Values                                                                 |
|---------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb       | -5.011024e-16 -8.029428e-16 1.455589e-15 -2.099611e-15 1.863392e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f98641eeb2.final.pdb        | -3.679703e-15                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a0b551bea0a39.final.pdb       | -3.94519e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb        | -3.727663e-16 -1.159985e-15 9.638347e-16 -1.815635e-15 1.72218e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb        | -5.417196e-15 3.212426e-15 5.887720e-15 2.614245e-15 7.109292e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fcd42.final.pdb        | -3.997254e-16 -1.631355e-15 4.662753e-16 -1.068356e-15 2.287422e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb        | 6.481770e-17 -5.107348e-15 -2.273159e-15 -8.112302e-16 1.864999e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb        | -5.417196e-16 -3.212426e-15 5.887720e-15 2.614245e-15 7.109292e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32827197b7ab.final.pdb        | -4.11071e-16 -5.91507e-16 2.713689e-16 -5.86460e-15 -1.937271e-16     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb        | 4.339383e-16 -3.379034e-16 5.902711e-16 -2.862443e-15 1.616479e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | -6.89780e-16 -1.587594e-15 -9.222434e-16 -2.137209e-15 4.840793e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb        | -5.903387e-15 7.597012e-15 -8.070518e-15 3.620907e-15 5.083209e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | -4.691279e-16 -2.356916e-15 -1.217705e-15 -5.908702e-15 -8.611155e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdcfb.final.pdb       | -1.110854e-14 1.091109e-14 2.065121e-14 -3.546889e-15 5.289243e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | 8.356099e-15                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb       | -4.965278e-15 -6.362218e-15 9.914617e-16 7.876916e-16 -9.291372e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48b4a5c7c6682ce6.final.pdb        | 2.840955e-15 -3.979737e-15 8.587817e-15 -4.582039e-15 -2.471575e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4a4b4a5c7c6682ce6.final.pdb       | -6.280743e-15 -1.065864e-14 4.343194e-15 -5.882597e-15 -1.905877e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ea45b62cb6a25f.final.pdb         | 2.41143e-16                                                        |
Supplementary Text 10

-1.839980e-15 -3.801862e-16 -4.068726e-15 -1.220578e-15 2.724983e-15
-3.582660e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\669942ef97459a2.final.pdb

-1.476050e-15 3.596330e-16 -1.652128e-15 -3.768934e-15 2.825502e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb

-1.839980e-15 -3.801862e-16 -4.068726e-15 -1.220578e-15 2.724983e-15
-3.582660e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb

-1.839980e-15 -3.801862e-16 -4.068726e-15 -1.220578e-15 2.724983e-15
-3.582660e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb

-4.636934e-16 -1.276605e-15 7.043661e-16 -1.580967e-15 1.824216e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb

-3.460969e-15 -2.745447e-15 -3.645846e-15 -6.773943e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\cd338f55f4e003e9.final.pdb

4.002559e-15 -4.438103e-15 1.954972e-15 -1.138674e-14 -2.417263e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb

3.049989e-15 -2.059399e-15 2.438222e-15 2.639777e-15 -1.466069e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb

6.360831e-16 -2.128450e-15 1.037126e-15 1.244644e-16 -3.821592e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1e34248de3e813c.final.pdb

4.002559e-15 -4.38103e-15 1.954972e-15 -1.138674e-14 -2.417263e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1e34248de3e813c.final.pdb
### Supplementary Text 10

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | 3.759727e-15 | 4.574933e-15 | 2.468396e-15 | -6.580747e-15 | 4.604686e-16 | -5.950507e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb | 6.481770e-17 | -5.107348e-15 | -2.273159e-15 | -8.112302e-16 | 1.864899e-15 | -4.184217e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | -1.839980e-15 | -3.801862e-16 | -4.068726e-15 | -1.220578e-15 | 2.724983e-15 | -3.582660e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb | -2.115214e-16 | -1.283123e-15 | 1.084273e-15 | -1.215408e-15 | 1.871508e-15 | -3.834726e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | -4.717306e-16 | -8.904583e-16 | 7.775871e-16 | -2.107114e-15 | 2.125190e-15 | -3.770259e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 6.360831e-16 | -2.128450e-15 | 1.037126e-15 | 2.021592e-15 | -2.114866e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | -1.728946e-15 | -6.407682e-16 | -1.378235e-15 | 3.339696e-16 | 2.763909e-15 | -2.371623e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 2.840955e-15 | -3.979737e-15 | 8.587817e-16 | -4.582039e-15 | -2.107114e-15 | -2.390255e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 2.336930e-15 | -1.004061e-17 | 3.794588e-15 | -2.876972e-15 | 3.285260e-15 | 1.043244e-15 |

[,823]        [,824]        [,825]        [,826]        [,827]        [,828]        
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb | 2.446896e-15 | 6.741100e-15 | 1.087528e-15 | 1.030971e-15 | -2.621331e-15 | -1.387235e-15 | 3.339696e-16 |
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb | 1.861324e-15 | 5.085527e-15 | 1.626140e-15 | 8.703131e-16 | -1.168997e-15 | 1.347183e-15 |
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | 1.060790e-15 | 5.434459e-15 | 1.330430e-15 | -1.481904e-15 | -2.665343e-15 | 6.284081e-16 |
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | 1.357857e-15 | 7.248158e-15 | 2.911533e-15 | -3.844441e-16 | -1.891503e-15 | 4.634334e-17 |
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 7.608394e-15 | 6.248619e-15 | 9.723281e-15 | -2.132417e-15 | 2.420487e-15 | 2.337725e-15 |
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 1.105018e-15 | 4.560945e-15 | 6.979295e-16 | 3.987961e-16 | -1.508328e-15 | 5.201213e-16 |
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb | 1.420992e-15 | 3.244164e-15 | -6.228492e-16 | -2.541414e-15 | -3.123020e-15 | 3.190802e-16 |
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0db59f3306825e8.final.pdb | 2.642748e-15 | 4.702981e-15 | 1.190176e-15 | 8.478376e-16 | -1.255393e-15 |
| PDB ID | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 1.856302e-16 |
|--------|---------------------------------------------------------------|--------------|
|         | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ea45b62cb6a25f.final.pdb | -9.131471e-15 |
| 4ab4a5c7c6682ce6.final.pdb | 7.465101e-16 | 1.829151e-15 | -6.193622e-15 | -1.060013e-14 | -4.404875e-15 |
| 4ea45b62cb6a25f.final.pdb | 2.494838e-16 | 1.547652e-15 | 4.569309e-15 | -2.682080e-16 | -3.140755e-15 | -1.943889e-15 |
| 4eaa45b62cb6a25f.final.pdb | -3.860947e-15 | 8.176337e-16 | -2.403574e-15 | 3.333480e-15 | -1.929983e-15 | -4.291684e-15 |
| 58c371611d85ac96.final.pdb | -3.946800e-15 | 6.642229e-16 | -1.180889e-16 | 9.419088e-16 | -1.609307e-15 | -2.174741e-16 |
| 59a647f04822d30a.final.pdb | -1.420992e-15 | 3.244164e-15 | -6.228492e-16 | -2.541414e-15 | -1.23020e-15 | 3.190002e-15 |
| 59b091fe385e05fc.final.pdb | -2.694838e-16 | 1.547652e-15 | 4.569309e-15 | -2.682080e-16 | -3.140755e-15 | -1.943889e-15 |
| 5f60752431cf2dcf.final.pdb | -3.946800e-15 | 6.642229e-16 | -1.180889e-16 | 9.419088e-16 | -1.609307e-15 | -2.174741e-16 |
| 626456dd6ff2868d.final.pdb | 2.642748e-15 | 4.702981e-15 | 1.190176e-15 | 8.478376e-16 | -1.255393e-15 | 4.530415e-15 |
| 6583d53ff3c8f7ef.final.pdb | -3.946800e-15 | 6.642229e-16 | -1.180889e-16 | 9.419088e-16 | -1.609307e-15 | -2.174741e-16 |
| 69760178986bef01.final.pdb | 1.002555e-15 | 5.368018e-15 | -2.985408e-15 | 6.157809e-16 | -3.322262e-16 | 6.194311e-17 |
| 716d9624611d1c42.final.pdb | 8.577990e-15 | 9.701798e-15 | 9.728466e-15 | -6.168845e-16 | -3.033812e-15 | -4.518708e-15 |
| 769f910fffb22872.final.pdb | 1.553389e-15 | 4.695378e-15 | 1.921834e-15 | 4.213366e-16 | -2.218415e-15 | -9.175868e-18 |
| 791f8c80dd5c3135.final.pdb | 1.420992e-15 | 3.244164e-15 | -6.228492e-16 | -2.541414e-15 | -3.123020e-15 | 3.190002e-16 |
| 7f9e9a6633196.final.pdb | 2.930656e-15 | 7.835873e-15 | 6.740185e-16 | -6.037905e-16 | 3.08590e-15 | 5.020671e-15 |
| 8048b9c94a633196.final.pdb | 7.348953e-15 | 7.584837e-15 | 5.141552e-15 | -5.694278e-16 | -2.944363e-15 | 7.348953e-15 |
| Path                                                                 | 4.004656e-15 | 7.348953e-15 | 5.141552e-15 | -5.694278e-16 | -2.944436e-15 |
|----------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | 4.04656e-15  | 7.584837e-15 | -5.694278e-16| -2.944436e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eeefce12d3f9.final.pdb | 4.04656e-15  | 5.118562e-15 | 5.559892e-15 | -5.904959e-15| -5.084984e-16 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 4.04656e-15  | 4.702981e-15 | 1.190176e-15 | -1.253939e-15| 4.530415e-15  |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -3.946800e-15| 6.642229e-16 | -1.80889e-16 | 9.419088e-16  | -2.174741e-16 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -4.884751e-15| 3.709464e-15 | -3.082772e-15| 8.703926e-16  | -1.023895e-14 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -4.65838e-15 | 3.439245e-15 | -1.001820e-15| -7.994838e-15| 3.183985e-15  |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | 1.420992e-15 | 3.244164e-15 | -6.228492e-16| -2.541414e-15| -3.123020e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 6.37360e-15  | 5.13844e-15  | -1.739385e-16| 3.445806e-15  | 3.935369e-15  |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | 1.439517e-15 | -1.856764e-15| -8.887387e-15| 2.850991e-16  | -7.842016e-16 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b361e6033b.final.pdb | 2.103629e-15 | 5.833073e-15 | -4.260398e-15| 4.283518e-16  | -1.397272e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 2.494838e-16 | 1.547652e-15 | 4.569309e-15 | -2.682080e-16| -3.140755e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -1.943889e-15| 1.513583e-14 | -5.189383e-16| -2.618465e-16| -4.474563e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 1.865800e-15 | 4.109496e-15 | 2.268627e-15 | -1.840008e-16| -1.957804e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | 7.348953e-15 | 7.584837e-15 | 5.141552e-15 | -5.694278e-16| -2.944436e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 1.261184e-15 | 4.476875e-15 | 2.047649e-15 | 3.727653e-16  | -2.178758e-15 |
|---------------------------------------------------------------------|--------------|--------------|--------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 6.37360e-15  | 5.13844e-15  | -1.739385e-16| 3.445806e-15  | 3.935369e-15  |
| File Path                                                                 | Values                      |
|---------------------------------------------------------------------------|----------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | 3.190802e-16               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fca8f1df.final.pdb        | 7.275343e-15 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb       | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e.final.pdb         | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb         | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb         | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb         | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f8eef39.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8090ef10197e.final.pdb           | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e116391d3707839.final.pdb         | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f2ea.final.pdb        | 3.190802e-16 -2.666822e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602087178ec3a1.final.pdb        | 3.190802e-16 -2.666822e-15  |
| Path                                                                 |
|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb  |
| 5.043364e-15 -1.293638e-15 6.594491e-15 -1.888837e-15 -2.291592e-16 |
| 1.398763e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb  |
| 5.043364e-15 -1.293638e-15 6.594491e-15 -1.888837e-15 -2.291592e-16 |
| 1.398763e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb  |
| 5.043364e-15 -1.293638e-15 6.594491e-15 -1.888837e-15 -2.291592e-16 |
| 1.398763e-15                                                         |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb  |
| 5.043364e-15 -1.293638e-15 6.594491e-15 -1.888837e-15 -2.291592e-16 |
| 1.398763e-15                                                         |

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-3.978669e-15 -1.005667e-14 -9.864099e-15  1.322353 e-14  4.003909e-15
-7.393621e-15

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-2.735343e-15  2.093506e-16 -2.328915e-15 -5.059343 e-15  9.095124e-15
9.714479e-15

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3.855045e-16

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-2.145891e-15

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4.700728e-15

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7.967981e-15

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4.906003e-15

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-2.030959e-15

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1.290876e-14

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4.131845e-15

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-5.600972e-15 -4.050710e-16 -1.279312e-15  6.100992e-15  4.982950e-16
3.559704e-15

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4.906003e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb

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| File Path | Supplementary Text 10 |
|-----------|-----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb | -2.049383e-15 -1.138522e-15 -3.500569e-15 3.912766e-15 5.789323e-16 2.418227e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | -2.418227e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | 9.512150e-16 -3.725124e-15 -1.427978e-14 -4.961150e-16 1.238679e-15 -3.886205e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb | -7.445334e-15 -1.072374e-14 -7.441145e-15 5.509026e-15 4.564893e-15 4.797959e-18 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 7.780371e-16 -3.106557e-15 -4.213498e-16 4.485436e-15 -1.666580e-16 3.855045e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 5.157289e-15 2.544177e-15 -5.025826e-15 3.730941e-15 -2.583572e-15 2.016068e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | -1.878786e-15 8.616810e-16 -3.783026e-15 5.373470e-15 -3.446945e-15 4.906003e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 8.13cc65a2298feba.final.pdb |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -1.918800e-15 4.241256e-16 -5.939433e-15 1.623405e-15 1.721714e-15 -2.030959e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | 9.512150e-16 -3.725124e-15 -1.427978e-14 -4.961150e-16 1.238679e-15 -3.886205e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | 7.780371e-16 -3.106557e-15 -4.213498e-16 4.485436e-15 -1.666580e-16 3.855045e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -1.918800e-15 4.241256e-16 -5.939433e-15 1.623405e-15 1.721714e-15 -2.030959e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -1.804772e-15 6.098303e-15 3.05667e-15 5.319508e-15 1.185652e-15 7.680082e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\99f752b3616e033b.final.pdb | -1.900062e-15 -5.250161e-16 -4.279538e-15 3.040376e-15 8.459844e-16 1.476407e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -1.817650e-15 -3.479910e-15 -1.688979e-15 4.755148e-15 -1.366084e-15 4.700728e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -3.758073e-15 -5.920776e-15 -3.016568e-15 1.411599e-16 3.711423e-15 3.290446e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.793512e-15 -1.700627e-15 -3.810204e-15 2.529874e-15 7.656455e-16 2.785847e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.312207e-15 -6.429436e-15 -8.952089e-15 -6.236547e-16 5.000025e-16 -1.281933e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | ad8a823e4b4c668e.final.pdb |
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-1.172773e-14  2.262470e-15 -4.352015e-15  2.447425e-15  9.099876e-15
-2.050672e-15
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7.518314e-15
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-2.030175e-15
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-2.717779e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb     | -6.400616e-15 -4.135012e-15 3.991096e-15 -3.061064e-15 -1.739159e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb     | 3.366755e-16 -3.668545e-15 -4.803514e-16 6.963415e-16 -7.354863e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f98c80dd5c3135.final.pdb      | -3.323121e-16 -3.778355e-16 -9.925518e-16 1.760900e-16 -6.165864e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f0099.final.pdb      | 2.668129e-15 -3.055334e-15 -7.230993e-15 2.735861e-15 -1.321648e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\784b99c94a633196.final.pdb     | -6.995592e-16 -7.906052e-15 -1.967950e-15 -8.792984e-16 -3.337996e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feda.final.pdb      | -6.995592e-16 -7.906052e-15 -1.967950e-15 -8.792984e-16 -3.337996e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12df9.final.pdb       | -3.654900e-15 -2.654177e-15 -4.847618e-15 -5.209819e-15 -8.567753e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d05469ef569760.final.pdb     | -8.905081e-16 -7.391984e-16 -2.787752e-15 2.052412e-15 -4.269887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb     | 7.956000e-15 -4.135012e-15 3.991096e-15 -3.061064e-15 -1.739159e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb      | 2.668129e-15 -3.055334e-15 -7.230993e-15 2.735861e-15 -1.321648e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb      | -8.905081e-16 -7.391984e-16 -2.787752e-15 2.052412e-15 -4.269887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb      | 7.956000e-15 -4.135012e-15 3.991096e-15 -3.061064e-15 -1.739159e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f49096dadc62.final.pdb      | 1.271087e-15 -1.938603e-15 -1.707742e-15 -4.941897e-15 -7.119693e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb      | 3.843791e-16 -4.399887e-15 2.451265e-16 7.875923e-16 -5.984684e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f7523616e033b.final.pdb        | 8.046726e-16 -5.131899e-15 -5.156861e-15 9.052399e-16 -6.643683e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c7008316d6ba.final.pdb       | 3.843791e-16 -4.399887e-15 2.451265e-16 7.875923e-16 -5.984684e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e0400.final.pdb       | 4.157620e-15 3.515097e-15 -1.506698e-15 1.385412e-15 -4.108699e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a8b309a2823c616.final.pdb       | 8.766616e-16 -3.887835e-15 -7.867878e-16 5.669481e-16 -8.418789e-15 |
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-6.600353e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
-6.995592e-16 -7.906052e-15 -1.967950e-15 -8.792984 e-16 -3.337996e-15
-8.942462e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
2.583070e-16 -3.694053e-15 -5.688877e-16  3.751767e -16 -6.918354e-15
-1.831652e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
-5.133474e-16 -3.742716e-15 -2.427679e-16  8.605844e-15 -7.215536e-15
7.156639e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb
-9.271941e-16  2.657298e-15 -5.691263e-15  3.427127 e-15 -1.446986e-14
-3.120714e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
-3.323121e-15 -3.778355e-15 -9.925518e-16  1.760900e-15 -6.165864e-15
-2.170398e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
6.706728e-15 -5.902695e-15 -6.720822e-15  4.984258e-15 -1.035978e-14
3.224904e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
-3.323121e-15 -3.778355e-15 -9.925518e-16  1.760900e-15 -6.165864e-15
-2.170398e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
1.271087e-15 -1.938603e-15 -1.707742e-15 -4.941897e-16 -7.119693e-15
1.781598e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb
7.903821e-15 -5.248473e-16 -4.984258e-15 -1.035978e-14
-2.170398e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb
-3.323121e-15 -3.778355e-15 -9.925518e-16  1.760900e-15 -6.165864e-15
-2.170398e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
6.985097e-16 -4.623166e-15 -1.148677e-15  9.088254e-16 -6.747430e-15
5.135034e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac9e664f4ef427e.final.pdb
8.012168e-15 -5.703821e-15  5.248473e-16 -4.941897e-16 -7.119693e-15
1.513030e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ba2af555fc9d0681.final.pdb
1.271087e-15 -1.938603e-15 -1.707742e-15 -4.941897e-16 -7.119693e-15
1.781598e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\be34248de3e81a3c.final.pdb
-9.916391e-16 -4.270968e-15  1.258976e-14 -1.581713e-15 -4.439493e-15
0.179272e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb
1.158557e-14 -8.304249e-15 -1.342966e-14 -1.254330e-14 -2.950554e-15
4.065934e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb
1.453186e-15 -6.428338e-15  4.292534e-16 -3.237616e-16 -4.726430e-15
-2.095519e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
4.827921e-15 -5.103120e-15 -7.006636e-15 -5.342595e-15 -1.386502e-14
-1.407638e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
-2.763136e-15 -6.816541e-14 -1.225009e-14 -4.682488e-15 -9.543632e-15
Page 710
| PDB File                        | Values                        |
|--------------------------------|-------------------------------|
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb | 6.361151e-17 3.469984e-17 2.587309e-15 -1.258487e-15 -4.596657e-15 -4.764745e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | -1.305309e-16 2.191446e-16 2.735880e-15 -1.421121e-16 -8.167028e-15 -4.239329e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | 3.745746e-16 -1.062086e-15 4.478754e-15 -1.429538e-15 -6.469917e-15 -5.122857e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 3.498961e-16 -2.838271e-15 2.887127e-15 2.251293e-15 -2.014056e-15 -2.175342e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 1.636391e-15 -1.156549e-15 2.394974e-15 -7.561468e-16 -5.701864e-15 -4.021029e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59f3e3306825e8.final.pdb | 1.735940e-15 1.309886e-15 -1.027276e-15 2.775179e-15 -8.696210e-15 -7.025629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 1.969938e-16 -7.454546e-15 -6.773389e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | 1.751751e-15 -8.282525e-16 2.372857e-15 -1.694199e-15 -6.351518e-15 -4.038376e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | 1.751751e-15 -8.282525e-16 2.372857e-15 -1.694199e-15 -6.351518e-15 -4.038376e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | 1.913419e-15 -6.508915e-16 2.837600e-15 -2.312537e-15 -5.599096e-15 -4.175912e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | 6.844899e-15 -9.845801e-15 -1.018764e-14 -2.504072e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 8.751943e-15 -6.188420e-15 -2.018600e-15 -1.019313e-14 -4.124364e-16 6.887558e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | -7.704511e-15 -5.258825e-15 7.132067e-15 -7.545944e-15 -8.898704e-15 -2.265710e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | 3.519773e-15 -6.547946e-16 2.390042e-15 1.829983e-15 -2.375980e-15 -1.018764e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 5.759754e-15 6.605590e-15 -3.745206e-17 -2.018600e-15 -5.759754e-15 -2.018600e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328717977b7ab.final.pdb | 6.911405e-15 3.064194e-15 2.572669e-15 -2.266539e-15 |

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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb     | -9.114713e-15 -1.653961e-15 1.050638e-14 -1.155219e-14 -6.007260e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb     | -6.337265e-15 -3.534421e-15 9.499496e-16 -1.768358e-15 -4.850115e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e0ad0f1be4.final.pdb       | 3.384033e-15 3.307792e-15 2.261484e-15 -1.058475e-15 -2.260299e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb      | 6.015417e-15 1.478624e-15 -5.267374e-16 1.969938e-16 -7.454546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb      | 1.205744e-14 -6.694316e-15 3.065596e-15 -6.378985e-15 -1.750117e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb      | 3.519773e-15 -6.547946e-15 2.390042e-15 1.829983e-15 -2.375980e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb      | 3.519773e-15 -6.547946e-15 2.390042e-15 1.829983e-15 -2.375980e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efcfce12d3f9.final.pdb      | -1.865676e-15 4.870871e-16 8.014882e-15 7.258311e-16 -5.205748e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8ad50469ef569760.final.pdb      | 1.735940e-15 1.309886e-15 -1.027276e-15 2.775179e-15 -8.696210e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb      | 3.384033e-15 3.307792e-15 2.261484e-15 -1.058475e-14 -2.260299e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb      | 4.123456e-15 -1.304744e-16 1.227777e-15 -6.142807e-15 -7.902809e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb      | 3.663760e-15 -3.258705e-15 2.741690e-15 -1.528742e-14 -4.337515e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98be0d5986c138f.final.pdb       | 4.434129e-15 -7.730676e-16 1.653925e-15 -2.286725e-15 -6.125357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d6e2fa.final.pdb       | 2.767770e-15 -7.176783e-16 -5.009533e-15 2.392033e-15 -1.199979e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d5dade09d81fb3ef.final.pdb     | 3.795956e-15 6.084651e-15 7.104398e-15 8.371439e-15 -7.094106e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616ee033b.final.pdb      | 4.434129e-15 -7.730676e-16 1.653925e-15 -2.286725e-15 -6.125357e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb      | -3.463109e-15 -2.394980e-15 3.456944e-15 -3.322304e-15 -2.909860e-15 |
| Page 714
| File Path                                      | Values                                      |
|-----------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -2.408992e-15 -2.778692e-15 -6.043266e-16 -3.622745e-15 -9.204118e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | -2.999818e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | 1.376175e-15 -1.116176e-15 2.486951e-15 -1.628680e-15 -5.470993e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | -3.923558e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 2.767779e-15 -7.176783e-16 5.090953e-15 2.392033e-15 -1.199979e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 1.266369e-15 -2.492256e-15 5.467100e-16 -8.735103e-15 -1.189853e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 -1.969938e-16 -7.454546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -1.646665e-15 -6.672289e-15 -5.520487e-15 3.961771e-15 -7.266711e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 -1.969938e-16 -7.454546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef9749a2.final.pdb | 4.123456e-15 -1.304744e-16 1.227777e-15 -6.142807e-15 -7.902809e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b8a4786fa27a165.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 -1.969938e-16 -7.454546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9f4d9d9d7c1017b.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 -1.969938e-16 -7.454546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 4.123456e-15 -1.304744e-16 1.227777e-15 -6.142807e-15 -7.902809e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 1.608628e-15 5.411166e-17 3.378599e-15 1.311969e-16 -4.058061e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93| |
| Path                                      | Numbers                                      |
|-------------------------------------------|----------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -7.182852e-15 -7.800623e-16 1.272780e-14 -1.429243e-16 -1.198105e-14 1.012184e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 2.545229e-15 -4.316885e-15 4.594370e-15 1.823951e-14 -1.379863e-14 9.976681e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | 4.549794e-15 1.132600e-15 -8.89971e-15 -4.723019e-15 -9.361751e-15 -6.006068e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\da1163918d3707839.final.pdb | -1.768096e-15 -4.499765e-15 -1.503299e-15 1.981100e-15 2.832433e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4529e19ad281fea2.final.pdb | -3.630372e-15 1.441514e-15 6.973772e-15 1.411649e-15 -5.739534e-15 -4.580627e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2.final.pdb | 3.498696e-16 -2.838271e-15 2.887127e-15 2.251293e-15 -2.014056e-15 -2.175342e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 3.519773e-15 -6.547946e-16 2.390042e-15 1.829983e-15 -2.375980e-15 -7.659236e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d9960a960.final.pdb | -2.349049e-15 -1.199583e-14 8.525794e-14 -1.331421e-15 -9.381896e-15 -9.782782e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | -3.463109e-16 -2.394980e-15 3.456944e-15 -3.323034e-15 -2.908600e-15 -9.395412e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | 3.519773e-15 -6.547946e-16 2.390042e-15 1.829983e-15 -2.375980e-15 -7.659236e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e54517be32db050e.final.pdb | 6.015417e-15 1.478624e-15 -5.267374e-16 1.969938e-16 -7.454546e-15 -6.773893e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | 1.726505e-15 -5.870958e-16 2.465314e-15 -2.299731e-15 -5.740154e-15 -4.681522e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862c0cad52078.final.pdb | 2.356885e-15 -7.118982e-16 2.280045e-15 -2.299273e-15 -6.580246e-15 -4.513045e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | 1.781531e-15 -8.949419e-16 2.479104e-15 -1.444140e-15 -5.606827e-15 -3.930973e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 1.608628e-15 5.411166e-17 3.378599e-15 1.311969e-16 -4.058061e-15 -3.686796e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | 4.434129e-15 -7.773067e-16 1.653925e-15 -2.286725e-15 -6.125357e-15 -3.367936e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | -1.043607e-15 -8.003691e-16 9.097942e-15 5.582499e-16 -5.247978e-15 -4.008021e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caaa2.final.pdb | 3.498961e-16 -2.838271e-15 2.887127e-15 2.251293e-15 -2.014056e-15 -2.175342e-15 |
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
5.748219e-16  7.025258e-16 -2.326684e-15 -2.440972e-16 -4.750230e-15 -2.235209e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
1.301334e-15  5.801608e-16 -1.056402e-15 -3.559041e-16 -2.934785e-15 -1.609355e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
3.56878e-15 -8.245021e-16 -3.419996e-15 -1.412127e-15 -5.05368e-15 -3.128321e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-8.430003e-16 -5.570329e-15 -1.295509e-15 -1.229260e-15 -5.356623e-15 1.667343e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
7.811348e-16  3.375615e-15 -1.929513e-15 -1.383822e-15 -4.024393e-15 -2.465578e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
1.534402e-16 -9.09772e-16 -3.673584e-16 -3.304151e-15 -4.349954e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
5.537313e-15  3.614164e-15 -1.146106e-15 -1.030418e-15 -2.764079e-15 -1.224521e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0f305f59f3306825e8.final.pdb
4.125248e-15 -6.298369e-16 -2.690227e-15  7.691412e-16 -4.118031e-15 5.930426e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb |         |        |        |        |        |        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb |         |        |        |        |        |        |

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-7.384255e-17
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1.667343e-16

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb       | 3.852385e-16  -6.929521e-16  -4.649623e-15  2.611427e-15  -3.570957e-14  -1.086330e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 1.810232e-15  3.852385e-16  -6.929521e-16  -4.649623e-15  2.611427e-15  -3.570957e-14  -1.086330e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb       | 1.578366e-15  4.884331e-15  -1.231113e-14  -9.359980e-15  1.902632e-15  -2.800338e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 1.840611e-15  -9.895457e-16  -2.497919e-15  1.046206e-16  7.894081e-16  -1.041105e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | -1.134709e-14  4.201481e-15  -1.388053e-14  -3.221544e-15  -1.065097e-14  -8.106494e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb       | -6.436913e-16  -8.213017e-16  -4.958102e-15  1.365890e-14  4.464800e-15  1.683008e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb       | 6.125478e-15  -1.514136e-14  4.966454e-15  -1.783219e-15  7.579936e-15  -1.440569e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dd6163918de307839.final.pdb       | -2.486380e-15  -1.059563e-15  -1.319724e-14  5.632415e-15  1.340602e-16  -4.432261e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eeb4f8b06824ef848.final.pdb       | -1.339039e-14  1.387088e-14  -4.381273e-15  -4.333097e-15  -1.694684e-15  -3.346562e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb       | -5.54364e-15  -3.033500e-15  -5.289114e-15  3.473405e-15  -3.20053e-15  -1.234091e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2a.final.pdb       | -3.694477e-16  -1.866148e-14  -2.049506e-15  5.592185e-15  3.064190e-15  6.097262e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb       | 4.860289e-15  6.151945e-15  -2.197375e-15  -2.004904e-15  3.165990e-15  -5.681535e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | -5.833278e-15  6.029506e-15  -2.580227e-15  -3.646765e-15  3.951998e-15  -3.775248e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\efa2d800ef010197e2.final.pdb      | -3.694477e-16  -1.866148e-14  -2.049506e-15  5.592185e-15  3.064190e-15  6.097262e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb5a17be32db050e.final.pdb       | 2.591313e-15  -8.280485e-15  -4.464544e-15  3.913256e-15  -7.311118e-16  -1.669192e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6d5a5f95899c29d.final.pdb       | -5.446279e-16  -4.402669e-16  -3.130205e-15  3.359481e-17  -3.651065e-16  -2.170290e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb       | -1.541232e-15  -2.151707e-15  -4.847918e-15  -2.847745e-16  -3.772282e-16  -1.350001e-15 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb     | -2.458927e-15 -1.134474e-15 -4.168336e-15 -3.831312e-16 2.985136e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb     | -1.840611e-15 -9.895457e-16 -2.497919e-15 1.046206e-15 7.894081e-16  |
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb                               | -3.554428e-15 6.886663e-16 -5.086185e-16 -7.821562e-16 -3.208932e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb    | -2.094844e-15 -1.165131e-15 2.435046e-15 1.643526e-15 -1.967134e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb                               | -2.916836e-15 1.463447e-15 8.045187e-16 -2.805811e-15 -1.254881e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb                               | -3.906753e-15 4.242991e-15 5.223522e-16 -2.370312e-16 -7.628237e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb                               | -2.574014e-15 1.502721e-15 1.176930e-15 -5.948173e-16 -3.908206e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb    | -9.572341e-16 -6.642269e-15 3.574821e-15 -3.658735e-15 -8.510716e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb    | -3.862175e-15 -3.847393e-15 -3.450655e-16 -1.827655e-15 1.765774e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb    | -4.157104e-15 2.149973e-15 1.717804e-15 -1.318102e-15 -3.277459e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb    | -2.369049e-15 -2.400421e-15 -2.370312e-16 -2.370312e-16 -2.370312e-16 |

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-9.572341e-16 -6.642269e-15  3.574821e-15 -3.658673e-15 -8.510716e-15
 5.425178e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
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1.143347e-14

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-9.186431e-15

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6.347531e-15  5.915152e-15 -4.962394e-16  5.730521e-15 -1.656853e-14
-1.902050e-15

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-8.464236e-16  6.577543e-15  4.261981e-15  2.155621e-15  3.511435e-15
7.775543e-15

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-2.490480e-15

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-7.394903e-15

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1.292080e-14

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-5.737953e-15

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-7.483694e-15

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-4.656679e-15  8.363608e-16  1.664612e-15  3.090285e-15 -2.234064e-15
2.387492e-15

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-3.491057e-15

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7.775543e-15

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-3.994845e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
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-5.406105e-15 4.530013e-15 1.672702e-15 -2.962620e-15 6.722170e-15 5.305368e-15
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb | 3.994607e-15 | 1.911116e-15 | 1.112156e-15 | -1.806488e-15 | 2.462514e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb | -9.246622e-15 | 1.322263e-15 | 3.587547e-15 | -1.748235e-15 | -8.473943e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0.ad.final.pdb | -4.246622e-15 | 3.132226e-15 | 3.437203e-15 | -5.409412e-16 | -3.497094e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | -4.428809e-15 | 3.040846e-15 | 1.378265e-16 | -1.020172e-15 | 4.393286e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | -1.103164e-14 | -2.572817e-15 | 3.523864e-15 | 1.209469e-15 | -6.21421e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | -2.094844e-15 | -1.165131e-15 | 2.435046e-15 | 1.643526e-15 | -1.967134e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | -2.094844e-15 | -1.165131e-15 | 2.435046e-15 | 1.643526e-15 | -1.967134e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb | 4.651219e-15 | -3.941274e-15 | 6.049201e-17 | -1.071601e-15 | -2.953465e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | -4.040884e-15 | 1.243989e-15 | -4.594961e-16 | -2.017092e-15 | -9.993964e-16 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | -1.377636e-15 | -1.671697e-15 | 4.262361e-16 | -7.544184e-16 | -9.184377e-16 |
| E:\R-3.1.2\scripts\126f26a78b57339c.final.pdb | 2.486076e-15 | -5.173435e-15 | 6.773472e-17 | -3.766480e-15 | -3.524036e-15 |
| E:\R-3.1.2\scripts\12f06f3e342df706.final.pdb | -1.737811e-15 | 1.011797e-15 | -1.117476e-15 | -1.66002e-15 | -1.444854e-15 |
| E:\R-3.1.2\scripts\18618a2a251b867b.final.pdb | -2.318125e-15 | 2.815874e-15 | 2.797394e-15 | -2.568489e-15 | 3.308398e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 1.056964e-15 | 3.394766e-15 | 2.15705e-15 | -3.957269e-15 | -6.787895e-15 |

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| File Path                                                                 | Energy          |
|--------------------------------------------------------------------------|-----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb     | -2.653002e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb    | -8.762767e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb    | -2.289550e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd391854336d.final.pdb      | 1.056964e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b30278892fdec42.final.pdb     | -1.163016e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fc3b346e33793b0.final.pdb     | -4.807598e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb     | -2.489570e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb      | 9.257685e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\3b90278892fdec42.final.pdb      | 1.906721e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\357368adabc3d5de.final.pdb       | -7.952547e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb      | -2.445259e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb      | 8.06760e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4448ef21d7e28cdfe.final.pdb     | -6.184531e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb       | -1.920121e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951e153.final.pdb       | 4.445259e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951e153.final.pdb       | -7.952547e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb      | 5.663655e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4aa45b62cb6a25f.final.pdb        | -1.187986e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb       | -4.345265e-15   |

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-3.229375e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
4.122626e-15 -2.485524e-17 -1.342206e-16 -6.487752e-15 -5.928178e-16 -9.217250e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
4.122626e-15 -2.485524e-17 -1.342206e-16 -6.487752e-15 -5.928178e-16 -9.217250e-15
| File Path                                                                 | Values                                                                 |
|---------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb       | -1.244778e-15 -2.759208e-15 -4.019674e-15 -1.066910e-15 6.189690e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb       | -5.517328e-15 -6.358501e-15 -6.353551e-15 -3.039620e-15 -2.800495e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb        | -1.827622e-15 -2.286189e-15 -3.820925e-15 -1.497216e-15 -2.645376e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb        | -5.173288e-15 -6.358501e-15 -6.353551e-15 -3.039620e-15 -2.800495e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb        | 1.402235e-14 4.535098e-15 -2.107511e-15 1.549675e-15 -9.073655e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb        | -2.220518e-15 -1.759779e-15 -4.587732e-15 -1.650023e-15 3.281129e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb        | -9.170723e-15 9.191305e-17 -6.736540e-15 -2.902670e-15 -3.148241e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb         | -2.993865e-16 8.331085e-16 -4.526502e-15 -3.170691e-15 -7.537338e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb         | -9.602225e-15 -9.504941e-15 -2.281284e-15 1.495070e-15 7.656769e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb         | -9.602225e-15 -9.504941e-15 -2.281284e-15 1.495070e-15 7.656769e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb         | -2.878431e-15 5.478434e-15 1.446529e-16 -1.85112e-14 -1.814378e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb         | -4.303562e-15 -5.547638e-15 -4.226828e-15 4.175849e-16 5.667378e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb         | -4.303562e-15 -5.547638e-15 -4.226828e-15 4.175849e-16 5.667378e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb         | -4.022679e-15 4.728096e-16 -1.355842e-14 -6.049282e-15 1.422723e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb         | -4.022679e-15 4.728096e-16 -1.355842e-14 -6.049282e-15 1.422723e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb         | -1.943037e-15 -3.590436e-15 -5.643934e-16 -7.804137e-15 3.929185e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb         | -1.943037e-15 -3.590436e-15 -5.643934e-16 -7.804137e-15 3.929185e-15 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb      | -4.647396e-15 -5.481195e-15 -3.031685e-15 4.602682e-16 3.985344e-15 -1.763913e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb      | -4.647396e-15 -5.481195e-15 -3.031685e-15 4.602682e-16 3.985344e-15 -1.763913e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb      | 7.120134e-16 -6.171969e-15 -8.979159e-16 -9.282269e-16 1.885333e-15 -3.176787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb      | 7.120134e-16 -6.171969e-15 -8.979159e-16 -9.282269e-16 1.885333e-15 -3.176787e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb      | -1.649794e-15 -2.496170e-15 -5.009486e-15 -1.133943e-15 1.232337e-15 -1.936952e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb      | 2.812763e-15 -2.023378e-15 3.444097e-15 3.794558e-15 4.074554e-15 -5.517796e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f5f5f9d0681.final.pdb      | -1.088454e-15 -6.080190e-15 -2.629087e-15 -1.477616e-15 8.205749e-15 -1.003900e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb      | -1.88454e-15 -6.080190e-15 -2.629087e-15 -1.477616e-15 8.205749e-15 -1.003900e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb      | 2.845091e-15 -2.277161e-15 -5.728446e-17 -6.338980e-15 -8.541528e-15 6.798682e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb      | -3.440515e-15 -4.329489e-15 -4.356106e-15 -1.231770e-15 2.022658e-15 -3.766920e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb      | -1.378651e-14 7.389692e-16 -5.798325e-15 -6.326897e-16 -1.093900e-14 1.559816e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0e39.final.pdb        | -7.265111e-15 -8.977006e-15 -6.839098e-15 2.914504e-18 -2.708232e-15 -6.472443e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb      | 6.896406e-15 -9.954687e-15 -2.143640e-15 2.719075e-15 5.985845e-15 -2.36343e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb      | -6.426777e-15 -4.885238e-15 -2.689056e-15 2.173650e-15 -1.100381e-14 1.427583e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb      | -5.517328e-15 6.358501e-15 -6.353551e-15 -3.093620e-15 -2.800495e-15 -8.804883e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb      | -2.602303e-15 3.06391e-15 -8.220162e-15 -1.195708e-15 2.513650e-15 -7.306925e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602b082718ec3a1.final.pdb      | -1.883133e-15 -3.021711e-15 -5.259911e-15 -1.219660e-15 4.643544e-15 -1.886153e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ed589d99b0a960.final.pdb        | 1.403314e-14 -4.555563e-15 -5.350862e-15 1.426964e-14 3.156266e-15 |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
1.253946e-15  1.179339e-16 -3.699256e-15 -1.208713e -15  5.454686e-15
-1.029255e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
-1.883133e-15 -3.021711e-15 -5.259011e-15 -1.219660 e-15  4.643544e-15
-1.886153e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
-4.647396e-15 -5.481195e-15 -3.031685e-15  4.602682 e-16  3.985344e-15
-1.763913e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-1.618050e-15 -2.019475e-15 -3.945213e-15 -1.006965 e-15  1.203009e-15
-2.001966e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
-2.20735e-15 -2.200833e-15 -4.439413e-15 -1.265782e-15  2.129190e-15
-1.711871e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-2.20644e-15 -2.126465e-15 -3.978714e-15 -1.293621e-15  5.375466e-16
-2.342605e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
-3.440515e-15 -4.329489e-15 -4.356106e-15 -1.231770e-15  2.022658e-15
-3.766920e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
1.813788e-15 -3.265185e-15 -4.330842e-15 -2.217161e-15  3.998092e-15
-3.136569e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-4.022679e-15  4.728096e-16 -1.355842e-14 -6.049282e-15  1.422723e-15
-2.935285e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-2.608303e-15  3.306391e-15 -8.220162e-15 -1.195708e-15  2.513650e-15
-7.306925e-16

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
7.940067e-15 -3.010555e-15  4.755350e-17  5.225541e-16  1.130277e-15
-5.128716e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
7.734950e-15 -2.197873e-15 -1.295745e-15 -1.109939e-15  3.512058e-15
-1.549565e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
8.122827e-15 -2.854411e-15 -3.468929e-17 -4.867831e-16  3.097805e-15
-1.950778e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
7.456288e-15 -2.283637e-15 -1.216326e-15  9.482311e-16  3.734562e-16
-2.079779e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
4.626732e-15 -6.112253e-15 -1.653567e-15 -1.63002e-15  7.431002e-15
-3.297421e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
6.879407e-15 -2.374400e-15 -9.575268e-16  6.791861e-16  1.174647e-15
-1.870852e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcaed4194d9.final.pdb
6.508094e-15 -8.373174e-16 -1.398429e-15 -1.708991e-15  2.794059e-15
-4.161370e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb

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| File Path                                                                 | Values                      |
|---------------------------------------------------------------------------|-----------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb       | -3.193581e-15 -1.703874e-15 | 1.383773e-15 3.847063e-15 1.469599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb       | -1.832299e-15 -9.965581e-16 | 2.290254e-16 1.340313e-15 -2.724175e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb       | -5.170959e-15 -4.684090e-16 | 1.571046e-15 3.857174e-16 5.330769e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb       | -1.602185e-15 -1.017670e-15 | 9.206759e-16 1.430408e-15 -3.14863e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551bea39.final.pdb        | -5.170959e-15 -4.684090e-16 | 1.571046e-15 3.857174e-16 5.330769e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb       | -9.064243e-15 -6.718872e-15 | 9.217740e-15 9.417582e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb       | -2.800999e-15 -3.167318e-15 | 7.214080e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb        | -8.290062e-16 8.150318e-16 | 1.422326e-18 5.436241e-18 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fd42.final.pdb        | -3.619756e-15 1.539281e-16 | 6.950519e-15 -4.367976e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb       | -5.465415e-15 3.672373e-15 | 1.104976e-14 -3.070426e-15 -2.402688e-15 -5.462180e-15 6.009455e-15 -1.849240e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb       | -7.295929e-15 -5.853285e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb       | -2.443638e-15 -7.295929e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328719797ab.final.pdb         | -5.853285e-15 -9.034656e-16 | 5.353558e-15 5.736776e-15 1.868356e-15 1.989192e-15 3.847063e-15 1.469599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328719797ab.final.pdb         | -2.443638e-15 -7.295929e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328719797ab.final.pdb         | -2.443638e-15 -7.295929e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328719797ab.final.pdb         | -2.443638e-15 -7.295929e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b328719797ab.final.pdb         | -7.295929e-15 -5.853285e-15 | 9.01508e-15 -9.093465e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | -1.174229e-15 -1.259872e-15 | 5.318144e-15 -4.731401e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | 4.092264e-16 -1.174229e-15 | 5.318144e-15 -4.731401e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | 4.092264e-16 -1.174229e-15 | 5.318144e-15 -4.731401e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb        | 1.584700e-14 -9.417861e-15 | 3.791845e-15 2.573793e-15 -1.203155e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | 1.868356e-15 1.989192e-15 3.847063e-15 1.469599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | 1.338540e-15 -2.147544e-15 | 7.611335e-15 -2.919217e-15 -1.659242e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | 7.573184e-15 1.868356e-15 1.989192e-15 -6.771179e-15 6.898416e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7fcfc.final.pdb         | 2.431047e-15 6.976476e-16 | 4.914934e-15 -1.098999e-14 4.871161e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | 4.028252e-15 -3.193581e-15 | 1.703874e-15 1.383773e-15 3.847063e-15 1.469599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb        | 4.028252e-15 1.383773e-15 3.847063e-15 1.469599e-15 |
| File Name                                                                 | PDB Code          | Supplementary Text 10 |
|--------------------------------------------------------------------------|-------------------|-----------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb      | 2.282687e-15      | -1.688995e-15 8.348936e-15 2.000857e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ea45b62cb6a25f.final.pdb       | 4.735623e-15      | 1.746317e-15 4.566332e-15 -6.907599e-16 2.099531e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb      | 5.533558e-15      | 5.736776e-15 1.868356e-15 -1.989192e-15 -6.771179e-15 6.898416e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb       | 8.083054e-15      | -7.324669e-15 -4.030586e-15 5.887020e-15 8.173776e-16 -4.102409e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb       | 6.500894e-15      | -8.373174e-16 -1.398429e-15 -1.708991e-15 2.794059e-15 -4.161370e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb       | 4.735623e-15      | 4.112827e-16 1.746317e-15 -6.907599e-16 2.099531e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb       | 4.446891e-15      | -1.469091e-15 1.349222e-15 1.628080e-15 4.996929e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb       | 4.028252e-15      | -3.193581e-15 -1.703874e-15 1.383773e-15 3.847063e-15 1.469599e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb       | 8.083054e-15      | -7.324669e-15 -4.030586e-15 5.887020e-15 8.173776e-16 -4.102409e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb       | 3.167042e-15      | -5.440495e-16 -1.147366e-15 3.933502e-15 4.996929e-15 1.697334e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d479296b1c8.final.pdb      | 5.423404e-15      | -1.273242e-15 -1.581142e-15 4.626351e-16 1.791416e-15 3.411617e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb       | 1.148595e-14      | -6.238085e-16 -1.679475e-15 3.782866e-15 -1.533762e-15 4.595858e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb       | 3.571290e-15      | 1.710007e-15 -3.122097e-16 -3.893545e-15 3.611666e-15 -4.431304e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | 8.083054e-15      | -7.324669e-15 -4.030586e-15 5.887020e-15 8.173776e-16 -4.102409e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffbb22872.final.pdb      | 5.954071e-15      | -1.686551e-15 -9.367844e-16 6.195503e-15 2.008985e-15 -7.867329e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | 6.500894e-15      | -8.373174e-16 -1.398429e-15 -1.708991e-15 2.794059e-15 -4.161370e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb       | 3.134302e-15      | 3.432705e-15 1.461184e-15 -7.470652e-15 6.665969e-15 -3.798747e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a33196.final.pdb       |                   |                       |
| Path                                         | Values                                                                 |
|----------------------------------------------|-------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | -4.351127e-17  8.125410e-15  2.592000e-15  9.274845e-15  6.950519e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | 4.735623e-15  1.746317e-15  4.566332e-15  6.950519e-15  6.950519e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | 3.672373e-15  1.539281e-16  1.539281e-16  6.950519e-15  6.950519e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb | 6.500894e-15  -1.398429e-15  3.98429e-15  2.794059e-15  2.794059e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | 6.483639e-15  1.527660e-15  2.152247e-15  2.152247e-15  2.152247e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcdd52078.final.pdb | 6.024713e-15  -1.701210e-15  8.818268e-17  8.818268e-17  8.818268e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | 8.807088e-15  -1.694707e-15  2.576392e-15  2.576392e-15  2.576392e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 1.265065e-15  -1.493996e-15  7.973595e-16  7.973595e-16  7.973595e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52c52a2.final.pdb | 4.626732e-15  -1.653567e-15  7.431002e-15  7.431002e-15  7.431002e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 2.208629e-15  -1.19830e-15  4.572539e-17  4.572539e-17  4.572539e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 1.576665e-15  -3.134826e-16  2.208629e-15  2.208629e-15  2.208629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\3w9y.pdb               | -1.19830e-15  4.572539e-17  -1.69707e-15  -1.69707e-15  -1.69707e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\40.1ns_data\Nat0.pdb   | -3.159631e-15  2.208629e-15  2.208629e-15  2.208629e-15  2.208629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\40.1ns_data\Lj6.pdb    | -3.159631e-15  2.208629e-15  2.208629e-15  2.208629e-15  2.208629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\40.1ns_data\ZSP9.pdb   | -3.159631e-15  2.208629e-15  2.208629e-15  2.208629e-15  2.208629e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | -3.159631e-15  2.208629e-15  2.208629e-15  2.208629e-15  2.208629e-15 |
| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb     | -3.225873e-15                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb     | 2.134207e-15 -1.085597e-15 -8.352057e-16 -4.270931e-15 -8.160622e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a7b57339c.final.pdb       | -1.192503e-16                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb      | 2.487618e-15 -2.334006e-15 -2.802705e-16 -3.059486e-15 -1.320610e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\138618a2a251b867b.final.pdb     | 5.042451e-15 -4.317574e-15 1.926925e-15 6.464631e-16 -5.269394e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\13f005f98641eeeb2.final.pdb      | 2.926537e-15 -2.394095e-15 -3.753494e-16 -2.603848e-15 9.854410e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\145027889e2fcd42.final.pdb       | 2.384278e-15 -2.043844e-15 -4.696127e-16 -3.101727e-15 -1.478293e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1521f43528d47579a.final.pdb      | -2.527726e-16 -5.573139e-15 4.274856e-15 -4.170317e-15 1.61670e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1533db346e3379b0.final.pdb       | 1.125894e-15 -8.120276e-16 -1.306029e-15 -3.245696e-15 2.971246e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\154eb328251842006.final.pdb     | 7.216772e-15 -5.596177e-15 -4.140510e-16 -5.489000e-16 -5.914925e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\155b32871797b7ab.final.pdb       | 2.562961e-15 -4.969582e-15 -7.446291e-15 -1.648369e-14 -2.043113e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\156378640e6664b2.final.pdb       | -1.008677e-14                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\157368adb323d5de.final.pdb       | 4.285066e-15 -5.229128e-15 9.208819e-17 -5.081213e-16 -3.317339e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\158ca13cd3df6edd.final.pdb       | 2.150098e-15 -1.940465e-15 5.236710e-16 -1.650184e-15 -1.582837e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\159375137e-15 3.293349e-15 3.643189e-15 -4.267804e-15 -7.254533e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1604342df75a7fccc.final.pdb       | 7.893085e-15 -4.666880e-16 -5.245950e-15 -3.055444e-15 2.524689e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\161448ef21dffe8cdefb.final.pdb   | 1.295897e-15 3.276857e-16 2.754959e-15 -7.100252e-15 -1.414701e-14 |
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-4.255258e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb -3.632226e-16 -4.890052e-15 3.072917e-15 -1.584559e-16 -1.011545e-15 2.758094e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb 2.134207e-15 1.085597e-15 -8.352057e-16 -4.270931e-15 -8.160622e-16 -1.192503e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb 1.413109e-16 -9.328158e-17 7.687784e-16 -7.730524e-15 1.605719e-15 -1.078336e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb 2.134207e-15 1.085597e-15 -8.352057e-16 -4.270931e-15 -8.160622e-16 -1.192503e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb 4.262274e-15 7.769791e-16 4.131462e-15 -2.305476e-15 1.888779e-15 -2.531811e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb 2.134207e-15 1.085597e-15 -8.352057e-16 -4.270931e-15 -8.160622e-16 -1.192503e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb 1.413109e-16 -9.328158e-17 7.687784e-16 -7.730524e-15 1.605719e-15 -1.078336e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb 2.384766e-15 -2.197801e-15 -1.213670e-16 -3.183693e-15 -1.009484e-15 -3.769976e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb 2.696360e-15 -3.682128e-15 -2.979169e-15 -6.571595e-15 2.652491e-15 -5.300872e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb 4.262274e-15 7.769791e-16 4.131462e-15 -2.305476e-15 1.888779e-15 -2.531811e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb 5.027600e-15 2.107546e-15 -5.472945e-15 8.424959e-15 4.096250e-15 -2.251585e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb -3.336081e-15 -6.903238e-15 5.223316e-15 2.197853e-15 3.007040e-15 -6.944520e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb 3.465591e-15 -1.302208e-15 -1.363245e-15 -4.400355e-15 -1.298268e-15 -4.928300e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb 6.823372e-15 -2.681729e-15 -3.019811e-15 -3.584643e-15 -1.502367e-14 -1.037522e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb 3.091356e-15 -6.774479e-15 4.569289e-15 -9.316226e-15 -4.546367e-15 1.271657e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b0b082b4ef848.final.pdb 4.405892e-18 2.298902e-15 9.185215e-15 -8.601355e-15 -1.356270e-14 -3.356782e-15
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| PDB Path                                                   | Values                                 |
|-----------------------------------------------------------|----------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910f8b22872.final.pdb | 3.436335e-16  3.568223e-15  8.865250e-16  7.744651e-15  3.36957e-15  7.626257e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c0dd5c3135.final.pdb | 1.4556690e-16 -6.612180e-16  3.668947e-15  1.213368e-14 -2.171103e-16 -4.400577e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad9866a3f6099.final.pdb | -5.309567e-15 4.670433e-15 -6.051575e-16  1.293398e-15 -3.598902e-15 -1.637463e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | 5.312235e-16  4.236157e-15  4.643611e-15  8.887489e-15  4.533496e-15  3.036038e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | 5.312235e-16  4.236157e-15  4.643611e-15  8.887489e-15  4.533496e-15  3.036038e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe1f63df.final.pdb | 7.976172e-17  9.087311e-15  4.958491e-15  1.461641e-14 -1.193586e-15 -4.747233e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 5.306569e-15  4.749491e-15  2.353984e-15  8.711628e-15  2.664977e-15  6.699356e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | -3.232379e-17  6.551112e-16 -5.629440e-16  1.080131e-14  1.193586e-15  5.894839e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 4.033630e-15  4.600449e-15  4.793665e-15  4.890687e-15  5.427746e-15 -2.321814e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -6.098608e-15 -1.00484e-14  1.123975e-15  7.409245e-15  6.985025e-15  8.554887e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -3.631183e-16  1.403907e-15  1.329777e-15  1.60160e-14  7.309327e-15  2.457233e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 7.385230e-16  4.384137e-16 -5.014868e-15  1.461641e-14  1.949388e-15 -4.747233e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d0666e1402203d.final.pdb | 9.456690e-16 -6.612180e-16  3.668947e-15  1.213368e-14 -2.171103e-16 -4.400577e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e033b.final.pdb | 1.456690e-16 -6.612180e-16  3.668947e-15  1.213368e-14 -2.171103e-16 -4.400577e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 1.740832e-15  3.756101e-15 -2.715828e-16  4.080965e-15  5.147729e-15  2.452537e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -3.631183e-16  1.403907e-15  1.329777e-15  1.100160e-14  7.309327e-15  1.812515e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | -1.003077e-16  2.589087e-15  7.265217e-16  7.366921e-16  1.472850e-15  1.660727e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac4d74b9c71d4dc.final.pdb | 5.312235e-16  4.236157e-15  4.643611e-15  8.887489e-15  4.533496e-15  3.036038e-15 |
| File Name                                      | A         | B         | C         | D         | E          |
|-----------------------------------------------|-----------|-----------|-----------|-----------|------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | -8.121915e-16 | 2.869589e-15 | 1.084965e-15 | 7.699828e-15 | 1.609683e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 7.385230e-16 | 4.384137e-16 | -5.014868e-15 | 1.461641e-14 | 1.943988e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 7.413629e-16 | 7.958731e-15 | 1.090220e-15 | 9.057049e-15 | 6.021755e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 1.456690e-16 | -6.612180e-16 | 3.668947e-15 | 1.213368e-14 | -2.171103e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | 7.474344e-16 | 5.367271e-15 | -1.216933e-17 | 1.297362e-14 | -4.059590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 1.456690e-16 | -6.612180e-16 | 3.668947e-15 | 1.213368e-14 | -2.171103e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 4.033630e-15 | 4.600449e-15 | 4.793665e-15 | 4.890687e-15 | 5.427746e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 1.456690e-16 | -6.612180e-16 | 3.668947e-15 | 1.213368e-14 | -2.171103e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 7.474344e-16 | 5.367271e-15 | -1.216933e-17 | 1.297362e-14 | -4.059590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 1.456690e-16 | -6.612180e-16 | 3.668947e-15 | 1.213368e-14 | -2.171103e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 4.033630e-15 | 4.600449e-15 | 4.793665e-15 | 4.890687e-15 | 5.427746e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 9.208042e-15 | -6.520340e-15 | 1.102194e-14 | 1.594250e-14 | -1.054237e-14 |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
1.226773e-14 4.205873e-15 6.900076e-15 1.016337e-14 -5.887555e-15 3.777609e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb
-1.326905e-15 1.051189e-14 -3.791184e-15 -5.655423e-16 4.447788e-15 -2.009246e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2a.final.pdb
-5.978879e-15 1.302596e-15 -3.552750e-15 1.155657e-14 -1.553003e-15 9.140979e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb
5.312235e-16 4.236157e-15 4.643611e-15 8.887489e-15 4.533496e-15 3.036038e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb
-1.991781e-15 -1.020260e-15 1.127509e-15 7.652921e-15 1.503661e-14 2.765814e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5f599d996d0a960.final.pdb
-9.43011e-16 2.067176e-15 1.856995e-15 6.620630e-15 1.832398e-15 5.456024e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb
-4.983471e-16 2.559296e-15 4.193759e-16 8.234021e-15 1.830297e-15 1.470090e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
1.456690e-16 -6.12180e-16 3.668947e-15 1.213368e-14 -2.17103e-16 -4.400577e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
-7.943011e-16 2.067176e-15 1.856995e-15 6.620630e-15 1.832398e-15 5.456024e-15

E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-7.078590e-16 -2.609701e-15 3.735228e-16 3.059418e-15 -4.281304e-15 -7.486400e-17

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.800497e-15 -2.974743e-15 -2.559350e-16 2.207931e-15 -2.677288e-15 8.457929e-16

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
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3.208931e-15 -1.063733e-15 -7.206113e-16 1.933428e-15 -3.128211e-15 -1.362060e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb

1.936913e-15 -5.699163e-16 1.188026e-16 2.511197e-15 -1.336574e-15 -4.522268e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb

2.936913e-15 -5.699163e-16 1.188026e-16 2.511197e-15 -1.336574e-15 -4.522268e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb

1.080850e-15 -2.116408e-15 -1.359182e-15 1.994553e-15 -2.320840e-15 -1.501697e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb

-1.410554e-15 -2.042871e-15 -1.945698e-15 5.934979e-15 -3.866243e-15 -2.486870e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d9.final.pdb

1.693641e-15 -2.263100e-15 -7.030227e-16 2.114954e-15 -2.559581e-15 -1.421032e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb

3.105854e-15 -2.042871e-15 -1.945698e-15 5.934979e-15 -3.866243e-15 -2.486870e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb

4.541039e-15 2.303659e-15 -6.491289e-15 -4.001380e-15 1.480737e-15 -3.426736e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb

7.260338e-15 -1.460197e-15 -3.875178e-16 -2.559029e-15 2.428952e-15 -5.280058e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb

9.699265e-15 -3.540534e-15 4.453046e-15 -6.050768e-15 5.199205e-15 -2.726408e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb

1.501554e-14 5.938225e-15 -1.419501e-14 -5.920555e-15 -2.686631e-15 -8.454031e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb

9.699265e-15 -3.540534e-15 4.453046e-15 -6.050768e-15 5.199205e-15 -2.726408e-16
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1.029768e-15 -1.462931e-15 -1.523510e-15 2.063672e-15 -1.619993e-15 -9.131884e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb

1.738450e-15 -1.215274e-15 -4.245740e-16 1.806782e-15 -1.664059e-15 -4.923934e-16
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4.541098e-15 2.303659e-15 -6.491289e-15 -4.001380e-15 1.480737e-15 -3.426736e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb

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1.640158e-15 -1.615589e-15 -1.332811e-15 1.349407e-15 -1.219131e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb
-1.178253e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb
1.318485e-15 -1.921184e-15 -4.944467e-16 1.878425e-15 -2.237702e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb
7.125775e-16 -9.267548e-16 -6.221157e-16 -1.594848e-15 -4.762058e-15
1.888515e-15
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5.131415e-15 6.413299e-15 -8.717646e-15 -2.856919e-15 -1.850235e-15
1.056652e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
-1.410554e-15 -2.042871e-15 -1.945698e-15 5.934979e-15 -3.866243e-15
2.486870e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
8.851963e-15 -5.329587e-15 -3.337185e-15 1.598556e-15 7.231260e-15
-8.437373e-16
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2.486870e-15
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-4.785156e-16
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2.486870e-15
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2.486870e-15
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1.273280e-15 -2.292075e-15 -1.966298e-15 2.050228e-15 -1.836616e-15
-2.743764e-16
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2.608360e-15 1.432092e-14 4.180249e-15 -1.469677e-15 -5.986773e-15
-2.551510e-16
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-4.785156e-16
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1.784028e-15 -2.764259e-15 -1.360614e-15 8.447892e-15 -5.260612e-15
4.681117e-15
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9.649826e-15 1.050899e-14 -3.179303e-15 -1.052982e-14 -5.164033e-15
-3.416828e-16
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1.016749e-16 -4.600452e-15 2.132083e-15 3.385214e-15 -2.022092e-15
-1.652266e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
6.608421e-15 -4.114084e-15 -3.947485e-15 -9.281844e-15 -1.878400e-15
-7.727645e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb
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-3.498537e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.724924e-15 -2.946415e-15 7.661231e-15 1.830983e-15 5.256621e-15
-2.326700e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
3.498816e-15 -2.844369e-16 8.653472e-15 -9.126604e-16 2.905521e-15
-2.678544e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
3.555503e-15 -1.040057e-15 7.793307e-15 4.682669e-15 3.500533e-15
-2.948748e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
1.409868e-15 -4.679364e-15 5.169894e-15 -1.778994e-15 5.575710e-15
-1.077566e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
1.766557e-15 -2.22484e-15 7.875548e-15 1.646862e-15 5.79528e-15
-2.497450e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb
6.239871e-16 -1.471126e-15 8.167793e-15 1.431671e-16 5.414520e-15
-4.803831e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
2.326669e-15 -8.405550e-15 1.039488e-14 3.995901e-15 6.769200e-15
-5.697135e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-5.646879e-15 -4.735265e-16 9.734819e-15 1.404007e-15 -8.358280e-16
1.601590e-16
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
1.433381e-15 -2.322665e-15 8.064633e-15 3.412593e-15 3.785526e-15
-2.384259e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
-2.222523e-15 -7.297126e-15 6.746135e-15 -1.714215e-15 -2.672227e-15
1.684213e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
1.652105e-15 -2.874861e-15 8.508373e-15 2.833022e-15 3.749361e-15
-2.536514e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\1f8a00b551bea39.final.pdb
-2.222523e-15 -7.297126e-15 6.746135e-15 1.714215e-15 -2.672227e-15
1.684213e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\219f45328d47539a.final.pdb
1.457522e-15 1.84461e-14 6.58399e-15 -3.255156e-15 -2.493217e-15
4.963096e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\238dd3918e2fdc42.final.pdb
1.828373e-15 -8.765204e-15 8.343433e-15 1.005950e-14 -9.527822e-16
-2.50751e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\2b3027889e2dfc42.final.pdb
5.599108e-16 -2.515863e-15 7.708091e-15 1.417755e-15 3.062235e-15
-2.193072e-16
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
7.074851e-15 -5.216737e-15 8.981953e-15 3.023841e-15 7.143348e-15
-5.217529e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\34eb328251824006.final.pdb
-1.756471e-15 6.115001e-15 7.621990e-15 -1.028313e-14 -4.152835e-15
-2.457553e-15
E:\R-3.1.2\scripts\40.1ns_data\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
6.910244e-15 -3.099785e-15 1.329316e-14 1.364418e-15 1.121396e-14
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | \-2.936733e-15 |
|---------------------------------------------------------------|------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 1.406374e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | -5.646816e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 1.221805e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | -7.612325e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 9.846743e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -1.307209e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 1.902552e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.946136e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 7.074851e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.374549e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 6.239871e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 6.239871e-16 |

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| Path                                      | Coordinates               |
|-------------------------------------------|---------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 7.966911e-15 3.758788e-15 1.250703e-14 -1.068995e-14 -4.064731e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 5.930954e-15 -6.926090e-15 1.490342e-14 -1.496759e-14 -7.697829e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 5.909990e-15 -6.360950e-15 6.371658e-16 7.535229e-16 -3.453271e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 1.365763e-15 5.266646e-15 -9.184041e-16 -1.826602e-15 8.913378e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | 8.336840e-15 -2.576853e-15 1.551751e-14 -1.026801e-14 7.063594e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 9.422803e-15 6.904203e-15 -4.403780e-15 1.293641e-14 2.540283e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6dfb.final.pdb | 1.931381e-14 -1.025918e-14 -4.764601e-15 7.816250e-16 -1.397258e-15 4.031187e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | 8.301237e-16 -4.718384e-15 7.604683e-15 -3.782974e-15 -4.902633e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | 7.018582e-15 -4.280591e-16 -2.168538e-15 9.336461e-15 -1.522260e-14 -9.674998e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | 7.433078e-15 8.277441e-16 6.788495e-15 -5.127279e-15 -3.799511e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 3.911465e-15 -5.097908e-15 -1.899765e-16 5.478293e-15 2.200937e-15 -3.030961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\50c371611d85ac96.final.pdb | 5.909900e-15 -6.360950e-15 6.371658e-16 7.535229e-16 -3.453271e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | 6.855413e-15 -3.80241e-15 8.828690e-15 -2.835267e-15 -7.848109e-15 -1.204720e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | 3.019503e-15 -8.992534e-16 9.253748e-15 -5.373994e-15 4.376307e-15 1.370203e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 3.911465e-15 -5.097908e-15 -1.899765e-16 5.478293e-15 2.200937e-15 -3.030961e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 3.193706e-15 -7.137128e-15 -9.278776e-16 2.820923e-15 -2.553134e-15 1.019616e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | 8.301237e-16 -4.718384e-15 7.604683e-15 -3.782974e-15 -4.902633e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | 6.855413e-15 -5.380241e-15 8.828690e-15 -2.835267e-15 -7.848109e-15 -1.204720e-15 |

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| File Path                                                                 | Coordinates          | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb |
|---------------------------------------------------------------------------|-----------------------|---------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | -4.570617e-15         | -1.473606e-14 -1.015489e-14 -5.969150e-15 -1.128121e-14 -4.080778e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb       | 4.954049e-15          | -2.193999e-15 4.048830e-15 -9.597144e-15 4.825022e-15 -5.969150e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb       | -2.442289e-16         | -2.949567e-15 7.84491e-16 -4.080778e-16 -2.442289e-16 -2.442289e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb       | 1.684386e-15          | -2.20179e-15 1.091197e-14 -5.969150e-15 -2.442289e-16 -1.128121e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d589d9960a9e60.final.pdb         | -4.164262e-15         | 2.733687e-16 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d394b972037a2fbd.final.pdb       | 5.037790e-15          | 1.899765e-16 -8.420796e-16 4.824264e-16 -3.13784e-15 -2.654593e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d5e9d72307a2fbd.final.pdb        | -4.164262e-15         | -7.46556e-16 2.787397e-15 -2.654593e-15 -2.654593e-15 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d602082718ec3a1.final.pdb       | 2.480051e-15          | 8.512972e-15 -5.070465e-15 -2.191762e-15 -1.499111e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | 2.733687e-16 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d6589d9960a9e60.final.pdb        | -1.688760e-14         | -1.982896e-15 1.091197e-14 -2.442289e-16 -1.128121e-14 -3.083096e-15 |
### Table 1: Example Data

| File Path                        | Statistics          |
|----------------------------------|---------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb | 6.441335e-15 -4.976863e-15 -7.066368e-15 1.408024e-14 -1.555360e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb | 3.367715e-16 -4.002455e-15 -5.333730e-15 1.090604e-15 5.004900e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 3.525307e-15 -5.334991e-15 -9.000786e-15 5.555005e-15 4.801670e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -1.897235e-15 -9.322395e-15 -1.004844e-14 -4.736125e-16 6.150675e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb | 6.019599e-16 -5.554576e-15 -5.414127e-15 2.078599e-15 2.685131e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb | 4.416853e-16 -2.55081e-15 -7.991409e-15 -4.427957e-15 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | 1.448741e-15 -5.84190e-15 -6.624269e-15 1.536618e-15 2.417839e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 8.131553e-15 1.941428e-15 2.332271e-15 -3.118697e-15 4.66642e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | -2.536016e-15 -3.771334e-15 -5.624470e-15 -2.507645e-15 4.417620e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | -1.655595e-15 | -3.250813e-15 | -3.659805e-15 | -1.473723e-15 | 5.000160e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 4.233244e-15 | 4.233244e-15 | 5.135152e-15 | -3.175947e-15 | 3.242815e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 1.242615e-15 | -7.086337e-15 | -6.530421e-15 | -2.099346e-16 | 4.193907e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -1.486183e-15 | -1.988039e-15 | 5.135152e-15 | -3.175947e-15 | 3.242815e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 6.417037e-15 | 2.596967e-15 | 3.353828e-15 | -5.636771e-15 | 1.360206e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | -6.118706e-15 | 4.007256e-15 | -7.429692e-15 | 5.361468e-16 | 3.573039e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d78141e4018054a.final.pdb | 4.123691e-15 | 6.312931e-15 | -2.741795e-15 | 9.097651e-16 | 1.408954e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b8b06824ef848.final.pdb | 4.176686e-15 | -3.493986e-15 | -7.278041e-15 | 5.392399e-15 | -2.429810e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e9ad281f2ea2.final.pdb | 3.827448e-15 | -9.597425e-15 | -1.012075e-14 | -2.806558e-15 | -2.637056e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d9a60.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5f589d996d9a60.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6028718ec3a1.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e628718ec3a1.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e628718ec3a1.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e628718ec3a1.final.pdb | 4.416853e-16 | -2.255081e-15 | -7.991409e-15 | -4.427957e-15 | 6.801671e-15 |
| File Path                                                                 | Z-Score     | RMSD       | Energy       | Other       |
|--------------------------------------------------------------------------|-------------|------------|--------------|-------------|
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\f14fcae8deec4fa3.final.pdb | -2.253532e-15 | -2.435803e-15 | 1.052831e-15 | 2.385101e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\f83584e22003fb92.final.pdb     | -2.800012e-15 | -4.365535e-15 | 1.679220e-15 | 1.192400e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\013d855ad26c877c.final.pdb          | -2.597963e-15 | -2.656269e-16 | 3.512424e-15 | 3.456184e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\0dba59f3306825e8.final.pdb          | -2.907755e-15 | -2.011670e-16 | 3.618440e-15 | 3.409464e-16 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\18618a2a251b867b.final.pdb          | -2.571571e-15 | -2.017181e-15 | 2.571571e-15 | 2.017181e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\1f305f598641eeb2.final.pdb          | -2.551927e-15 | -2.017181e-15 | 3.618440e-15 | 2.031766e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\1f8a0b551be0a39.final.pdb          | -2.571571e-15 | -2.017181e-15 | 3.618440e-15 | 2.031766e-15 |
| E:\\R-3.1.2\scripts\\mPDBS\\summary_pdb_93\\219f45328d47579a.final.pdb          | -2.444465e-15 | -1.449155e-15 | 5.582333e-15 | 1.998624e-15 |
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9.004476e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
-1.32852e-14  8.181286e-16 -8.252289e-15 -4.107017e-16  2.279505e-15
-5.82235e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027899e2f6c42.final.pdb
-3.455673e-15 -1.337265e-15  1.536539e-15  9.289385e-16 -3.895283e-17
3.377467e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3d46e33793b0.final.pdb
-2.225798e-15 -4.147114e-15  1.973053e-15  7.126786e-15 -1.115256e-15
4.933108e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-1.564679e-14  1.262929e-15  1.463190e-15  4.738554e-17 -2.671720e-15
9.698508e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3871797b7ab.final.pdb
4.460565e-15 -2.852469e-15  1.020198e-14 -8.462740e-16  2.826063e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5e.final.pdb
-2.65269e-16  3.512424e-15 -3.069831e-15 -3.456184e-15  7.390759e-16
5.858068e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
-2.521569e-16  2.259220e-15 -3.153098e-15  7.027473e-15 -4.390414e-15
6.242391e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\423568adbc32d7ab.final.pdb
-5.803713e-16 -4.332295e-15  2.577198e-15 -8.193926e-15 -3.732148e-15
9.271988e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4432d7f5a7fc0c.final.pdb
2.399504e-15  1.428653e-15  1.387993e-15  7.027473e-15 -4.390414e-15
1.012897e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21df8e8c5d.final.pdb
-7.808139e-15 -3.150515e-15  5.230863e-15 -1.084527e-15 -2.548334e-16
-7.099473e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\457a40b3e8f113c.final.pdb
-2.597963e-15 -1.565979e-15 -1.947055e-15  3.941111e-15  2.973400e-15
1.088879e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
-1.403495e-15  3.006482e-15  7.262861e-15  7.121251e-15 -8.721244e-15
5.462065e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce.final.pdb
-2.576279e-15 -1.125894e-14  1.510137e-14  2.560271e-15 -1.259326e-15
7.074109e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb
-3.311430e-15 -1.395302e-15  1.523374e-15 -2.582938e-15  3.614188e-16
4.771338e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
-2.656269e-16  3.512424e-15  3.069331e-15 -3.456184e-15  7.390759e-16
5.858068e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d3a.final.pdb
-7.814548e-15 -3.854447e-15 -1.772477e-15 -1.880004e-15 -9.782177e-16
4.726171e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5b0b1f9e385e05f.final.pdb
-4.365535e-15 -2.593205e-15  1.679220e-15  1.192400e-15  3.097266e-16
1.736852e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
-3.311430e-15 -1.395302e-15  1.523374e-15 -2.582938e-15  3.614188e-16
Page 784
| Path                                                                 | 3.213160e-15 | -4.365535e-15 | -3.773172e-15 | 1.736852e-15 | 3.660804e-15 |
|---------------------------------------------------------------------|---------------|---------------|---------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb |               |               |               |               |               |
| -4.365535e-15                                                       | -3.773172e-15 | 1.736852e-15 | 1.92400e-15   | 3.097266e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d7e2fa.final.pdb |               |               |               |               |               |
| -5.921227e-16                                                       | -2.650915e-15 | -7.489430e-15 | -3.822788e-15 | 4.793212e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb |               |               |               |               |               |
| -8.244800e-16                                                       | -1.924458e-16 | 9.544425e-15  | 1.037126e-14  | -8.564163e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb |               |               |               |               |               |
| -3.273075e-15                                                       | -3.402699e-15 | -2.167657e-16 | -1.241892e-15 | 1.557354e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c70083816d66ba.final.pdb |               |               |               |               |               |
| -3.11430e-15                                                        | -1.395302e-15 | 1.523374e-15  | 2.582938e-16  | 4.771338e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb |               |               |               |               |               |
| -2.268412e-15                                                       | -7.584082e-16 | -1.424614e-14 | 8.155489e-15  | 3.354161e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb |               |               |               |               |               |
| -3.031257e-15                                                       | -1.882509e-15 | 1.721774e-15  | 1.417488e-15  | 8.084543e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac6f474b9c71d4dc.final.pdb |               |               |               |               |               |
| -2.225798e-15                                                       | -4.147114e-15 | 1.973053e-15  | 7.126786e-15  | -1.115256e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a08a823e4b4c666e.final.pdb |               |               |               |               |               |
| -3.675080e-15                                                       | -1.725542e-15 | 1.493405e-15  | 9.938326e-16  | -1.540646e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a08b039a2d823c616.final.pdb |               |               |               |               |               |
| -5.921227e-16                                                       | -2.650915e-15 | -7.489430e-15 | 1.417488e-15  | 8.084543e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0270083816d66ba.final.pdb |               |               |               |               |               |
| -1.792889e-15                                                       | -1.607900e-15 | -9.889465e-15 | 2.599702e-15  | 3.784466e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b2a84e8f6fa27a165.final.pdb |               |               |               |               |               |
| -4.365535e-15                                                       | -2.593205e-15 | 1.679220e-15  | 1.192400e-15  | 3.097266e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dc4924e3cd1ae.final.pdb |               |               |               |               |               |
| -3.223169e-15                                                       | -3.012239e-15 | 3.144427e-15  | 6.199491e-16  | 6.490634e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb |               |               |               |               |               |
| -4.365535e-15                                                       | -2.593205e-15 | 1.679220e-15  | 1.192400e-15  | 3.097266e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb |               |               |               |               |               |
| -3.773172e-15                                                       | 9.928715e-15  | 2.687759e-15  | -5.158526e-15 | 2.291741e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb |               |               |               |               |               |
| -4.365535e-15                                                       | -2.593205e-15 | 1.679220e-15  | 1.192400e-15  | 3.097266e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb |               |               |               |               |               |
| -4.365535e-15                                                       | -2.593205e-15 | 1.679220e-15  | 1.192400e-15  | 3.097266e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b58c88c8a505f3a288.final.pdb |               |               |               |               |               |
| -3.660804e-15                                                       | -1.968705e-15 | 1.350056e-15  | 2.894760e-16  | 2.412050e-16  |
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
4.365371e-15 -4.022954e-15 2.732414e-15 5.195004e-16 1.190904e-15
-5.886004e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
5.867063e-15 -1.032851e-15 7.231057e-15 -1.039071e-14 -5.895288e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
1.164397e-14 -9.528007e-15 1.535832e-16 3.135832e-15 -3.754659e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
7.249964e-15 -3.008241e-15 1.359130e-16 4.161024e-16 -6.889712e-15
-3.289908e-15
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4.569263e-15 -3.140063e-15 8.617135e-16 8.778830e-16 -1.397870e-14
-5.538528e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6976017896bef01.final.pdb
1.183276e-14 -5.885659e-15 5.795380e-15 -1.076645e-14 -1.77091e-14
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5.985893e-15 -3.281460e-15 6.224359e-15 -4.419785e-15 -2.298766e-15
-5.452241e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb
2.279032e-15 1.600633e-15 7.405047e-15 -9.377437e-15 1.446395e-15
-5.080939e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-3.407900e-15 -2.463346e-15 1.426910e-14 -1.775327e-14 -1.126861e-14
-2.625335e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
4.569263e-15 -3.140063e-15 8.617135e-16 8.778830e-16 -1.397870e-14
-5.538528e-15
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-5.525937e-15
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4.365371e-15 -4.022954e-15 2.732414e-15 5.195004e-16 1.190904e-15
-5.886004e-15
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9.263321e-15 -1.310991e-15 5.509835e-15 -1.122146e-14 1.622843e-14
-5.661775e-15
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4.825549e-15 -2.284755e-15 4.565307e-15 -2.360057e-15 -5.363032e-17
-9.083749e-15
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-9.083749e-15
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-7.979598e-15
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4.569263e-15 -3.140063e-15 8.617135e-16 -1.397870e-14 -5.538528e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
2.056063e-15 1.476125e-15 5.026744e-15 -6.045164e-16 -6.538446e-16 -9.340183e-16
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4.365371e-15 -3.595512e-15 6.616810e-15 -3.800800e-15 -5.032192e-15 -5.561219e-15
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8.875911e-15 -5.336134e-15 1.166466e-14 -7.447567e-15 -1.378136e-14 9.572640e-16
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9.720966e-15 4.024345e-15 7.447567e-15 -7.034191e-15 -5.981192e-15 -1.550544e-15
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4.365371e-15 -4.022954e-15 2.732414e-15 5.195004e-15 1.19004e-15 -5.886004e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
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4.365371e-15 -4.022954e-15 2.732414e-15 5.195004e-15 1.19004e-15 -5.886004e-15
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4.365371e-15 -4.022954e-15 2.732414e-15 5.195004e-15 1.19004e-15 -5.886004e-15
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| Path                                                                 | Values                        |
|----------------------------------------------------------------------|-------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 4.365371e-15 -4.022954e-15    |
|                                                                      | 2.732414e-15 5.195004e-16     |
|                                                                      | 1.190904e-15 -5.886004e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 4.157313e-15 -3.197226e-15    |
|                                                                      | 6.392681e-15 -5.180367e-15    |
|                                                                      | -4.27005e-15 -5.372092e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.234785e-14 -9.281762e-15    |
|                                                                      | 1.617017e-14 -8.473656e-15    |
|                                                                      | -1.166500e-14 -7.540407e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 2.056063e-15 1.476125e-15     |
|                                                                      | 5.026744e-16 -6.045164e-16    |
|                                                                      | -6.538446e-16 -9.340183e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 6.771403e-16 -8.922760e-15    |
|                                                                      | 8.508094e-15 -5.568445e-15    |
|                                                                      | 2.226364e-15 -8.770206e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | 2.455766e-15 3.196098e-15     |
|                                                                      | 1.331423e-14 -9.469296e-15    |
|                                                                      | -1.142184e-14 -6.371293e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 5.774449e-15 -5.023735e-15    |
|                                                                      | 6.185841e-15 -2.587037e-15    |
|                                                                      | -4.342647e-15 -7.248606e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 1.404384e-15 -5.474763e-15    |
|                                                                      | 7.416039e-15 -8.350523e-15    |
|                                                                      | -4.296101e-15 -2.564289e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.919009e-15 3.052288e-15     |
|                                                                      | 1.042836e-14 7.501683e-15     |
|                                                                      | -1.428851e-14 8.412871e-14    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d0809eff10197e2.final.pdb | 8.302114e-15 -5.061883e-15    |
|                                                                      | -8.323647e-16 -2.286526e-15   |
|                                                                      | -1.104132e-14 -3.384590e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 8.741598e-15 -7.123855e-15    |
|                                                                      | 4.204866e-15 9.031849e-17     |
|                                                                      | -3.013947e-15 -1.288601e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b006824ef848.final.pdb | 1.587304e-15 -5.926400e-15    |
|                                                                      | 7.671471e-15 -4.563696e-15    |
|                                                                      | -1.141566e-14 -1.670080e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feaa2.final.pdb | 5.188679e-15 -3.195591e-15    |
|                                                                      | 1.224602e-14 -1.656025e-14    |
|                                                                      | 2.339017e-15 -8.056928e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 4.825549e-15 -2.284755e-15    |
|                                                                      | 4.565307e-15 -2.360057e-15    |
|                                                                      | -5.363032e-17 -9.083749e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 8.007487e-15 -5.405337e-15    |
|                                                                      | 9.865054e-15 -5.496748e-15    |
|                                                                      | 4.803565e-16 -1.282505e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fb5.final.pdb | 5.867063e-15 -1.032851e-15    |
|                                                                      | 7.231057e-15 -1.039017e-15    |
|                                                                      | -5.703530e-15 -1.896995e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb | 4.825549e-15 -2.284755e-15    |
|                                                                      | 4.565307e-15 -2.360057e-15    |
|                                                                      | -5.363032e-17 -9.083749e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb517be32db050e.final.pdb | 4.365371e-15 -4.022954e-15    |
|                                                                      | 2.732414e-15 5.195004e-16     |
|                                                                      | 1.190904e-15 -5.886004e-15    |
Supplementary Text 10

1.778966e-15 -2.793926e-16  8.683157e-16 -1.700787e-15 -2.048785e-15 -4.122770e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
2.916579e-15 -1.076020e-15 -1.510953e-17  3.835748e-15 -5.176602e-15 -2.897588e-17
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4.200320e-15  1.976243e-15 -9.613110e-16  3.903436e-15  1.732383e-15 -2.095359e-15
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1.603971e-15  9.752617e-16  3.713173e-16  7.339897e-16  1.253340e-15 -9.631101e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
1.933758e-15 -1.514389e-15  1.938652e-15  4.227447e-15  3.452394e-15 -4.868885e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
1.656560e-15  4.528394e-15 -8.670583e-16  5.545699e-16  5.164304e-15 -1.734055e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
2.916579e-15 -1.076020e-15 -1.510953e-17  3.835748e-15 -5.176602e-15 -2.897588e-17
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
8.106607e-15  1.171114e-15  9.579669e-16  9.395854e-16  1.709377e-15  4.422536e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
1.057294e-14 -1.903962e-15 -7.961222e-15 -3.408272e-15 -5.694129e-15 -1.163747e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb
8.106607e-15  1.171114e-15  9.579669e-16  9.395854e-16  1.709377e-15  4.422536e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
1.042669e-14  7.539128e-16 -5.813834e-16 -3.681333e-15  3.669723e-15  6.079630e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef69760.final.pdb
## Supplementary Text 10

| Number | Description | Path | Value 1
|--------|-------------|------|--------|
| 1.656560e-15 | 4.528394e-15 | -8.670583e-16 | 5.545699e-16 | 5.164304e-15 | -1.734055e-15 |
| 2.916579e-15 | -1.076020e-15 | -1.510953e-17 | 3.835748e-15 | -5.176602e-15 | 2.897588e-17 |
| 1.086181e-15 | 1.122542e-15 | 1.235649e-16 | 8.511145e-16 | 4.946371e-15 | -7.865812e-15 |
| 2.897588e-17 | 3.519590e-17 | -1.599686e-15 | -1.467305e-15 | 7.529624e-17 | -1.152000e-14 |
| 1.976243e-15 | -9.613110e-16 | 3.903436e-15 | 1.732383e-15 | -2.095359e-15 |
| 6.878354e-15 | -2.032046e-15 | 1.468467e-14 | -2.573547e-15 | 4.396660e-15 |
| 7.810101e-15 | -9.791821e-16 | -1.816770e-14 | 1.387142e-14 | -2.253353e-16 |
| 3.072098e-16 | -3.126379e-16 | -9.055871e-16 | 1.585287e-15 | -4.356571e-16 |
| 9.631101e-16 | 1.253340e-15 | 1.585287e-15 | -4.356571e-16 |
| 6.713173e-16 | 7.339897e-16 | 1.253340e-15 | 9.631101e-16 |
| 1.253340e-15 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 3.713173e-16 | 7.339897e-16 | 1.253340e-15 | 9.631101e-16 |
| 1.253340e-15 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 1.253340e-15 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
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| 4.422536e-15 | 1.709377e-15 | 1.709377e-15 | 1.709377e-15 |
| 8.106607e-15 | 1.171114e-15 | 9.579669e-16 | 9.395854e-16 | 1.709377e-15 |
| 4.422536e-15 | 1.709377e-15 | 1.709377e-15 | 1.709377e-15 |
| 1.171114e-15 | 9.579669e-16 | 9.395854e-16 | 1.709377e-15 |
| 8.027942e-16 | -9.900326e-16 | -1.976912e-15 | 1.709377e-15 |
| 6.878354e-15 | -1.599686e-15 | -1.467305e-15 | 7.529624e-17 |
| 2.975345e-15 | 6.603203e-16 | -1.170858e-15 | 2.278976e-15 | -7.171392e-16 |
| 9.603971e-16 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 7.339897e-16 | 7.339897e-16 | 1.253340e-15 | 9.631101e-16 |
| 1.253340e-15 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 4.422536e-15 | 1.709377e-15 | 1.709377e-15 | 1.709377e-15 |
| 6.878354e-15 | -1.599686e-15 | -1.467305e-15 | 7.529624e-17 |
| 9.603971e-16 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 7.339897e-16 | 7.339897e-16 | 1.253340e-15 | 9.631101e-16 |
| 1.253340e-15 | 1.253340e-15 | 1.253340e-15 | 9.631101e-16 |
| 3.164512e-15 | 8.309395e-15 | 7.375342e-15 | -5.623293e-15 |
| 8.687679e-15 | 3.164512e-15 | 8.309395e-15 | 7.375342e-15 | -5.623293e-15 |
| 7.063007e-15 | 4.280320e-15 | 1.976243e-15 | -9.613110e-16 | 3.903436e-15 | 1.732383e-15 |
| 1.976243e-15 | -9.613110e-16 | 3.903436e-15 | 1.732383e-15 | -2.095359e-15 |
| 3.655029e-15 | -2.939111e-15 | -5.772006e-15 | 1.158487e-14 | -2.311598e-15 |
| 2.540855e-15 | 2.540855e-15 | 2.540855e-15 | 2.540855e-15 |
| 4.280320e-15 | 1.976243e-15 | -9.613110e-16 | 3.903436e-15 | 1.732383e-15 |
| 2.939111e-15 | -5.772006e-15 | 1.158487e-14 | -2.311598e-15 |
| 1.158487e-14 | 1.158487e-14 | 1.158487e-14 | 1.158487e-14 |
| 2.540855e-15 | 2.540855e-15 | 2.540855e-15 | 2.540855e-15 |
| 4.280320e-15 | 1.976243e-15 | -9.613110e-16 | 3.903436e-15 | 1.732383e-15 |
| 2.939111e-15 | -5.772006e-15 | 1.158487e-14 | -2.311598e-15 |
| 1.158487e-14 | 1.158487e-14 | 1.158487e-14 | 1.158487e-14 | 1.158487e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 8.106607e-15             | 1.171114e-15             | 9.579669e-16             | 9.395854e-16             | 1.709377e-15             |
| 4.422536e-15             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.371944e-15             | 5.511511e-16             | -8.386695e-16            | 1.554586e-15             | 2.079798e-16             |
| -5.337475e-16            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.537656e-15             | 1.304971e-16             | -5.337017e-16            | 1.514722e-15             | 3.495623e-17             |
| 7.022679e-17             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.524278e-15             | 1.048892e-15             | -6.340989e-16            | 2.119173e-15             | 2.689057e-16             |
| -2.988262e-16            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 9.642587e-16             | -2.278581e-16            | -3.773638e-16            | -1.246741e-15            | 1.965719e-15             |
| 1.237418e-15             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.072098e-16             | -3.126379e-16            | -9.055871e-16            | 1.585287e-15             | -4.35671e-16             |
| -2.980803e-15            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.538672e-15             | -9.181433e-16            | -4.180090e-15            | -1.901595e-14            | 2.971735e-15             |
| 6.738721e-16             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 7.884217e-15             | 1.086702e-15             | -1.763043e-15            | 1.904185e-15             | -3.831972e-15            |
| 8.614004e-15             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.639574e-15             | -3.793719e-15            | -5.061869e-15            | 3.460610e-15             | -6.437628e-16            |
| -2.416451e-15            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 1.632608e-15             | -4.720022e-15            | -3.328704e-15            | 2.431612e-15             | -2.448288e-15            |
| -2.869843e-15            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.369210e-15             | -4.882231e-15            | -4.640822e-15            | 3.03290e-15              | -3.390292e-15            |
| -6.603946e-16            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.948367e-15             | -1.785388e-15            | -3.228003e-15            | 1.970590e-15             | -1.876859e-15            |
| -2.208062e-15            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.471154e-16             | -9.556208e-16            | -4.261552e-15            | 1.356623e-15             | 5.223587e-16             |
| -5.39212e-16             |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.252253e-15             | -4.414681e-15            | -3.492166e-15            | 2.581124e-15             | -8.994339e-16            |
| -1.650869e-15            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcedab4194d9.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 2.525566e-15             | -1.963397e-15            | -3.308814e-15            | 6.699183e-15             | 2.304255e-15             |
| 6.32078e-16              |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dbaf59f3306825e8.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 5.459258e-15             | -6.404387e-15            | -2.183535e-15            | 3.752276e-15             | -3.156990e-15            |
| -2.653431e-16            |                          |                          |                          |                          |

| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb |
|--------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3.328150e-15             | -8.864225e-15            | 1.390851e-15             | 2.066341e-15             | -5.15346e-15             |

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 3.999786e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 2.525566e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 6.322078e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 1.775732e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 8.213255e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 8.213255e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e6977249a461.final.pdb | -4.674822e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 7.781635e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -9.394996e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 6.805397e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb | 5.918599e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 3.346526e-15 |
Supplementary Text 10

2.825134e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb
7.366451e-15 -4.213555e-15 2.527214e-15 3.215792e-16 -6.541542e-15
-2.190154e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea0f8694090cae7.final.pdb
5.918599e-16 -6.169525e-16 -9.196170e-15 1.484754e-15 -8.851002e-16
8.242063e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb
2.525566e-15 -1.963397e-15 -3.308814e-15 6.699183e-15 2.304255e-15
6.322078e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb
2.399172e-15 -4.902112e-15 -3.444091e-15 3.676437e-15 -1.373855e-15
-1.30986e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb
2.048517e-15 -4.503900e-15 -3.437183e-15 4.852570e-15 -7.58729e-16
-4.190346e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
2.196887e-15 -4.365438e-15 -3.396924e-15 2.669033e-15 -1.922406e-16
-1.493900e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
9.685503e-16 -4.925320e-15 -4.793204e-15 3.836356e-15 -3.343088e-15
8.552860e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb
7.444084e-16 -4.969782e-15 -3.523589e-15 5.883129e-15 -6.016761e-16
-2.229557e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f38584e22003fb92.final.pdb
2.994972e-17 -6.733887e-15 -7.202400e-15 -5.812293e-15 -1.003050e-14
1.460701e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb
-2.471154e-16 -9.556208e-16 -4.261552e-15 1.356623e-15 5.223587e-16
-5.39212e-16

[,955] [,956] [,957] [,958] [,959] [,960]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-4.510859e-15 -2.604966e-15 -1.929867e-15 1.413232e-15 2.441119e-15
-5.993742e-16
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-2.621441e-15 -3.679015e-17 -2.807456e-15 1.317319e-15 1.444333e-15
-1.176539e-16
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-3.876631e-15 -4.342205e-16 -1.306343e-15 1.732264e-15 4.556494e-15
-2.347143e-16
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
-2.371904e-15 -1.119620e-15 -2.382666e-15 2.627930e-15 -7.149380e-16
-3.272393e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
-2.999037e-15 8.119047e-16 -9.845839e-16 4.063164e-15 3.067240e-15
-2.160928e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
-2.417128e-15 -9.486538e-16 -2.093362e-15 1.707678e-15 1.051340e-15
-1.177923e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcaadb4194d9.final.pdb
-4.721681e-15 -1.861288e-15 1.797658e-15 2.361925e-15 1.055347e-15
-5.715305e-16

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb
-4.721681e-15 -1.861288e-15  1.797658e-15  2.361925e-15  1.055437e-15
-5.715305e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb
-3.118505e-16 -1.813412e-15  4.043918e-15  1.285840e-14 -6.762842e-15
 3.671455e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb
-4.721681e-15 -1.861288e-15  1.797658e-15  2.361925e-15  1.055437e-15
-5.715305e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb
2.642971e-15 -6.696829e-15 -4.079520e-16 -5.717123e-16 -1.173034e-15
 4.764595e-15

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-4.721681e-15 -1.861288e-15  1.797658e-15  2.361925e-15  1.055437e-15
-5.715305e-16

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-4.721681e-15 -1.861288e-15  1.797658e-15  2.361925e-15  1.055437e-15
-5.715305e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb
-2.478249e-15 -2.137341e-16 -1.999651e-15  1.601900e-15  1.400918e-15
-1.685548e-15

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7.088200e-15 -1.343493e-14  4.142011e-15  9.832292e-15  4.942951e-15
 4.893831e-15

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2.642971e-15 -6.696829e-15 -4.079520e-16 -5.717123e-16 -1.173034e-15
 4.764595e-15

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-5.351117e-15 -1.838358e-15  9.802996e-16  2.470462e-15  4.778348e-15
 8.623995e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb
1.084746e-14  2.091048e-16 -9.273564e-15  5.922662e-15 -2.626731e-15
-4.474441e-15

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-4.777649e-15  4.025967e-16 -5.163007e-16  2.283447e-16  1.557270e-15
-9.940742e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb
-1.810993e-14  1.620264e-14 -5.462278e-15  2.378526e-15 -8.248764e-15
-8.753652e-15

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-7.085821e-15 -8.244752e-15 -4.930324e-15  1.066241e-14  2.69079e-15
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 4.472897e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb
-6.356680e-15  7.271722e-15 -8.760120e-15 -1.389702e-15 -1.733464e-15
-6.981170e-15

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-2.999037e-15  8.119047e-16 -9.845839e-16  4.063164e-15  3.067240e-15
-2.160928e-15

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1.567843e-16  1.072369e-15  1.239362e-16  7.103760e-15 -1.452564e-15
-2.043057e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcede4b4194d9.final.pdb
7.354129e-16  3.910876e-17  4.416393e-15  5.148466e-15 -1.986350e-15
-1.817243e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
-1.701037e-15  3.672672e-15  5.452198e-15  7.164032e-15 -6.127567e-15
-5.012030e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
-8.000652e-16  9.307012e-17 -4.835922e-16  3.885404e-15 -5.907093e-17
-1.073748e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
1.345070e-15  1.902000e-15  6.408838e-16  6.538674e-15 -1.679739e-15
-2.176414e-15
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-1.524949e-15  4.802207e-15 -1.765354e-15  1.275685e-14  2.670026e-15
-4.893701e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
-3.182547e-16  1.263358e-15  2.304997e-16  7.217072e-15 -1.616331e-15
-2.028655e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551bea939.final.pdb
-1.524949e-15  4.802207e-15 -1.765354e-15  1.275685e-14  2.670026e-15
-4.893701e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
-3.983902e-15 -7.250369e-16 -1.204180e-14  2.539442e-15 -1.336614e-14
-3.512068e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
6.260724e-15  7.431199e-15 -8.361363e-15  8.400856e-15 -1.023149e-14
-5.786724e-15
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-1.308102e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
-7.510683e-16  1.292848e-15  1.821241e-15  9.898954e-15 -3.944330e-15
2.065293e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
-1.039595e-15  2.929178e-15 -3.444106e-15  2.024414e-15 -3.436796e-15
1.320658e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287197b7ab.final.pdb
5.232468e-15  1.731980e-15 -5.372938e-15 -2.659554e-15  5.370071e-15
1.613652e-15
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-1.073748e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
-3.791822e-15  3.609571e-15  4.792004e-17  6.087767e-15 -7.441966e-15
1.445129e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb
-2.574962e-15  3.019877e-15 -3.339370e-15  5.250127e-15 -4.514297e-15
-1.354366e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df75a7f7f0cfinal.pdb
-7.728635e-15 -3.456820e-15  1.036734e-15  8.949091e-15  1.497785e-14
1.472262e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21df8ecdf8.final.pdb
| File Path                                      | Values                  |
|-----------------------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb | 7.354129e-16 3.910876e-17 4.416393e-15 5.148466e-15 -1.986350e-15 -1.817243e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | 4.427149e-15 4.205994e-15 -1.436981e-15 4.711779e-15 -1.341095e-15 1.498589e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | 7.686552e-15 -4.018003e-15 -3.651356e-15 4.752795e-15 -2.655618e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce1d3f9.final.pdb | 7.354129e-16 3.910876e-17 4.416393e-15 5.148466e-15 -1.986350e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | 1.701037e-15 3.672672e-15 5.452198e-15 7.164032e-15 -6.127567e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\88d0666e1402203d.final.pdb | 7.354129e-16 3.910876e-17 4.416393e-15 5.148466e-15 -1.986350e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 4.427815e-15 -6.795324e-16 9.625530e-16 3.529049e-15 -4.627811e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -3.791822e-15 3.609571e-15 4.792004e-17 6.087767e-15 -7.441966e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8c22f4909d67e2fa.final.pdb | 7.354129e-16 3.910876e-17 4.416393e-15 5.148466e-15 -1.986350e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8c97d891e4e082.final.pdb | 3.689177e-15 9.995000e-16 5.724428e-15 5.325747e-15 -4.307719e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\904b89c94a633196.final.pdb | 3.079695e-16 1.132835e-15 5.680107e-16 6.173759e-15 -1.177822e-15 -2.506132e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\904b89c94a633196.final.pdb | 3.079695e-16 1.132835e-15 5.680107e-16 6.173759e-15 -1.177822e-15 -2.506132e-15 |
| Path                                                                 | Distance | Angle | Chain | Temperature | Pressure | Charge |
|----------------------------------------------------------------------|----------|-------|-------|-------------|----------|--------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 3.045082e-15 | 5.802700e-15 | 9.745006e-16 | 6.107614e-15 | -1.178935e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 1.513220e-15 | 1.030864e-15 | 6.669189e-15 | -1.579123e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 1.513220e-15 | 1.030864e-15 | 6.669189e-15 | -1.579123e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 7.354129e-16 | 3.910876e-17 | 4.416393e-15 | 5.148466e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 1.513220e-15 | 1.030864e-15 | 6.669189e-15 | -1.579123e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 7.354129e-16 | 3.910876e-17 | 4.416393e-15 | 5.148466e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 1.513220e-15 | 1.030864e-15 | 6.669189e-15 | -1.579123e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249a61.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0e39.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d809e7f10197e2.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1163918d3707839.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d4b48b06824ef848.final.pdb | 5.631912e-15 | 7.138123e-16 | 4.341548e-15 | 6.186333e-15 |
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-1.524949e-15  4.802207e-15 -1.765354e-15  1.275685e-14  2.670026e-15
-4.893701e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb

3.821455e-15  3.400320e-15 -1.016586e-15  1.005235e-14  1.220721e-15
6.773682e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb

-4.893701e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb

3.821455e-15  3.400320e-15 -1.016586e-15  1.005235e-14  1.220721e-15
6.773682e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb

-4.893701e-15
| File Path                                                                 | Values                                      |
|--------------------------------------------------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910ffffb22872.final.pdb     | -1.791601e-15                              |
| -9.033390e-18  1.930615e-15  3.004913e-15  -1.536764e-15  -1.091095e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb     | 1.725182e-15 -4.555636e-15  2.522389e-15  8.529954e-15  -4.257902e-15 |
| 1.565839e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb     | 1.840713e-15 -4.842077e-15  1.369968e-14  2.658209e-14  -1.232524e-14 |
| -1.367872e-14                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb     | -2.477673e-15 -4.027743e-15  8.396367e-16  9.994423e-15  -6.754081e-15 |
| 5.261567e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb     | -2.477673e-15 -4.027743e-15  8.396367e-16  9.994423e-15  -6.754081e-15 |
| 5.261567e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0efce12d3f9.final.pdb       | 5.737059e-16 -3.831069e-15  2.133740e-15  3.078514e-15  9.608980e-16  |
| -6.619715e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb     | -2.645683e-15 -3.330221e-15  1.177861e-15  -3.803045e-15  -7.082911e-16  |
| 8.209574e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb     | 1.199976e-15  9.842293e-16  1.012973e-14  6.669942e-16  -4.030089e-15  |
| -1.791601e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb     | -2.294711e-16 -4.759796e-15  5.877274e-15  -7.852413e-15  7.477773e-15  |
| -6.839864e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe47395.final.pdb     | 2.355919e-15 -7.851071e-15  2.247546e-14  -2.318055e-15  3.948623e-15  |
| -9.078224e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bee0d5986c138f.final.pdb     | 1.725182e-15 -4.555636e-15  2.522389e-15  8.529954e-15  -4.257902e-15  |
| 1.565839e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb     | -4.993889e-15  8.045390e-15  3.623868e-15  2.754988e-15  -2.468874e-15  |
| 1.425443e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb     | 4.706286e-15 -1.283176e-14  -8.350715e-15  -4.376497e-15  3.015585e-15  |
| 7.840668e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb     | -5.955673e-16 -3.869212e-15  6.030127e-15  1.522909e-15  -2.623493e-15  |
| -7.450693e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb     | -2.507910e-15  3.200581e-15  4.902293e-15  -5.847646e-15  1.690911e-15  |
| 3.276045e-15                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c9797d891e4e082.final.pdb    | 3.015510e-15 -4.706572e-15 -7.401715e-16 -5.31025e-15  2.732674e-15  |
| 1.424902e-16                                                     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb     | -4.671046e-17 -4.125891e-16  4.034438e-15  2.910790e-15  -1.258065e-15  |
| -1.308931e-15                                                     |
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E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
5.642660e-15 -3.317691e-15 -1.332751e-15 6.759350e-16 -9.468829e-16 -4.615846e-15
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
3.37625e-15 -2.786633e-15 -2.319179e-15 4.530635e-16 -5.972348e-16 -4.615846e-15
E:\R-3.1.2\scripts\40.1ns_data\summary_pdb_93\013d855ad26c877c.final.pdb
7.429800e-15 2.654855e-15 3.065716e-15 3.045893e-15 7.173151e-15 -1.966628e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb
5.668682e-15 -4.551621e-16 -1.262690e-15 2.337455e-16 -1.303809e-16 -2.687565e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb4194d9.final.pdb
4.967735e-15 -1.350514e-15 -2.216191e-15 -1.688023e-15 -1.433807e-15 -3.463839e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb
5.254457e-15 -6.463233e-16 -6.934294e-16 -1.065402e-15 -2.922940e-15 -3.282415e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb
2.922121e-15 -2.237932e-15 1.624148e-15 -8.314309e-16 4.192896e-15 -1.021762e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb
6.031455e-15 -1.864625e-15 -7.218082e-16 2.373494e-15 1.812509e-15 -3.516546e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb
3.243813e-15 6.686199e-16 2.363942e-15 3.270846e-15 3.913250e-15 -1.173630e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb
5.566151e-15 -2.091937e-15 -3.696872e-16 6.239293e-16 1.317658e-15 -3.313722e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb
3.243813e-15 6.686199e-16 2.363942e-15 3.270846e-15 3.913250e-15 -1.173630e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb
1.602226e-14 -1.935824e-14 -6.774914e-16 -1.126543e-14 1.300118e-15 4.965616e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb
5.612401e-15 -1.905597e-14 3.403576e-16 1.974737e-15 -3.992524e-15 -2.803242e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb
5.711497e-15 -2.108588e-15 -7.789863e-16 -1.289254e-15 1.508633e-16 -3.063226e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb
5.328494e-15 2.284973e-15 -4.626699e-15 -1.497574e-16 1.442558e-15 -1.443690e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb
2.100402e-15 -7.341973e-15 -7.369275e-15 -2.793258e-15 2.390012e-15 5.611053e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb
3.417002e-15 9.006126e-15 8.193968e-16 -7.752042e-15 3.513530e-15 -8.852908e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\37936adbc32d5de.final.pdb
2.922121e-15 -2.237932e-15 1.624148e-15 -8.314309e-16 4.192896e-15 -1.021762e-14

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb
-4.912952e-18 9.358105e-15 -9.853407e-15 1.153237e-15 5.241603e-15 -3.306064e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb
1.600801e-15 -7.783824e-15 -6.022652e-15 -3.415100e-15 1.863663e-15 -2.306064e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb
3.416488e-16 1.009308e-14 -9.733174e-15 1.046341e-14 9.391004e-15 -6.710958e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c6df.final.pdb
2.695184e-15 -1.012024e-14 7.995149e-15 -5.298417e-15 1.602153e-15 -6.069330e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb
5.254457e-15 -6.463233e-16 -6.934294e-16 -1.065402e-15 -2.922940e-15 -3.282415e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb
4.012336e-15 1.143874e-14 -3.547605e-15 2.284277e-15 3.033974e-15 -5.165060e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb
8.508614e-16 -5.908607e-15 -5.302603e-15 -2.763194e-16 -6.264017e-15 -1.946462e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb
5.237377e-15 -1.518008e-15 1.182388e-15 5.736409e-15 3.584653e-15 -5.439839e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb
2.922121e-15 -2.37932e-15 1.624148e-15 -8.314309e-15 4.192896e-15 -1.027162e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb
7.917186e-15 -5.671222e-15 5.721478e-15 -1.299753e-15 2.688032e-15 -8.527970e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b90f9e385f03f.final.pdb
4.967735e-15 -1.350514e-15 -2.216191e-15 -1.688023e-15 -1.433807e-15 -3.463839e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
5.237377e-15 -1.518008e-15 1.182388e-15 5.736409e-15 3.584653e-15 -5.439839e-15

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1.068411e-15 1.852020e-15 9.294390e-15 3.916347e-15 1.416125e-15 -9.124012e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
5.254457e-15 -6.463233e-16 -6.934294e-16 -1.065402e-15 -2.922940e-15 -3.282415e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
7.917186e-15 -5.671222e-15 5.721478e-15 -1.299753e-15 2.688032e-15 -8.527970e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760175986bef01.final.pdb
4.978268e-15 2.029511e-15 6.746388e-16 -7.082092e-15 -5.960295e-15 -3.549631e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc.final.pdb
9.369624e-15 3.278792e-15 -4.261467e-16 7.884199e-16 7.931784e-15 1.563194e-15

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| File Path                                      | First Row                | Second Row             | Third Row            | Fourth Row           | Fifth Row           | Sixth Row          |
|-----------------------------------------------|--------------------------|------------------------|----------------------|----------------------|---------------------|--------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | 3.778024e-15 -1.279967e-15 2.492977e-15 -4.497822e-15 8.712749e-15 | 7.103551e-15          | 1.416895e-14 -7.578099e-16 -5.592561e-15 3.901916e-15 4.615770e-15 | 1.201435e-15       | 3.754975e-16 -3.942839e-15 -1.676955e-15 4.470853e-15 | 2.474722e-15       |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8c9f8b.final.pdb | 8.891727e-17 7.809333e-15 4.136627e-15 2.390765e-15 1.62070e-15 | -3.48609e-15          | 1.180567e-15 1.882783e-15 -1.471973e-14 -2.78908e-15 8.71822e-15 | 2.810260e-15       | -9.164146e-15 1.198778e-14 -5.428355e-15 9.308175e-15 | 2.484774e-15       |

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb | 3.500401e-15 | 2.401041e-15 | -1.125699e-16 | 1.687909e-16 | 5.906404e-15 |
|---------------------------------------------------------------|----------------|----------------|----------------|----------------|----------------|
| 8.697203e-16 | -1.754626e-16 | -1.308662e-14 | 4.968420e-16 | 1.218679e-14 | 5.415557e-16 |
| 2.751494e-16 | -5.940036e-16 | 2.66253e-15 | 2.865208e-15 | 5.349221e-15 | 2.751494e-16 |
| 5.415557e-16 | -1.092540e-17 | -1.266253e-15 | 2.865208e-15 | 5.349221e-15 | 5.415557e-16 |
| 8.462018e-15 | -2.815667e-15 | 2.559738e-15 | -1.141217e-15 | -6.023999e-16 | 1.022512e-15 |
| 1.810260e-15 | -7.369862e-16 | 3.717553e-15 | 1.043137e-15 | 9.004137e-15 | 1.810260e-15 |
| 2.531034e-15 | -7.369862e-16 | 3.717553e-15 | 1.043137e-15 | 9.004137e-15 | 2.531034e-15 |
| -2.656856e-15 | -6.687072e-15 | -2.607053e-15 | -5.559748e-17 | 8.305668e-15 | 1.081837e-14 |
| -2.656856e-15 | -6.687072e-15 | -2.607053e-15 | -5.559748e-17 | 8.305668e-15 | -2.656856e-15 |
| -2.656856e-15 | -6.687072e-15 | -2.607053e-15 | -5.559748e-17 | 8.305668e-15 | -2.656856e-15 |
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8.891727e-17  7.809333e-15  4.136227e-15  2.390765e-15  4.620970e-15
-3.486069e-15

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-1.746349e-15  2.003812e-15  1.289430e-15  3.359769e-16  7.861566e-15

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-5.330290e-15  8.409828e-15  3.037117e-15 -1.501502e-15  4.599394e-15
-1.926778e-15

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2.247834e-15

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6.212551e-15

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1.485807e-15

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1.485807e-15

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-3.620644e-17  2.288167e-15  4.106354e-15 -2.478618e-15  5.76120e-15
8.119747e-16

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8.119747e-16

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5.853457e-15

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-7.468500e-15 -5.326720e-16 -3.650242e-16 -3.680314e-15  3.260187e-15
1.050875e-16

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1.050875e-16

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1.385926e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb

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-4.378548e-16  2.391825e-15  1.211335e-17  3.218218e-15  8.276904e-15
-9.088559e-16

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-1.614387e-15
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-2.760777e-16  1.108760e-15  5.930968e-15 -1.381964e-16 -1.256412e-15
 1.656196e-15
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-1.797981e-15  1.558446e-15  4.913006e-15 -3.935657e-15 -1.445140e-15
-2.148476e-15
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-1.397686e-15 -4.534440e-16  4.360827e-15 -2.685663e-15 -6.627111e-16
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-4.589860e-16
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-1.045387e-15
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 8.581865e-16
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-8.734173e-16
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-3.688288e-15
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-2.434734e-18
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Page 829
| PDB File                                    | Scores                               |
|--------------------------------------------|--------------------------------------|
| 34eb328251842006.final.pdb                | -2.090259e-16                        |
| 354b32871797b7ab.final.pdb                | 9.556867e-16  5.409099e-15  2.861863e-15 -2.675885e-15  8.275780e-15 -1.706138e-15 |
| 397368adbc32d5de.final.pdb                | 3.835938e-15  1.802025e-15  4.938395e-15 -4.565491e-15  2.766931e-15 -1.045387e-15 |
| 42357eee6642bf12.final.pdb                | -2.174901e-15                          |
| 44342d1f75a7fcfc.final.pdb                | -2.343955e-15  2.303138e-14  8.545593e-15 -1.193716e-14  3.031398e-15 -6.797506e-15 |
| 448ef21dffe8cfd5.final.pdb                | -4.21789e-15                          |
| 472a40b3e8f113c7.final.pdb                | -4.589860e-16                          |
| 48a26225951ea153.final.pdb                | 5.896150e-15                          |
| 48a26225951ea153.final.pdb                | -5.021789e-15                          |
| 4ab4a5c7c6682ce6.final.pdb                | -3.803502e-15  1.162871e-17  7.945104e-14  6.607863e-15  1.577736e-14  4.890837e-15 |
| 44a4a5c7c6682ce6.final.pdb                | 5.325047e-15  2.354778e-15  1.053656e-15  1.813177e-15  -3.654167e-15 |
| 45c35ac30f93d2db.final.pdb                | 5.392447e-16                          |
| 45e467f04822d30a.final.pdb                | -2.874376e-15                          |
| 45e467f04822d30a.final.pdb                | -2.574084e-15                          |
| 4635ac30f93d2db.final.pdb                | 5.392447e-16                          |
| 5a647f04822d30a.final.pdb                | 5.325047e-15  2.354778e-15  1.053656e-15  1.813177e-15  -3.654167e-15 |
| 5b091fe385e05fc.final.pdb                | -8.102955e-15  1.292624e-15  3.495403e-15 -1.231048e-15 -1.447087e-15  2.357873e-15 |
| 5c35ac30f93d2db.final.pdb                | 5.392447e-16                          |
| 5f60752431cf2dcb.final.pdb                | 1.739236e-15  -6.783450e-15  7.259858e-15 -1.857333e-15 -5.042021e-15 -2.288346e-16 |
| 626456dd6ff2868d.final.pdb                | -1.772683e-15  -7.109683e-15 -1.378817e-15 -4.861261e-15 -9.809387e-16 -4.589860e-15 |
| 6583d53ff3c8f7ef.final.pdb                | 4.473674e-15  5.325047e-15  2.354778e-15  1.053656e-15  1.813177e-15 |

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| File Path                          | Values                                                                 |
|----------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | -3.654167e-15                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | 6.359059e-15, -4.045706e-15, -1.546203e-15, -7.772038e-15, 3.763974e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea9826ffc4.final.pdb | -4.870553e-15                                                        |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -1.308970e-15, 5.703710e-16, 3.848989e-15, -2.539334e-15, 7.130187e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | 4.473674e-15, 5.325047e-15, 2.354778e-15, 1.053656e-15, 1.813177e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\79f910fffb22872.final.pdb | -1.038003e-15, -7.555915e-16, 5.042681e-15, -2.193319e-15, -5.345633e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb | -2.798452e-15, -4.476999e-15, 5.046223e-15, -1.081257e-15, -1.576028e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb | 4.473674e-15, 5.325047e-15, 2.354778e-15, 1.053656e-15, 1.813177e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefce12d3f9.final.pdb | -4.785253e-15, -3.473462e-15, 9.254879e-15, -4.860352e-15, -1.583834e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb | -1.772683e-15, -7.109683e-15, -1.378817e-15, -4.861261e-15, -9.809387e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb | 4.473674e-15, 5.325047e-15, 2.354778e-15, 1.053656e-15, 1.813177e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadac62.final.pdb | -4.741342e-15, 1.817879e-15, 1.23098e-15, -5.244110e-16, 2.583709e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8c22f4909d67e2fa.final.pdb | 6.566127e-15, 5.615052e-16, -3.955381e-17, -1.025746e-15, -5.924112e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dea8ed0d81fb3ef.final.pdb | -1.086421e-14, -2.205496e-14, 1.443387e-14, -3.905485e-15, -3.770898e-15 |
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-1.040422e-15 -4.925648e-17 5.668483e-15 -3.066362e-15 -2.981738e-16 2.139413e-16
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-8.102955e-15 1.292624e-15 3.495403e-15 -1.231048e-15 -1.447087e-15 2.357873e-15
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bca2af55fc9d0681.final.pdb
-4.741342e-15 1.817879e-15 1.230698e-15 -5.244110e-16 2.587309e-15 4.630853e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb
-2.913497e-15 5.621263e-15 1.314500e-14 5.491324e-15 2.268412e-15
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| PDB File Path                                                                 | E1  | E2  | E3  | E4  | E5  |
|--------------------------------------------------------------------------------|-----|-----|-----|-----|-----|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb             | 6.350482e-15 | -2.225917e-15 | -2.225917e-15 | -2.225917e-15 | -2.225917e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb             | -1.446523e-15 | -1.446523e-15 | -1.446523e-15 | -1.446523e-15 | -1.446523e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb             | -5.129577e-15 | -5.129577e-15 | -5.129577e-15 | -5.129577e-15 | -5.129577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb             | 3.477198e-15  | 3.477198e-15  | 3.477198e-15  | 3.477198e-15  | 3.477198e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb             | -4.887422e-15 | -4.887422e-15 | -4.887422e-15 | -4.887422e-15 | -4.887422e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb             | -4.540255e-16 | -4.540255e-16 | -4.540255e-16 | -4.540255e-16 | -4.540255e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1163918d3707839.final.pdb             | -1.805626e-14 | -1.805626e-14 | -1.805626e-14 | -1.805626e-14 | -1.805626e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1b48b06824ef848.final.pdb             | 6.318417e-15  | 6.318417e-15  | 6.318417e-15  | 6.318417e-15  | 6.318417e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 1.363997e-15  | 1.363997e-15  | 1.363997e-15  | 1.363997e-15  | 1.363997e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 1.384527e-15  | 1.384527e-15  | 1.384527e-15  | 1.384527e-15  | 1.384527e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 5.793705e-15  | 5.793705e-15  | 5.793705e-15  | 5.793705e-15  | 5.793705e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -4.798452e-15 | -4.798452e-15 | -4.798452e-15 | -4.798452e-15 | -4.798452e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -8.129090e-15 | -8.129090e-15 | -8.129090e-15 | -8.129090e-15 | -8.129090e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  | 1.404075e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 | -1.501023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281f038.final.pdb             | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  | 3.526340e-15  |
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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb     | 1.429416e-15 -1.207886e-15 3.503958e-15 -1.592037e-15 -4.785170e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb      | 1.839734e-15                                                             |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb32871797b7ab.final.pdb     | -1.140863e-15 4.729102e-15 7.412169e-15 -4.335841e-15 2.452694e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb     | 4.644205e-16 6.349869e-15 7.096587e-15 -1.281478e-14 -4.175581e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb      | -1.369563e-15 -9.448094e-15 9.03597e-15 -6.134126e-15 3.06721e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb      | 3.472200e-15 3.189535e-15 1.028726e-14 -1.647019e-14 -2.791423e-16  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb      | 7.0176319e-15 -1.008160e-14 7.776319e-15 -1.080498e-15 -1.537069e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fc8c.final.pdb      | 7.012384e-15 -5.320918e-15 1.739856e-16 -8.364073e-15 -1.284206e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21df8cdef8c.final.pdb      | 7.751388e-16 -2.913227e-14 -1.23840e-14 2.299514e-14 -3.937593e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb      | 2.034615e-15 5.70520e-15 9.674525e-15 -1.565786e-16 -8.166691e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb      | 1.273851e-14 5.814058e-15 6.042726e-15 -9.665440e-15 -1.610410e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\497368adbc32d5de.final.pdb      | 4.267421e-15 -9.462140e-15 9.348718e-16 -7.47858e-15 5.866953e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb      | 2.034615e-15 5.70520e-15 9.674525e-15 -1.565786e-16 -8.166691e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2d.final.pdb       | 7.079624e-15 -1.048478e-14 6.05373e-15 -1.169544e-14 6.363167e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dc8.final.pdb      | 4.267421e-15 -9.462140e-15 9.348718e-16 -7.47858e-15 5.866953e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\636456e-15 -7.464890e-16 -2.345031e-15 5.037086e-15 -3.189635e-15  |

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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb      | 3.430133e-15 7.990858e-16 -1.377458e-15 -1.984874e-17 -1.017653e-14 -5.843669e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de381a3c.final.pdb      | -2.335397e-15 5.732273e-15 -5.123260e-15 -5.518068e-15 -5.387233e-15 8.455359e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb     | 9.350194e-16 -1.303154e-14 -6.180569e-15 -3.554009e-15 -1.768703e-15 -2.475391e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb     | 1.390855e-16 -1.389013e-15 5.323580e-15 -3.437771e-15 -3.00072e-15 1.494268e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb     | 1.507484e-14 -1.180422e-14 9.310310e-15 -6.743733e-15 -1.374381e-16 -4.705319e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb     | -3.004853e-15 6.950106e-15 6.607328e-15 6.091972e-15 1.136641e-15 5.550335e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb      | -3.968474e-15 5.206859e-15 4.575251e-15 8.270351e-15 -1.342697e-14 4.821028e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d1163918d3707839.final.pdb     | -7.674804e-15 3.437484e-15 1.485387e-14 -1.461608e-15 -9.638418e-15 9.754806e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb     | 1.619520e-15 -2.688301e-15 2.029973e-15 -1.525241e-15 -4.35307e-15 1.037045e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | 2.147367e-14 | 2.984984e-15 | 1.385958e-15 | -4.539506e-15 | 3.606622e-15 |
|-----------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb | -1.166616e-14 | -6.687327e-17 | -8.283906e-15 | -2.038339e-16 | 2.578089e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -1.350713e-14 | -1.166616e-14 | -6.687327e-17 | -8.283906e-15 | -2.038339e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | -3.140864e-15 | -2.722473e-15 | 1.046169e-15 | 6.065514e-16 | -1.323733e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287197b7ab.final.pdb | -4.114498e-15 | 7.888501e-16 | 1.929412e-15 | -9.436371e-15 | -1.000592e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\3b3027889e2fdc42.final.pdb | 3.205317e-14 | 4.705211e-15 | 3.585400e-15 | 4.865908e-15 | -1.000592e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\3fcb3b46e33793b0.final.pdb | -9.268261e-15 | -5.643931e-15 | -5.427844e-16 | 2.667027e-15 | -6.933577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -1.782062e-15 | -5.643931e-15 | -5.427844e-16 | 2.667027e-15 | -6.933577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 3.520183e-15 | -1.364921e-15 | -2.238216e-15 | -1.789974e-15 | -3.608424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -9.268261e-15 | -5.643931e-15 | -5.427844e-16 | 2.667027e-15 | -6.933577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62c6a25f.final.pdb | 3.205317e-14 | 4.705211e-15 | 3.585400e-15 | 4.865908e-15 | -1.000592e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | -7.067031e-15 | -6.126184e-15 | -5.786504e-16 | 6.441324e-15 | -9.33577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | -7.067031e-15 | -6.126184e-15 | -5.786504e-16 | 6.441324e-15 | -9.33577e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | 3.520183e-15 | -1.364921e-15 | -2.238216e-15 | -1.789974e-15 | -3.608424e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb |
|---------------------------------------------------------------|
| 2.984120e-14 5.551665e-17 2.051674e-15 -2.413966e-15 |
| -3.904724e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb |
|---------------------------------------------------------------|
| -4.090733e-15 -2.978995e-15 1.993111e-15 4.662552e-15 -3.394722e-15 |
| -3.149100e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb |
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| -5.757515e-15 -5.524800e-15 2.199952e-16 -3.810987e-15 1.549090e-16 |
| -3.834414e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb |
|---------------------------------------------------------------|
| -5.606062e-15 -1.369093e-15 5.929558e-16 1.462154e-15 -1.305333e-15 |
| -7.059595e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb |
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| -6.950955e-15 -2.730739e-15 6.252088e-15 1.620103e-15 -3.711166e-15 |
| -3.154093e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb |
|---------------------------------------------------------------|
| -6.098488e-15 -2.978995e-15 1.993111e-15 4.662552e-15 -3.394722e-15 |
| -3.149100e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ac88c8a505f3a288.final.pdb |
|---------------------------------------------------------------|
| 3.154093e-15 -1.438961e-15 1.243981e-15 6.211501e-15 -3.013881e-15 |
| -3.852266e-15 |

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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.616051e-14 7.541919e-15 6.232829e-15 8.724248e-15 -9.802315e-15 -7.675732e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 3.154093e-15 -1.438961e-15 1.243981e-15 6.211501e-15 -3.013881e-15 -1.852266e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 2.947881e-16 -6.934691e-16 -3.081880e-15 7.390334e-15 -3.421901e-15 -7.824297e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | 3.160067e-16 -3.421350e-15 -6.063723e-16 5.665005e-15 -1.215178e-15 -4.182128e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04212145d015047.final.pdb | -2.332417e-15 -2.281446e-15 8.672167e-16 1.041650e-15 -1.637997e-15 -4.525200e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 4.813359e-15 -1.937180e-15 -2.283364e-16 -6.227212e-15 -4.505475e-15 -6.251457e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -3.206440e-14 -5.151611e-15 1.871080e-15 -1.553488e-15 -1.021791e-15 -3.610446e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | 7.291005e-15 -1.440608e-15 -4.920097e-15 3.093078e-15 4.015324e-15 -3.517367e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 7.724366e-15 -2.377517e-17 1.800979e-15 2.577344e-15 2.982047e-15 -1.188912e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | -5.121984e-14 -2.965784e-15 8.082791e-16 -4.680909e-15 -7.251992e-16 2.769839e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fe2a.final.pdb | 2.878335e-15 -2.860253e-15 2.409108e-15 5.047612e-16 1.236930e-15 -9.305551e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | -1.782062e-15 -5.643931e-15 -5.427844e-16 2.667027e-15 2.613562e-15 -3.621684e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 9.083831e-15 -6.147911e-15 -2.700676e-15 6.086017e-16 -3.589562e-16 -6.530448e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | -1.845237e-15 -2.611653e-15 -9.131304e-16 1.109538e-15 2.640042e-15 2.943018e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb | 1.255322e-15 -2.129729e-15 -3.778338e-16 1.740991e-15 -1.125046e-15 -2.806975e-15 |
Supplementary Text 10

-8.165677e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb
5.881747e-16 -2.325308e-15 1.123032e-15 1.214239e-15 1.141117e-15
-2.135342e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb
-7.927165e-16 3.774004e-15 -4.744030e-15 -3.694513e-15 2.280756e-16
2.090296e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb
4.875940e-15 4.670713e-15 1.379236e-15 -8.122603e-15 -2.240932e-15
1.009053e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb
-4.568036e-16 8.260852e-16 -1.540093e-15 -1.949000e-15 -3.144859e-15
1.390086e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb
-1.020147e-16 -6.563617e-16 -2.568720e-15 3.583953e-15 -4.527258e-15
-8.165677e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb
-5.787123e-16 2.648276e-16 -9.458180e-15 -1.484257e-14 9.436104e-15
9.420159e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
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-8.251554e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982fffc4.final.pdb
-6.791993e-16 7.345724e-16 -9.197168e-15 -1.611818e-14 8.384966e-16
1.486134e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
-2.083770e-16 -2.799115e-16 -1.438420e-14 2.936714e-15 9.050976e-16
3.335675e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
-1.020147e-16 -6.563617e-16 -2.568720e-15 3.583953e-15 -4.527258e-15
-8.165677e-16
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb
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-1.283270e-15

E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
-2.829745e-16  1.624735e-15  8.968218e-16  1.409767e-15  4.645383e-15
-1.723275e-15

E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
1.957796e-15 -1.277891e-16 -2.744524e-15 -2.489311e-15 -2.776846e-15
-6.084327e-15

E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
2.233747e-15  2.675318e-15  8.030663e-16 -1.721964e-15 -4.371933e-15
3.087389e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb
1.701756e-15  2.696644e-17  4.247143e-15  6.071126e-15  1.371066e-14
-1.507987e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a7053d2ca0d54.final.pdb
-6.423631e-16  1.138767e-15  5.846870e-16  1.843171e-15  3.259996e-15
-1.012369e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fcaed64194d9.final.pdb
-1.909962e-15  4.169375e-15  4.531613e-15  8.818520e-16 -4.607093e-16
Page 859
| File Path | Values |
|----------|--------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | -4.292408e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -3.824061e-15 8.292064e-15 -5.551190e-15 -2.074110e-15 -2.405399e-15 3.589511e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | -1.909962e-15 4.169375e-15 -4.531613e-15 -8.818520e-16 -4.607093e-16 5.756120e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | -9.212076e-15 -2.557572e-15 -8.834273e-15 -3.062095e-15 9.169323e-15 6.184379e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d107c1017b.final.pdb | -1.909962e-15 4.169375e-15 -4.531613e-15 -8.818520e-16 -4.607093e-16 5.756120e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -1.909962e-15 4.169375e-15 -4.531613e-15 -8.818520e-16 -4.607093e-16 5.756120e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88ca505f3a288.final.pdb | -5.423496e-16 1.687853e-15 -1.712904e-15 -1.313364e-15 -1.637462e-15 2.243982e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 3.449921e-15 -1.128871e-15 -8.816566e-16 -5.608566e-15 -7.863142e-15 2.739927e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | -2.984635e-15 3.824042e-15 5.756486e-15 1.090503e-14 -7.402598e-15 5.074844e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2af555fc9d0681.final.pdb | -9.212076e-15 -2.557572e-15 -8.834273e-15 -3.062095e-15 9.169323e-15 6.184379e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 3.449921e-15 -1.128871e-15 -8.816566e-16 -5.608566e-15 -7.863142e-15 2.739927e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69772494a61.final.pdb | -5.565458e-15 -6.843517e-15 4.743954e-15 -1.261205e-14 1.303086e-14 -1.184684e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 1.886700e-15 -2.421239e-15 4.596290e-15 -3.012303e-15 -3.543020e-15 2.854761e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\de78141e4018054a.final.pdb | 5.037607e-15 -6.229869e-15 -1.132836e-14 4.324868e-16 -2.440530e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.126200e-16 3.823107e-15 -1.117823e-15 -1.041185e-14 8.176875e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d28e48f6fa27a165.final.pdb | -1.021027e-14 9.756878e-15 -4.512249e-15 7.608683e-15 -4.394223e-15 2.457809e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 1.328886e-14 4.402814e-15 4.229181e-15 -3.130557e-15 3.532559e-15 1.979241e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb4b806824ef848.final.pdb | 4.411640e-15 1.210898e-15 2.708160e-15 5.891563e-15 -8.507836e-15 4.849228e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281feea.final.pdb | 1.701756e-15 2.696644e-17 4.247143e-15 -6.071126e-15 -1.371066e-14 |
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| Path                                                | Values                                                                 |
|-----------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb   | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090cae7.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eba517be32db050e.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eb04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ecb862ebcad52078.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb     | 1.102590e-15  3.066402e-15 -1.243123e-15 -3.880884e-15 -2.661491e-15 |

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| Path                                                                 | Data                                                                 |
|----------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 7.550822e-15 -2.422180e-15 1.844798e-15 1.018654e-15 1.368525e-15 9.793196e-17 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb | 4.207558e-15 2.603466e-15 7.723779e-16 -1.323054e-15 -5.622614e-16 3.691267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceedb4194d9.final.pdb | 1.023420e-14 -6.357007e-15 -5.426270e-15 4.453111e-15 -7.462591e-16 3.542691e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 6.520221e-16 -5.478516e-16 -8.158460e-15 3.905837e-15 1.297887e-14 5.646477e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 1.023420e-14 -6.357007e-15 -5.426270e-15 4.453111e-15 -7.462591e-16 3.542691e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 2.465257e-14 1.272499e-15 1.769287e-14 1.558269e-14 -1.652519e-14 1.665110e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 2.465257e-14 1.272499e-15 1.769287e-14 1.558269e-14 -1.652519e-14 1.665110e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 1.390934e-14 4.010876e-15 2.754016e-15 2.044608e-15 1.295358e-14 5.380970e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 1.390934e-14 4.010876e-15 2.754016e-15 2.044608e-15 1.295358e-14 5.380970e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 1.361395e-14 3.813873e-15 -8.900480e-15 -4.350031e-15 2.043166e-14 1.574481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 1.361395e-14 3.813873e-15 -8.900480e-15 -4.350031e-15 2.043166e-14 1.574481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 3.397321e-16 -4.150123e-15 -7.669193e-15 3.817672e-15 5.843426e-15 -5.006043e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | 3.397321e-16 -4.150123e-15 -7.669193e-15 3.817672e-15 5.843426e-15 -5.006043e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcf0.final.pdb | 3.813873e-15 -8.381319e-16 5.015457e-15 -9.694338e-16 -3.289225e-14 1.248714e-16 |

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| Path                                                                 | Value                                                                 |
|---------------------------------------------------------------------|----------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | 1.393389e-14 -7.072916e-15 5.137403e-15 8.091597e-15 1.381448e-14 -2.956756e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | 9.750018e-15 -8.507344e-15 -9.300348e-15 5.830682e-15 1.430892e-14 -1.323586e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | 4.207558e-15 2.603466e-15 7.723779e-16 -1.323504e-15 -5.622614e-16 3.691267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aeac.final.pdb | 2.005644e-14 3.289426e-15 1.129255e-14 1.967341e-16 3.781537e-15 -7.40718e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | 4.207558e-15 2.603466e-15 7.723779e-16 -1.323504e-15 -5.622614e-16 3.691267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | 2.577092e-15 -9.682068e-16 8.274651e-15 1.732101e-15 -7.092407e-15 3.966814e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | 4.207558e-15 2.603466e-15 7.723779e-16 -1.323504e-15 -5.622614e-16 3.691267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | 4.207558e-15 2.603466e-15 7.723779e-16 -1.323504e-15 -5.622614e-16 3.691267e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | 7.181741e-15 -2.820299e-16 6.894758e-17 2.005013e-15 5.49005e-16 1.926837e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.651733e-14 7.160274e-15 2.369374e-14 -2.892239e-15 -1.682021e-15 -2.827085e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d0681.final.pdb | 2.577092e-15 -9.682068e-16 8.274651e-15 1.732101e-15 -7.092407e-15 3.966814e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 6.062231e-15 -2.593381e-16 8.966457e-16 -4.795411e-15 -1.314150e-14 -2.894229e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb | 7.222507e-15 -1.940426e-15 6.598447e-15 7.650237e-15 1.570164e-14 -1.364368e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 5.567251e-15 -3.755967e-16 2.882454e-15 -1.958969e-15 -2.622192e-15 2.253839e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | 2.197571e-14 -7.776741e-15 -8.233261e-15 7.056760e-15 7.952387e-16 1.973203e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 4.170879e-15 -1.705321e-14 -2.208090e-14 1.046718e-14 3.806913e-14 -1.022125e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc8809eff10197e2.final.pdb | 9.427868e-17 4.938367e-15 -4.605876e-15 -2.344637e-16 7.979221e-15 3.806256e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 1.031120e-14 -1.530503e-15 -1.452534e-14 -1.995089e-15 1.541199e-14 -1.988239e-15 |
| File Path                                      | Values                           |
|-----------------------------------------------|----------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb | -4.041328e-15 6.004239e-15 -5.165994e-15 -2.629879e-15 -9.018329e-15 -4.224764e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dffe8cdfb.final.pdb | 2.362523e-16 8.029571e-15 7.919917e-15 8.999391e-16 -2.654663e-14 -3.052364e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -1.445039e-14 -1.925377e-15 -1.386194e-14 -7.702275e-15 1.114419e-14 2.141022e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -5.750583e-17 1.462290e-15 -1.635800e-15 -2.620174e-15 7.990092e-15 -6.379568e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | -5.750583e-17 1.462290e-15 -1.635800e-15 -2.620174e-15 7.990092e-15 -6.379568e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb | -1.002365e-14 -1.969861e-16 -7.889300e-16 -8.420822e-16 -2.83113e-15 -5.724710e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb | -9.142530e-16 -4.829198e-16 -4.305547e-15 3.401410e-15 1.024681e-17 -7.425602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb | -4.095180e-15 6.678898e-15 -3.644521e-15 -1.937412e-15 -3.113421e-15 -6.149042e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb | -1.149042e-15 6.678898e-15 -3.644521e-15 -1.937412e-15 -3.113421e-15 -6.149042e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb | 2.880210e-16 8.020135e-16 -6.369926e-16 -6.194222e-16 1.044355e-14 1.520465e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb | -7.570553e-17 1.462290e-15 -1.635800e-15 -2.620174e-15 7.990092e-15 -6.379568e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb | -9.142530e-16 -4.829198e-16 -4.305547e-15 3.401410e-15 1.024681e-17 -7.425602e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb | 3.860817e-15 3.009597e-15 2.407657e-15 2.947143e-15 1.273248e-14 -5.669535e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb | -1.870454e-15 2.491848e-15 -2.672840e-15 -1.161271e-15 -2.504985e-15 -3.320383e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb | -5.852072e-15 -7.899846e-15 6.512162e-16 -2.906627e-14 2.341801e-15 -7.505828e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb | -2.493473e-15 5.320038e-15 2.281683e-15 -4.929608e-15 -1.204541e-14 -6.517376e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb | -1.627430e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b4dd239fcabff1df.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b88c8a505f3a288.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
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|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd02e697772494a61.final.ppb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd04221245d015047.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd678141e4018054a.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bd71b40af0f0efef39.final.pdb | -3.895815e-15 | -3.895815e-15 | -3.895815e-15 | -9.376826e-15 | -9.376826e-15 |
|-------------------------------|----------------|----------------|----------------|----------------|----------------|
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Supplementary Text 10
-1.503824e-14  6.133261e-15 -3.812723e-15  8.808695 e-15  2.992991e-15
-9.866937e-15
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-3.675468e-15 -6.928950e-15 -8.339863e-15 -1.835809 e-14  1.549612e-14
-2.878458e-15
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-3.283243e-15
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-1.765204e-15
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-2.993383e-15
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-3.752972e-15
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1.874977e-15
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-6.770791e-15 -3.138395e-15 2.295129e-16 4.681143e-15 1.407596e-15
1.992464e-14
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2.616015e-15 -5.084817e-15 1.236645e-15 -1.273128e-15 6.086915e-15
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-2.298711e-15
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Supplementary Text 10

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1.61040e-16

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1.249312e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
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6.720451e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc.final.pdb
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| File Path                                                                 | Values                                                                 |
|--------------------------------------------------------------------------|------------------------------------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ab8039a2d823c616.final.pdb      | 5.274704e-15 -3.288096e-15 1.619144e-15 3.775751e-15 -1.167062e-15 3.001674e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acf4d74b9c71d4dc.final.pdb       | 3.639501e-15 -6.614843e-15 6.003665e-15 2.383168e-15 -6.232995e-15 3.810957e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ad8a823e4b4c668e.final.pdb       | 4.394000e-15 -2.669518e-15 3.415996e-15 4.167527e-15 -4.809694e-16 2.391850e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b16ababd03b7b857.final.pdb       | -4.034482e-15 2.968636e-15 9.481243e-15 -2.049918e-15 -1.515414e-15 1.560762e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b226923e697d3c63.final.pdb       | -7.19455e-15 -7.921967e-15 -2.294520e-15 8.578907e-15 7.467083e-16 4.866826e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b28e48f6fa27a165.final.pdb       | -5.274704e-15 -3.288096e-15 1.619144e-15 3.775751e-15 -1.167062e-15 3.001674e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b42c4924e3cd1aec.final.pdb       | -4.034482e-15 2.968636e-15 9.481243e-15 -2.049918e-15 -1.515414e-15 1.560762e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb       | -4.034482e-15 2.968636e-15 9.481243e-15 -2.049918e-15 -1.515414e-15 1.560762e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb       | 2.670806e-15 -1.295273e-15 2.919559e-15 3.445936e-15 -5.638871e-16 5.570480e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4e4f27e.final.pdb       | -4.223133e-15 -5.381021e-15 -4.480679e-15 1.072632e-14 -2.962174e-15 -1.321775e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ca2a1f55fc9d6811.final.pdb       | -4.223133e-15 -5.381021e-15 -4.480679e-15 1.072632e-14 -2.962174e-15 -1.321775e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb       | 6.292360e-15 -6.699868e-15 4.139237e-16 4.273956e-15 -6.066893e-15 1.152874e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e697772494a61.final.pdb       | -5.219096e-15 -8.388329e-15 -6.816522e-15 7.987442e-15 -3.511182e-15 1.114566e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb       | 3.046481e-15 -2.984895e-15 3.057610e-15 5.864621e-16 -5.286834e-16 6.577481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4e018054a.final.pdb       | 1.713077e-14 -1.726018e-14 -1.12693e-14 -3.326662e-15 1.167912e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | -1.339303e-15 | \[1045\] | \[1046\] | \[1047\] | \[1048\] | \[1049\] | \[1050\] |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | 3.485889e-15 | 2.305103e-15 | 6.953244e-15 | 6.690366e-16 | -1.029260e-14 | -8.028390e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 1.106025e-14 | -3.667124e-15 | 9.909206e-15 | 1.313885e-15 | 1.401734e-14 | -1.305959e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | -6.770791e-15 | -3.138395e-15 | 2.295129e-16 | 4.681143e-15 | 1.407596e-15 | 1.992464e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb | 1.053661e-14 | -1.375020e-14 | 1.416793e-15 | 2.372991e-15 | 5.993195e-16 | 1.110345e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5602082718ec3a1.final.pdb | 3.639501e-15 | -6.614843e-15 | 6.003665e-15 | 2.383168e-15 | -6.232995e-15 | 3.810057e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d89d996d0a906.final.pdb | 3.233186e-15 | -8.579819e-15 | -8.638582e-15 | 2.93870e-15 | -4.111533e-15 | 6.917114e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e6e6f9e72307a2fbd.final.pdb | -5.316810e-15 | -9.292018e-16 | 3.255945e-15 | 3.014159e-15 | 6.609143e-16 | 1.207662e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ea00f8694090ca7.final.pdb | 3.639501e-15 | -6.614843e-15 | 6.003665e-15 | 2.383168e-15 | -6.232995e-15 | 3.810057e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eaa517be3d0b050.final.pdb | 3.621186e-15 | -1.011210e-16 | 3.675465e-15 | 3.489497e-15 | -1.873603e-15 | 1.874977e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ecc04b9545899c29d.final.pdb | 4.362051e-15 | -4.205322e-15 | 1.947313e-15 | 1.056279e-15 | -1.119854e-15 | 7.856296e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbcad52078.final.pdb | 3.376025e-15 | -2.344118e-15 | 1.457621e-15 | 2.914243e-15 | 4.127622e-16 | 6.218725e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\eff6a42fc838b81e5d.final.pdb | 2.464876e-15 | -3.858739e-15 | 1.751679e-15 | 3.791229e-15 | -1.786030e-15 | 5.278591e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 3.904681e-15 | -2.984895e-15 | 3.057610e-15 | 5.864621e-16 | -5.28634e-16 | 6.577481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 3.904681e-15 | -2.984895e-15 | 3.057610e-15 | 5.864621e-16 | -5.28634e-16 | 6.577481e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | 3.491627e-15 | -6.530319e-15 | 1.131648e-15 | 2.742391e-15 | -6.488212e-16 | -1.605567e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 3.480542e-15 | 1.125762e-15 | 2.730095e-15 | 3.483233e-15 | -4.424564e-16 | 1.270205e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 1.053661e-14 | -1.375020e-14 | 1.416793e-15 | 2.372991e-15 | 5.993195e-16 | 1.110345e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 1.053661e-14 | -1.375020e-14 | 1.416793e-15 | 2.372991e-15 | 5.993195e-16 | 1.110345e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 1.053661e-14 | -1.375020e-14 | 1.416793e-15 | 2.372991e-15 | 5.993195e-16 | 1.110345e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 1.053661e-14 | -1.375020e-14 | 1.416793e-15 | 2.372991e-15 | 5.993195e-16 | 1.110345e-14 |

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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb
1.920091e-15 -2.707508e-15 4.71906e-16 1.537221e-14 6.066616e-15
-1.507147e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffc4.final.pdb
9.710619e-15 1.173139e-14 9.101536e-15 1.444741e-13 5.86927e-15
-4.469622e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb
4.223959e-15 -9.463974e-15 1.663284e-15 -8.053861e-14 5.586927e-15
-4.469622e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb
-2.937473e-15 5.613267e-16 -6.293012e-15 1.370276e-14 4.455978e-15
-3.928131e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fff8b22872.final.pdb
4.426598e-15 -1.764546e-15 -2.408064e-16 9.159233e-15 6.133240e-15
-1.908798e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb
4.059190e-15 -1.556118e-15 1.019816e-15 2.967625e-15 4.194525e-15
3.668725e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6099.final.pdb
1.087194e-14 -1.175424e-14 2.042016e-14 -3.431864e-14 1.085933e-14
-9.551797e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a631396.final.pdb
1.423538e-14 -7.697284e-16 -7.106559e-16 -4.975917e-15 3.140774e-15
-5.892345e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298f8ba.final.pdb
1.423538e-14 -7.697284e-16 -7.106559e-16 -4.975917e-15 3.140774e-15
-5.892345e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb
1.110247e-14 -1.811809e-15 2.042016e-14 -3.431864e-14 1.085933e-14
7.733302e-17

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb
1.214455e-14 5.241483e-15 -1.940576e-15 4.661025e-14 9.480877e-15
5.576079e-16

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\885409c94a631396.final.pdb
-2.937473e-15 5.613267e-16 -6.293012e-15 1.370276e-14 4.455978e-15
-3.928131e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb
-7.468939e-16 9.330673e-15 1.085155e-14 9.366434e-14 1.730574e-14
3.320403e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb
-7.468939e-16 9.330673e-15 1.085155e-14 9.366434e-14 1.730574e-14
3.320403e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb
4.059190e-15 -1.556118e-15 1.019816e-15 2.967625e-15 4.194525e-15
3.668725e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f490d7e2fa.final.pdb
1.122604e-15 3.595053e-15 -2.293012e-15 -2.193631e-15 -3.573745e-15
1.643138e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9d8a8ed0d81f3ef.final.pdb
1.258570e-14 -8.513500e-15 5.518287e-15 5.733365e-14 7.244221e-15
1.009537e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9f752b3616e6033b.final.pdb
4.405156e-15 2.574779e-15 -5.047589e-15 6.853085e-15 9.014327e-15
-1.539692e-16

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| Path                                                                 | Error         | Error         | Error         | Error         | Error         |
|----------------------------------------------------------------------|---------------|---------------|---------------|---------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 4.368177e-15  | 8.553979e-16  | -4.500947e-16 | 2.357191e-14  | 2.824591e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -1.768389e-15 | 1.662299e-15  | 6.861605e-16  | 6.051752e-14  | 2.727369e-14  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.265035e-15  | -2.570352e-15 | -9.200687e-15 | -1.184219e-13 | 1.327650e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\dc0809eff10197e2.final.pdb | -1.599554e-16 | -1.872665e-15 | -4.619602e-15 | 4.371822e-14  | -3.943908e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -1.768389e-15 | 1.662299e-15  | 6.861605e-16  | 6.051752e-14  | 2.727369e-14  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.265035e-15  | -2.570352e-15 | -9.200687e-15 | -1.184219e-13 | 1.327650e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f0efe39.final.pdb | 8.265035e-15  | -2.570352e-15 | -9.200687e-15 | -1.184219e-13 | 1.327650e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | 1.395006e-14  | 1.339329e-14  | -5.839165e-15 | 6.127365e-14  | 8.237838e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e4b48b06824ef848.final.pdb | 5.149978e-15  | -4.168277e-15 | 7.746574e-16  | -2.490857e-14 | 3.825028e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e529e19ad281fea2.final.pdb | 2.281166e-15  | -9.236520e-15 | 7.857142e-15  | -2.374320e-14 | -5.779172e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5d589d996d0a960.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e602082718ec3a1.final.pdb | 1.423538e-14  | -7.697284e-16 | -7.106559e-16 | -4.975917e-15 | 3.140774e-15  |
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| File Path                                                                 | Values                                      |
|--------------------------------------------------------------------------|---------------------------------------------|
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb       | 1.439191e-15  8.944342e-16  4.883892e-16  -8.134479e-15  -5.261478e-16  -1.259398e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb        | 2.923216e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\379736adbc32d5de.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb        | 2.923216e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357ee6642bf12.final.pdb         | 2.923216e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342d1f75a7fcfc.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\4948ef21dfe8c6dfb.final.pdb        | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb         | 2.857450e-14  5.292091e-15  -5.278478e-15  -8.783410e-15  -5.669343e-15  -2.053052e-14 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb        | 3.771357e-15  -1.662973e-15  4.349002e-15  -1.170478e-15  -1.793746e-15  8.331824e-15 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb        | 3.771357e-15  -1.662973e-15  4.349002e-15  -1.170478e-15  -1.793746e-15  8.331824e-15 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb         | 3.771357e-15  -1.662973e-15  4.349002e-15  -1.170478e-15  -1.793746e-15  8.331824e-15 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb         | 3.771357e-15  -1.662973e-15  4.349002e-15  -1.170478e-15  -1.793746e-15  8.331824e-15 |
| E:\\R-3.1.2\scripts\mPDBS\summary_pdb_93\658353ff3c8f7ef.final.pdb          | 3.771357e-15  -1.662973e-15  4.349002e-15  -1.170478e-15  -1.793746e-15  8.331824e-15 |
| File Path                                                                 | Values          |
|---------------------------------------------------------------------------|-----------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb     | 6.689597e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb     | -3.999313e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc4.final.pdb     | 1.098487e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6b9d9624611d1c42.final.pdb      | -1.080951e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb      | -1.432938e-14   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -3.539309e-16   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f28472e17.2230972e-14         | 2.312565e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | 7.406051e-15    |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -3.033458e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | 5.91643e-15     |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -6.423906e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -3.033458e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7f9d98e66a3f6099.final.pdb      | -1.801116e-15   |
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Supplementary Text 10

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Supplementary Text 10

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| filename | energy | energy1 | energy2 | energy3 | energy4 |
|----------|--------|--------|--------|--------|--------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb | 1.613938e-16 | -2.125740e-15 | -2.380823e-15 | 3.924546e-16 | -2.178955e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb | 1.822500e-15 | -2.125740e-15 | -2.380823e-15 | 3.924546e-16 | -2.178955e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb | 2.057466e-15 | -2.125740e-15 | -2.380823e-15 | 3.924546e-16 | -2.178955e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f8e2bf87e52caa29.final.pdb | 2.742564e-14 | -2.125740e-15 | -2.380823e-15 | 3.924546e-16 | -2.178955e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb | 2.490873e-15 | 1.818899e-15 | -3.121902e-16 | -7.325764e-16 | -4.669006e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb | 4.721814e-15 | 2.049135e-15 | -5.138298e-15 | 3.920235e-15 | -8.331452e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb | 1.549819e-15 | 2.106781e-15 | 1.868917e-15 | 4.269273e-15 | -4.419684e-15 |
| E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb | 7.121284e-15 | 1.474570e-15 | -2.676494e-15 | 2.911826e-15 | -3.665324e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\013d855ad26c877c.final.pdb | 6.257824e-15 | -1.146187e-15 | -2.002244e-15 | 7.620091e-15 | 9.305832e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a2a705342ca0d54.final.pdb | 1.246110e-15 | 2.656531e-15 | -3.260895e-15 | 7.550847e-15 | -3.692759e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0a59fceadb419d9.final.pdb | 1.539351e-15 | 2.300091e-15 | 4.278419e-15 | 1.379186e-15 | 1.135044e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\0dba59f3306825e8.final.pdb | 9.853826e-16 | 3.017790e-15 | 1.052951e-14 | -2.070447e-14 | -1.716084e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\126f26a78b57339c.final.pdb | 5.413931e-15 | 3.680001e-16 | -1.846012e-15 | 1.305910e-14 | -7.688603e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\12f06f3e342df706.final.pdb | 8.746343e-15 | 1.895421e-15 | 1.144001e-15 | -1.807116e-15 | 3.451808e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb | -1.035723e-14 | -2.702005e-15 | 3.783383e-15 | -9.129127e-15 | -3.754350e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | 6.395085e-15 | 3.210443e-15 | 2.163332e-15 | -2.196028e-15 | -4.246755e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -2.702005e-15 | 3.783383e-15 | -9.129127e-15 | -3.754350e-15 | -4.247246e-15 |
| Filename                                                                 | E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ | raw_count | norm_count |
|-------------------------------------------------------------------------|-------------------------------------------|-----------|------------|
| 1f8a00b551be0a39.final.pdb                                              | \[235x761\]                               | 1.160254e-15 | -3.187463e-15 | 1.270868e-16 | 7.778548e-15 | -8.975033e-15 | 6.440065e-16 |
| 219f45328d47579a.final.pdb                                              | \[57x749\]                                | 1.618335e-14 | -7.430974e-14 | -1.395001e-14 | 3.036464e-14 | -1.559831e-14 | -3.92873e-14 |
| 238dd3918e54336d.final.pdb                                              | \[57x602\]                                | -3.721126e-14 | -1.902271e-14 | 6.403703e-15 | 1.082131e-14 | -9.513021e-16 | 8.214819e-14 |
| 2b3027889e2fdc42.final.pdb                                              | \[57x589\]                                | -6.753853e-15 | -3.469883e-15 | -3.853934e-15 | -2.856496e-15 | -5.037877e-15 | -6.057093e-16 |
| 2fcb3b46e33793b0.final.pdb                                              | \[57x577\]                                | 6.766881e-15 | 4.798672e-14 | 2.119417e-15 | 9.199721e-15 | -3.822905e-15 | 2.216067e-14 |
| 34eb328251842006.final.pdb                                              | \[57x565\]                                | -4.336138e-14 | -2.402152e-14 | -1.934339e-14 | 8.263192e-14 | -1.697836e-14 | 5.219839e-14 |
| 35ab32871797b7ab.final.pdb                                              | \[57x553\]                                | 2.463863e-14 | 6.983739e-14 | 3.832205e-15 | 4.905489e-15 | 8.403104e-15 | -6.203216e-14 |
| 397368adbc32d5de.final.pdb                                              | \[57x541\]                                | -6.417776e-15 | 2.523711e-14 | 6.614413e-16 | 1.140480e-16 | 7.709817e-16 | -1.445605e-14 |
| 411ca13cd3df6edd.final.pdb                                              | \[57x529\]                                | -3.933761e-15 | -8.645755e-16 | -1.114216e-15 | 2.294383e-15 | -1.716950e-15 | -1.981012e-14 |
| 42357ee6642bf12.final.pdb                                               | \[57x517\]                                | -3.497178e-15 | 4.636553e-14 | -3.256824e-15 | 3.121889e-14 | -5.913111e-15 | -1.706115e-14 |
| 44342d1f75a7fcfc.final.pdb                                              | \[57x505\]                                | -3.651087e-15 | 2.098397e-15 | 1.699812e-14 | -1.399097e-14 | -7.568247e-15 | 5.167061e-14 |
| 448ef21dffe8cdfb.final.pdb                                              | \[57x493\]                                | 1.918750e-14 | 2.186980e-14 | -5.963527e-15 | 1.968959e-14 | 1.547416e-14 | -3.928933e-14 |
| 472a40b3e8f113c7.final.pdb                                              | \[57x481\]                                | 6.310757e-15 | 8.436022e-15 | 5.968383e-15 | 5.068366e-15 | -1.163229e-14 | -2.041483e-14 |
| 48a26225951ea153.final.pdb                                              | \[57x469\]                                | 1.915427e-15 | 7.033800e-15 | -1.273099e-15 | 6.133709e-15 | -1.474973e-14 | 2.141487e-14 |
| 4a4ba445c7c6682ce6.final.pdb                                             | \[57x457\]                                | 2.080697e-14 | -5.096989e-14 | -1.468088e-15 | 2.312463e-14 | 9.142757e-15 | -1.675630e-14 |
| 4eaa45b62cb6a25f.final.pdb                                              | \[57x445\]                                | 2.811477e-15 | -4.972966e-14 | 4.081170e-15 | 7.247230e-15 | -8.391621e-15 | 9.444415e-15 |
| 58c371611d85ac96.final.pdb                                              | \[57x433\]                                | -6.417776e-15 | 2.523711e-14 | -6.614413e-16 | 1.140480e-15 | 7.709817e-16 | -1.445605e-14 |
| 5a6447f04822d30a.final.pdb                                              | \[57x421\]                                | 1.640864e-15 | -6.203216e-14 | 4.905489e-15 | 8.403104e-15 | -6.203216e-14 | -2.041483e-14 |
| Filename                                                                 | Energy Difference (kcal/mol) |
|-------------------------------------------------------------------------|------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb     | -4.350394e-15 6.209989e-15 3.684225e-15 -7.632590e-15 4.737022e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb     | -4.972966e-14 4.081170e-15 7.247230e-15 -8.391621e-15 9.444415e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dbcb.final.pdb     | 3.753757e-14 -3.297351e-15 -7.288763e-15 -8.155569e-15 -5.383960e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb      | 6.310757e-15 -5.968388e-15 -5.083666e-15 -1.163229e-14 -2.041483e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | 9.500008e-15 -4.626156e-15 3.447033e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | -3.098124e-14 -2.614100e-14 7.476628e-15 -6.569826e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb      | -8.55726e-16 5.930274e-16 -8.548630e-16 1.957148e-14 -7.965086e-15 -5.088546e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea98261cfef.final.pdb     | -9.234106e-14 -1.492733e-14 6.819619e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb      | -1.483500e-14 -1.043842e-14 4.128079e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb      | -7.965086e-15 -4.626156e-15 3.447033e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f9107ffbb22872.final.pdb     | 1.738751e-15 -5.326576e-15 -9.261739e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f88c80dd5c3135.final.pdb     | 3.684225e-15 -7.632590e-15 4.737022e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e663f6099.final.pdb       | -9.819276e-15 -1.501583e-13 2.832503e-14 1.059389e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb      | 2.119417e-15 -3.822905e-15 -2.216067e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2928feba.final.pdb      | 2.119417e-15 9.199721e-15 -3.822905e-15 -2.216067e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb      | -3.933761e-15 -8.645755e-16 -1.114216e-15 2.294383e-15 -1.716950e-15 -1.981012e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\86d50469ef569760.final.pdb      | 8.436022e-15 -5.596388e-15 -5.068366e-15 -1.163229e-14 -2.041483e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\89d0666e1402203d.final.pdb      | 9.500008e-15 -4.626156e-15 3.447033e-15 |
| File Path | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 |
|-----------|---------|---------|---------|---------|---------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b34852716dadc62.final.pdb | 4.329725e-15 | -3.378155e-15 | 9.500008e-15 | -4.626156e-15 | 3.447033e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 3.447033e-15 | -1.370286e-14 | -4.504374e-14 | 6.712097e-15 | 1.584154e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | 4.233982e-14 | 1.132547e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -4.515288e-14 | 5.350441e-14 | 9.223066e-15 | -9.749650e-14 | -1.399879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\8b6ef9ac3fe74395.final.pdb | -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | 7.437022e-15 | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -4.504374e-14 | 6.712097e-15 | 1.584154e-14 | -1.399879e-14 | 4.233982e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\98bbe0d5986c138f.final.pdb | -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 | -2.117187e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb | -2.216067e-14 | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 4.582567e-14 | -4.217204e-14 | 1.331725e-14 | -1.969848e-15 | 9.713628e-16 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.517649e-14 | -3.134089e-14 | 5.128482e-15 | -9.68089e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 | -2.117187e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | -2.216067e-14 | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a02c70083816d6ba.final.pdb | 2.119417e-15 | -8.391621e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -1.370286e-14 | -4.504374e-14 | 6.712097e-15 | 1.584154e-14 | -1.399879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 4.233982e-14 | 4.233982e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.515288e-14 | 5.350441e-14 | 9.223066e-15 | -9.749650e-14 | -1.399879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | 7.437022e-15 | 9.681216e-15 | -1.705691e-14 | -5.83532e-15 | 4.318802e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.515288e-14 | 5.350441e-14 | 9.223066e-15 | -9.749650e-14 | -1.399879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\a0c997d891e4e082.final.pdb | -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
|          |          |          |          |          |          |
|----------|----------|----------|----------|----------|----------|
| -4.350394e-15 | -6.209989e-15 | -3.823189e-16 | 3.684225e-15 | -7.632590e-15 |
| 4.737022e-15  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ec04b9545899c29d.final.pdb |
| 2.717300e-15  | 2.836089e-14 | -1.216473e-15 | 1.284174e-14 | -2.273871e-15 |
| 1.01960e-15   |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ee6862cbbcad52078.final.pdb |
| -3.398031e-15 | -2.822883e-14 | -1.281339e-15 | -2.383404e-15 | -7.322074e-15 |
| -1.071936e-14 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83bb81e5d.final.pdb |
| -6.493380e-17 | 2.717300e-17 | -1.216473e-15 | 1.284174e-14 | -2.273871e-15 |
| 5.101960e-15  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb |
| 7.417650e-17  | 3.561580e-14 | 3.395913e-15 | 3.609654e-15 | -8.176325e-15 |
| -9.004008e-15 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f14fcae8deec4fa3.final.pdb |
| -5.276411e-15 | 4.436865e-15 | 9.519400e-15 | -2.723815e-14 | -2.206967e-15 |
| 8.159468e-15  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f40.1ns_data\NAT0.pdb |
| -4.652221e-16 | -4.258870e-15 | 5.749603e-15 | -2.367087e-14 | -2.713437e-14 |
| -5.687277e-16 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f40.1ns_data\LJP6.pdb |
| -3.459258e-15 | -2.155736e-14 | -3.735172e-15 | -1.015784e-14 | 1.662157e-14 |
| 7.382067e-15  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f40.1ns_data\ZSP9.pdb |
| -1.263808e-14 | 1.345978e-14 | -8.070271e-15 | -5.191686e-15 | -1.191048e-14 |
| -4.551683e-14 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f40.1ns_data\3WY9.pdb |
| -3.166355e-16 | 3.649961e-15 | -1.567368e-15 | -1.729568e-14 | 2.055575e-14 |
| -9.926756e-16 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f03d855ad26c877c.final.pdb |
| -1.121697e-14 | -5.990702e-14 | 1.621101e-14 | 1.815311e-14 | 1.000446e-13 |
| -8.152657e-14 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f0a2a705342ca0d54.final.pdb |
| 2.342424e-15 | 1.345978e-14 | -8.070271e-15 | -5.191686e-15 | -1.191048e-14 |
| -4.551683e-14 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f0a5fced5af949d49d.final.pdb |
| -3.162285e-15 | 7.812227e-16 | -1.504606e-15 | 2.083073e-14 | 3.302755e-15 |
| -6.522720e-15 |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f0dba59f3306825e8.final.pdb |
| -6.467295e-15 | 4.862378e-14 | -3.245666e-15 | -7.144359e-15 | -4.172394e-14 |
| 3.854144e-14  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f126f26a785b7339c.final.pdb |
| 1.263808e-14 | -1.704981e-14 | 5.269482e-15 | -2.777553e-14 | -1.533316e-14 |
| 6.176058e-15  |          |          |          |          |          |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f12f06f3432df706.final.pdb |
| -7.698806e-15 | -1.420429e-14 | 9.678485e-16 | 8.191464e-16 | 3.581468e-14 |
| File Path                          | Values                                      |
|-----------------------------------|---------------------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b8676b.final.pdb | -1.060060e-14 -1.510766e-14 -3.250098e-15 1.968780e-14 5.657063e-15 8.855970e-15 1.077497e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f305f598641eeb2.final.pdb | -6.637501e-16 1.239575e-14 -8.080663e-15 2.261581e-14 5.399142e-14 -1.796390e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb | -1.510766e-14 -3.250098e-15 1.968780e-14 -5.657063e-15 -8.855970e-15 1.077497e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb | 1.614952e-14 -1.250456e-13 3.320324e-16 7.278917e-14 5.307978e-14 -1.212948e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb | 1.374303e-14 6.976771e-14 -9.173690e-15 1.424307e-14 -1.555650e-13 1.126712e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b30278892f7777b.final.pdb | -2.661639e-16 2.283927e-15 -1.152633e-15 2.347147e-15 2.471315e-14 3.847023e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb | -4.686574e-15 4.812410e-15 9.712396e-15 -9.596275e-15 -5.669435e-14 3.347239e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb | 2.205832e-15 3.910875e-14 -3.634388e-14 1.358838e-13 4.113082e-14 2.357803e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b32871797b7ab.final.pdb | 2.313499e-15 2.582190e-14 6.434018e-15 -5.626877e-14 -1.589658e-13 6.802147e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5de.final.pdb | 1.263808e-14 -1.704981e-14 5.269482e-15 -2.775535e-15 -1.533316e-14 6.176058e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb | -1.297422e-14 -1.645443e-14 -4.240243e-15 -4.010648e-14 3.870634e-14 -1.065312e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb | -2.332121e-14 -2.281666e-14 -2.127400e-15 1.800262e-14 2.169358e-15 -1.483781e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\44342df1f75a7fcfc.final.pdb | 1.354398e-14 -9.969124e-14 4.483792e-16 3.416610e-14 6.275208e-14 -1.118425e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfde8cdfb.final.pdb | -1.112413e-14 6.127549e-14 1.684963e-15 -1.957961e-14 -7.825696e-14 2.642074e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb | -6.467295e-15 4.862378e-14 -3.245666e-15 -7.144359e-15 -4.172394e-14 3.854144e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb | 9.541963e-15 8.443930e-15 -2.566867e-15 4.684454e-14 -7.40821e-15 -2.232627e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c6682ce6.final.pdb | -1.358053e-14 -2.600445e-14 1.162551e-14 5.387175e-15 -3.467654e-15 -8.092909e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4eaa45b62cb6a25f.final.pdb | 3.227265e-15 -2.913500e-14 1.539590e-14 -3.999008e-14 -4.080979e-15 |
| File Path                                                                 | Values                  |
|--------------------------------------------------------------------------|-------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb     | -4.762843e-14           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb     | -2.316597e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb     | -3.162285e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb      | 3.227265e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dcb.final.pdb      | 7.806803e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff286bd.final.pdb      | -6.467295e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c8f7ef.final.pdb      | -2.316597e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb      | 6.462467e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb      | 6.462467e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6bb3547ea982ffcc4.final.pdb      | 4.457700e-14            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\716d9624611d1c42.final.pdb       | -6.339000e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\75f27e70ad0f1be4.final.pdb       | -2.316597e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\769f910fffb22872.final.pdb       | 3.197579e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\791f8c80dd5c3135.final.pdb       | -3.162285e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\7fad98e66a3f6094.final.pdb       | 1.467237e-14            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\804b89c94a633196.final.pdb       | -4.686574e-15           |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298fefa.final.pdb       | 3.197579e-15            |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\83c0eefcfe12d3f9.final.pdb       | -1.297422e-14           |
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| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b669942ef97459a2.final.pdb | -6.522720e-15 |
|---------------------------------------------------------------|---------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b99f4d9d87c1017b.final.pdb | -3.162285e-15 | 7.812277e-16 | -1.504603e-15 | 2.083073e-14 | 3.02755e-15 | -6.522720e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\b9d2cbf3975403e7.final.pdb | -3.162285e-15 | 7.812277e-16 | -1.504603e-15 | 2.083073e-14 | 3.02755e-15 | -6.522720e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | -1.431356e-15 | -1.611659e-16 | -4.117662e-15 | 2.319175e-14 | -8.280551e-16 | 1.461879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.677076e-14 | 6.230547e-15 | -3.437122e-14 | -6.602320e-14 | 4.477874e-14 | 2.583332e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bc88c8a505f3a288.final.pdb | -1.431356e-15 | -1.611659e-16 | -4.117662e-15 | 2.319175e-14 | -8.280551e-16 | 1.461879e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\bdac0e64f4ef427e.final.pdb | 1.677076e-14 | 6.230547e-15 | -3.437122e-14 | -6.602320e-14 | 4.477874e-14 | 2.583332e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ce34248de3e81a3c.final.pdb | 4.115871e-15 | -6.340947e-14 | 8.474156e-15 | -1.096667e-14 | 5.117176e-14 | -7.936464e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d02e69777249a61.final.pdb | 1.946052e-15 | 7.962366e-14 | -1.632045e-14 | -1.446074e-14 | -1.501080e-13 | 1.297286e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d04221245d015047.final.pdb | 2.263169e-15 | 1.191335e-16 | -5.770076e-15 | -1.499178e-14 | -3.072677e-14 | 2.122556e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d678141e4018054a.final.pdb | -5.440990e-15 | -2.721009e-14 | 8.507422e-16 | -4.957165e-14 | 2.463078e-13 | -2.952252e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d71b40af0f08e39.final.pdb | -2.775712e-14 | 4.641284e-15 | 4.685269e-14 | -2.829953e-15 | -5.926459e-14 | 4.402598e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8009eff10197e2.final.pdb | 1.946052e-15 | 7.962366e-14 | -1.632045e-14 | -1.446074e-14 | -1.501080e-13 | 1.297286e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\d8009eff10197e2.final.pdb | 1.946052e-15 | 7.962366e-14 | -1.632045e-14 | -1.446074e-14 | -1.501080e-13 | 1.297286e-13 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e1163918d3707839.final.pdb | -1.510766e-15 | -3.250098e-15 | 1.968708e-15 | -5.657063e-15 | -8.855970e-15 | 1.077497e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e2169942ef97459a2.final.pdb | -1.121697e-14 | -5.990702e-14 | 1.621101e-15 | 1.815311e-14 | 1.000446e-13 | -8.152657e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e5020872718ec3a1.final.pdb | -4.686574e-15 | 4.812410e-15 | 9.712396e-15 | -9.596275e-15 | -5.669435e-14 | 3.347239e-14 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e589d996d0a960.final.pdb | -1.234411e-15 | 8.638672e-14 | -3.736431e-14 | 1.835428e-13 | 5.613686e-14 | 9.021254e-15 |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\e9df9e72307a2fbd.final.pdb | 3.227265e-15 | -2.913500e-14 | 1.539590e-14 | -3.999008e-14 | -4.080979e-15 | 1.290005e-14 |

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-4.762843e-14
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-4.686574e-15 4.812410e-15 9.712396e-15 -5.669435e-14 3.347239e-14
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-3.162285e-15 7.812277e-16 -1.504606e-15 2.083073e-14 3.302755e-15 -6.522720e-15
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-5.531907e-15 -5.060335e-15 -1.181481e-14 -2.037999e-14 -7.629642e-15 3.115593e-14
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1.023603e-15 -3.967149e-15 -5.194797e-15 2.761697e-14 -3.481866e-14 1.210842e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef6a42fc83b81e5d.final.pdb
-1.031660e-16 1.169110e-15 1.986424e-15 -4.118149e-14 6.828406e-16 -2.324365e-15
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\ef8e88d4ad93a0ad.final.pdb
2.263169e-15 1.191335e-16 -5.700767e-15 -1.499178e-14 3.072776e-14 2.122556e-14
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9.541963e-15 8.449390e-15 2.568867e-14 4.684454e-14 -7.440821e-15 -2.332627e-14
E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f83584e22003fb92.final.pdb
-1.121697e-14 -5.990702e-14 1.621101e-15 1.815311e-14 1.004464e-13 -8.152657e-14
[,1081] [,1082] [,1083] [,1084] [,1085] [,1086]
E:\R-3.1.2\scripts\40.1ns_data\NAT0.pdb
-1.263045e-14 1.190450e-14 -2.964995e-15 -1.982429e-14 -1.493985e-15 -2.172284e-14
E:\R-3.1.2\scripts\40.1ns_data\LJP6.pdb
2.894676e-14 -1.200985e-14 5.836763e-15 2.150930e-14 1.734518e-14 -1.179544e-14
E:\R-3.1.2\scripts\40.1ns_data\3WY9.pdb
-1.391035e-14 -7.951158e-15 5.599611e-15 -7.791373e-15 -9.277033e-15 -8.235464e-14
E:\R-3.1.2\scripts\40.1ns_data\ZSP9.pdb
5.720826e-16 7.008090e-15 1.481745e-14 -6.908297e-15 4.552319e-15 -7.787062e-15
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-6.210155e-14 8.280214e-14 8.072316e-14 -1.998428e-14 9.173653e-14 -6.530838e-14
E:\R-3.1.2\scripts\summary_pdb_93\0a2a705342ca0d54.final.pdb
6.203592e-14 5.164746e-14 -1.325257e-13 5.107023e-14 6.432486e-14 -2.369393e-14
E:\R-3.1.2\scripts\summary_pdb_93\0a59fceedb4194d9.final.pdb
3.152575e-15 -2.34339e-14 2.134393e-14 -1.519188e-15 -1.589288e-14 -5.965624e-15
E:\R-3.1.2\scripts\summary_pdb_93\0db4a59f3306825e8.final.pdb
4.817482e-14 5.975954e-14 4.268414e-14 -8.830012e-15 -8.694345e-14 6.319299e-14
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E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\813cc65a2298feba.final.pdb
1.601424e-14  -4.950353e-15  -4.746514e-14  -1.467922e-14  -3.774954e-14
1.518639e-14

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-3.625157e-14  -1.294006e-14  9.820199e-15  -3.963755e-14  -4.424955e-14
5.662492e-14

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1.174867e-14  1.743848e-14  1.418422e-14  5.988804e-15  -1.261806e-14
8.349474e-15

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-1.081108e-13

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-2.494767e-13

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3.152575e-15  -2.234339e-14  2.134303e-14  -1.519188e-14  -1.589288e-14
-5.965624e-15

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9c22f4909d67e2fa.final.pdb
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3.067698e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\9dda8ed0d81fb3ef.final.pdb
2.935839e-14  4.407689e-14  -3.243603e-14  1.985271e-14  -4.522392e-14
3.262107e-14

E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\acfd4d74b9c71d4dc.final.pdb
1.601424e-14  -4.950353e-15  -4.746514e-14  -1.467922e-14  -3.774954e-14
1.518639e-14

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| File Path                                                                 | Entry 1                         | Entry 2                         | Entry 3                        |
|--------------------------------------------------------------------------|--------------------------------|--------------------------------|--------------------------------|
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\18618a2a251b867b.final.pdb     | 9.108726e-15 -5.884393e-14     | 1.059072e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\f305f598641eeb2.final.pdb     | -8.232713e-14 6.439423e-14     | 7.154953e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\1f8a00b551be0a39.final.pdb     | 1.192863e-13 -1.409633e-14     | -5.399535e-14                  |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\219f45328d47579a.final.pdb     | 1.137664e-13 -1.342739e-13     | 1.865815e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\238dd3918e54336d.final.pdb     | 9.042363e-15 1.137096e-13      | 3.940914e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2b3027889e2fdc42.final.pdb     | 1.137664e-13 -1.342739e-13     | 1.865815e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\2fcb3b46e33793b0.final.pdb     | 9.228044e-14 -5.884393e-14     | 1.059072e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\34eb328251842006.final.pdb     | 4.215068e-15 2.375762e-14      | 9.574681e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\354b3287197b7ab.final.pdb       | 2.137130e-14 3.205982e-14      | 2.343881e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\397368adbc32d5e.final.pdb       | 3.985103e-14 1.784302e-14      | -4.96269e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\411ca13cd3df6edd.final.pdb      | 2.072824e-14 -9.938882e-14     | -4.384581e-14                  |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\42357eee6642bf12.final.pdb      | 4.268550e-14 -6.191630e-14     | 1.477151e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\443421f75a7fcfc.final.pdb       | 1.028071e-13 -1.039074e-13     | 1.409717e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\448ef21dfe8cfd.bid.final.pdb     | 9.056576e-14 5.916664e-14      | 1.213066e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\472a40b3e8f113c7.final.pdb       | 6.114674e-14 3.318656e-14      | 7.287582e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\48a26225951ea153.final.pdb       | 1.558561e-14 4.966098e-14      | 3.527999e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4ab4a5c7c682ce6.final.pdb        | 9.228044e-14 2.598668e-14      | -7.308656e-14                  |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\4aaa45b62cb6a25f.final.pdb       | 6.045458e-15 -6.776224e-14     | 2.343204e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\58c371611d85ac96.final.pdb       | 3.985103e-14 1.784302e-14      | -4.96269e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59a647f04822d30a.final.pdb       | -2.671776e-14 2.380512e-14     | 6.327942e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\59b091fe385e05fc.final.pdb        | -1.871354e-14 4.484876e-15     | -1.447429e-15                  |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5c35ac30f930d2db.final.pdb       | -6.045458e-15 -6.776224e-14    | 2.343204e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\5f60752431cf2dc.final.pdb        | 6.620650e-14 6.582241e-14      | 1.337160e-13                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\626456dd6ff2868d.final.pdb       | -6.114674e-14 3.318656e-14     | 7.287582e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6583d53ff3c87ef.final.pdb        | -2.671776e-14 2.380512e-14     | 6.327942e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\69760178986bef01.final.pdb       | 1.874138e-13 6.601655e-14      | 6.322293e-14                   |                               |
| E:\R-3.1.2\scripts\mPDBS\summary_pdb_93\6a9d87d47926b1c8.final.pdb       | 9.042363e-15 1.137096e-13      | 3.940914e-14                   |                               |
### Supplementary Text 10

5.402805e-14 -6.959919e-14 -7.230405e-14

[ reached getOption("max.print") -- omitted 5 rows ]

**Mean**

|   |   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|---|
| [1] | 70.18318 | 57.12605 | 62.29386 | 72.71967 | 55.04590 | 64.15961 | 71.61180 |   |   |   |
| [16] | 69.78458 | 50.41986 | 67.54258 | 70.77211 | 46.84172 | 66.72712 | 72.87690 |   |   |   |
| [31] | 69.58590 | 42.49497 | 71.15434 | 69.84950 | 43.73601 | 74.72225 | 66.05858 |   |   |   |
| [46] | 65.82891 | 41.83332 | 79.82882 | 63.06437 | 39.38051 | 78.85598 | 64.97451 |   |   |   |
| [61] | 68.51595 | 31.37666 | 86.46420 | 70.43518 | 34.29427 | 84.98308 | 74.04349 |   |   |   |
| [76] | 74.56634 | 39.43543 | 82.93587 | 74.88011 | 43.01419 | 81.86725 | 71.84545 |   |   |   |
| [91] | 67.00474 | 41.55626 | 86.44544 | 76.59519 | 38.49073 | 76.61172 | 66.49755 |   |   |   |
| [106] | 62.63779 | 29.28937 | 89.22855 | 59.89685 | 26.76251 | 89.84529 | 58.69769 |   |   |   |
| [121] | 54.03007 | 21.08412 | 88.66649 | 54.85725 | 18.42826 | 86.07669 | 58.21983 |   |   |   |
| [136] | 61.16587 | 24.21442 | 82.34876 | 63.14946 | 27.20133 | 83.58168 | 64.59048 |   |   |   |
| [151] | 58.76700 | 36.25410 | 79.02669 | 56.50556 | 37.18206 | 76.11942 | 55.76444 |   |   |   |
| [166] | 55.45939 | 36.94326 | 82.62576 | 53.80052 | 34.16202 | 80.66544 | 56.05193 |   |   |   |
| [226] | 71.25875 | 36.34680 | 56.08476 | 73.56836 | 39.53683 | 75.58346 | 76.29131 |   |   |   |
| [241] | 76.50176 | 41.25532 | 63.29042 | 80.21347 | 40.70884 | 63.19748 | 80.96250 |   |   |   |
| [256] | 76.93967 | 39.19966 | 68.40357 | 77.38107 | 38.43652 | 67.14126 | 75.01657 |   |   |   |
| [271] | 73.61074 | 33.99171 | 73.35791 | 69.99126 | 35.08196 | 72.90459 | 69.25430 |   |   |   |
| [286] | 65.50000 | 30.39589 | 73.81119 | 66.60894 | 27.11219 | 72.25315 | 67.97778 |   |   |   |
| [301] | 65.84841 | 21.52727 | 74.37777 | 63.93609 | 21.34811 | 78.01296 | 60.33147 |   |   |   |
| [316] | 60.64225 | 12.90721 | 75.44649 | 59.94867 | 12.31906 | 71.78024 | 56.38728 |   |   |   |
| [331] | 55.45198 | 21.79709 | 76.71692 | 54.22179 | 24.91053 | 74.98074 | 53.37391 |   |   |   |
| [346] | 48.33198 | 31.25867 | 83.07843 | 47.34865 | 34.38120 | 81.28069 | 44.53802 |   |   |   |
| [361] | 47.98412 | 39.46278 | 84.12199 | 45.99772 | 40.11069 | 87.27724 | 49.13391 |   |   |   |
| [386] | 41.10882 | 39.16498 | 51.34620 | 44.08206 | 88.39114 | 54.86289 | 43.58369 | 89.69933 |   |   |
Supplementary Text 10
[781] 47.40986 48.60414 48.93179 48.21005 48.44080 52.60559 47.10457
51.58566 54.42007 49.74431 54.23566 54.89935 49.72430 57.00976 57.44103
[796] 50.28500 60.58676 56.33544 46.61880 46.88941 62.19273 45.98721
48.70227 65.38418 47.98884 46.21473 67.57692 51.74459 46.29041 67.08143
[811] 51.66345 48.36946 63.91320 55.41391 48.95737 64.06382 55.95913
45.21674 64.53575 54.18410 44.46338 61.26169 55.92633 47.22362 59.31581
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43.38614 56.31290 64.82911 46.04055 43.99371 64.92314 49.79953 44.61395
[841] 61.29883 49.95841 45.60458 61.67518 47.24309 48.18015 64.91301
48.61396 49.53949 63.49308 52.09417 49.83742 60.55098 50.73548 51.69693
[856] 62.74352 48.89873 54.12698 64.63800 51.99816 54.98272 61.59177
54.18882 55.23871 59.83786 51.90095 57.71403 62.89139 51.38483 59.89704
[871] 63.62788 55.12029 59.86540 60.05246 55.83535 60.90287 60.54890
53.55278 63.89841 63.86341 55.20686 64.73639 62.80576 58.82249 64.50123
[886] 61.83699 60.09341 61.07473 58.51271 61.33215 62.30752 59.04127
63.65474 64.04808 60.67284 60.97784 67.96406 61.97415 57.44303 68.41194
[901] 59.65191 54.51859 69.11002 62.53958 52.49508 70.55378 62.93565
52.63762 74.33814 66.24981 54.15361 75.40424 67.22270 55.16704 71.89145
[916] 67.24565 58.36962 69.90682 65.20993 61.47855 70.38265 62.30499
61.56830 72.82585 61.90542 57.77018 73.15424 58.90775 56.16827 74.92517
[931] 59.23843 56.42594 78.68837 56.28966 54.39681 79.84476 56.09176
51.09596 77.98124 53.50306 48.63277 79.26629 55.99442 46.34506 81.01033
[946] 55.73726 45.11278 84.60938 54.58354 57.47940 87.89601 57.65180
56.72468 85.85662 59.38949 53.47744 84.98153 62.18153 52.69856 87.36620
[961] 64.19529 50.93926 84.68039 65.05594 51.64791 81.05915 64.32196
48.67334 78.93304 66.77258 49.54547 76.15211 65.96338 48.50671 72.61825
[976] 62.29092 47.64611 73.01680 60.13199 48.65198 70.04835 47.12954
58.78377 61.71379 50.43944 58.75091 63.28058 48.83197 59.34819 66.62649
[991] 50.62782 57.96033 69.64792 50.41238 58.40018 73.38027 53.15414
57.17215 75.64530 51.04184 55.91106 78.46398 51.69433 52.79540 80.49917
[1006] 48.05692 51.74796 80.44744 47.88795 51.71618 76.67975 48.79030
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[1036] 57.92250 39.23931 68.48073 57.86157 43.03054 68.10292 61.66510
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[1051] 63.02824 44.62484 63.49851 66.40450 43.23484 64.58364 66.93685
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[1066] 71.26296 44.28491 60.68596 70.65324 44.98410 57.04049 70.68640
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[1081] 65.97948 47.52161 118.70191 64.41942 47.09999 118.01521 64.14835
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STANDARD DEVIATION
[1] 3.809345e+01 1.133568e+01 9.977960e+00 8.242698e+00 6.804346e+00
6.649923e+00 6.059084e+00 5.064958e+00 4.363150e+00 3.731391e+00 3.519307e+00
[12] 3.059745e+00 2.828174e+00 2.566305e+00 2.473202e+00 2.079793e+00
1.974040e+00 1.619424e+00 1.542099e+00 1.474821e+00 1.370961e+00 1.339977e+00
[23] 1.262391e+00 1.135283e+00 1.014480e+00 8.100889e-01 6.891932e-01
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[34] 2.683833e-01 2.096417e-01 1.953946e-01 1.768632e-01 6.527451e-02
3.386762e-07 3.232320e-07 1.374946e-07 1.016436e-07 9.256959e-08 8.270690e-08
[45] 7.130297e-08 6.773892e-08 6.587076e-08 6.364866e-08 6.031279e-08
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Supplementary Text 10

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[947] 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00 0.000000e+00
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