Dec 17, 2021 – 05:13 PM JST

Deposition ID : D_1300026375

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the symbol.

The following versions of software and data (see references) were used in the production of this report:

- EMDB validation analysis : 0.0.0.dev97
- Mogul : 1.8.5 (274361), CSD as541be (2020)
- MolProbity : 4.02b-467
- Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
- Ideal geometry (proteins) : Engh & Huber (2001)
- Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
- Validation Pipeline (wwPDB-VP) : 2.24
1 Overall quality at a glance

The following experimental techniques were used to determine the structure: ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

| Metric         | Whole archive (#Entries) | EM structures (#Entries) |
|----------------|--------------------------|--------------------------|
| Clashscore     | 158937                   | 4297                     |
| Ramachandran outliers | 154571                   | 4023                     |
| Sidechain outliers | 154315                   | 3826                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1016   |                  |
| 2   | B     | 1000   |                  |
| 3   | C     | 1000   |                  |
| 4   | O     | 118    |                  |
| 4   | P     | 118    |                  |
| 4   | U     | 118    |                  |
| 5   | Q     | 107    |                  |
| 5   | S     | 107    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | V     | 107    | ![Quality Bar](image) |
| 6   | D     | 3      | ![Quality Bar](image) |
| 6   | E     | 3      | ![Quality Bar](image) |
| 6   | F     | 3      | ![Quality Bar](image) |
| 7   | G     | 2      | ![Quality Bar](image) |
| 7   | H     | 2      | ![Quality Bar](image) |
| 7   | I     | 2      | ![Quality Bar](image) |
| 7   | J     | 2      | ![Quality Bar](image) |
| 7   | K     | 2      | ![Quality Bar](image) |
| 7   | L     | 2      | ![Quality Bar](image) |
| 7   | M     | 2      | ![Quality Bar](image) |
| 7   | N     | 2      | ![Quality Bar](image) |
| 7   | R     | 2      | ![Quality Bar](image) |
| 7   | T     | 2      | ![Quality Bar](image) |
## Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29187 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- **Molecule 1** is a protein called spike chain A.

| Mol | Chain | Residues | Atoms          | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 1   | A     | 1006     | Total C N O S  | 0       | 0     |
|     |       |          | 7761 4956 1292 1478 35 |         |       |

- **Molecule 2** is a protein called chain B of spike.

| Mol | Chain | Residues | Atoms          | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 2   | B     | 1000     | Total C N O S  | 0       | 0     |
|     |       |          | 7732 4938 1283 1476 35 |         |       |

- **Molecule 3** is a protein called chain C of spike.

| Mol | Chain | Residues | Atoms          | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 3   | C     | 1000     | Total C N O S  | 0       | 0     |
|     |       |          | 7677 4903 1270 1469 35 |         |       |

- **Molecule 4** is a protein called heavy chain of R33.

| Mol | Chain | Residues | Atoms          | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 4   | U     | 118      | Total C N O S  | 0       | 0     |
|     |       |          | 928 594 151 178 5 |         |       |
| 4   | O     | 118      | Total C N O S  | 0       | 0     |
|     |       |          | 928 594 151 178 5 |         |       |
| 4   | P     | 118      | Total C N O S  | 0       | 0     |
|     |       |          | 928 594 151 178 5 |         |       |

- **Molecule 5** is a protein called light chain of R33.

| Mol | Chain | Residues | Atoms          | AltConf | Trace |
|-----|-------|----------|----------------|---------|-------|
| 5   | V     | 107      | Total C N O S  | 0       | 0     |
|     |       |          | 824 520 137 164 3 |         |       |
| 5   | Q     | 107      | Total C N O S  | 0       | 0     |
|     |       |          | 824 520 137 164 3 |         |       |

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Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
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| Mol | Chain | Residues | Atoms       | AltConf | Trace |
|-----|-------|----------|-------------|---------|-------|
| 7   | R     | 2        | Total C N O | 28 16 2 10 | 0 0   |
| 7   | T     | 2        | Total C N O | 28 16 2 10 | 0 0   |

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

![Image of NAG molecule]

| Mol | Chain | Residues | Atoms       | AltConf |
|-----|-------|----------|-------------|---------|
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | A     | 1        | Total C N O | 98 56 7 35 | 0     |
| 8   | B     | 1        | Total C N O | 154 88 11 55 | 0   |
| 8   | B     | 1        | Total C N O | 154 88 11 55 | 0   |

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| Mol | Chain | Residues | Atoms       | AltConf |
|-----|-------|----------|-------------|---------|
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | B     | 1        | Total C N O | 0       |
|     |       |          | 154 88 11 55|         |
| 8   | C     | 1        | Total C N O | 0       |
|     |       |          | 112 64 8 40 |         |
| 8   | C     | 1        | Total C N O | 0       |
|     |       |          | 112 64 8 40 |         |
| 8   | C     | 1        | Total C N O | 0       |
|     |       |          | 112 64 8 40 |         |
| 8   | C     | 1        | Total C N O | 0       |
|     |       |          | 112 64 8 40 |         |
| 8   | C     | 1        | Total C N O | 0       |
|     |       |          | 112 64 8 40 |         |
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: spike chain A

Chain A:
• Molecule 2: chain B of spike

Chain B:

• Molecule 3: chain C of spike

Chain C:
• Molecule 4: heavy chain of R33

Chain U:

- Molecule 4: heavy chain of R33
Chain O:

- Molecule 4: heavy chain of R33

Chain P:

- Molecule 5: light chain of R33

Chain V:

- Molecule 5: light chain of R33

Chain Q:

- Molecule 5: light chain of R33

Chain S:

- Molecule 5: light chain of R33

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- **Molecule 6**: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

- **Molecule 6**: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

- **Molecule 6**: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

- **Molecule 7**: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

- **Molecule 7**: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

Chain T:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose
## 4 Experimental information

| Property                                      | Value                                      | Source     |
|----------------------------------------------|--------------------------------------------|------------|
| EM reconstruction method                     | SINGLE PARTICLE                            | Depositor |
| Imposed symmetry                             | POINT, Not provided                       |            |
| Number of particles used                     | Not provided                               |            |
| Resolution determination method              | Not provided                               |            |
| CTF correction method                         | Not provided                               |            |
| Microscope                                   | Not provided                               |            |
| Voltage (kV)                                 | Not provided                               |            |
| Electron dose ($e^-/\text{Å}^2$)             | Not provided                               |            |
| Minimum defocus (nm)                         | Not provided                               |            |
| Maximum defocus (nm)                         | Not provided                               |            |
| Magnification                                | Not provided                               |            |
| Image detector                               | Not provided                               |            |
| Maximum map value                            | 1.657                                      | Depositor |
| Minimum map value                            | -0.780                                     | Depositor |
| Average map value                            | -0.000                                     | Depositor |
| Map value standard deviation                 | 0.036                                      | Depositor |
| Recommended contour level                    | 0.177                                      | Depositor |
| Map size (Å)                                 | 432.000003, 432.000003, 432.000003         | wwPDB     |
| Map dimensions                               | 400, 400, 400                              | wwPDB     |
| Map angles (°)                               | 90.0, 90.0, 90.0                           | wwPDB     |
| Pixel spacing (Å)                            | 1.08, 1.08, 1.08                           | Depositor |
5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | Bond angles |
|-----|-------|--------------|-------------|
|     |       | RMSZ | #|Z| >5 | RMSZ | #|Z| >5 |
| 1   | A     | 1.33 | 6/7936 (0.1%) | 0.83 | 7/10811 (0.1%) |
| 2   | B     | 0.51 | 1/7907 (0.0%) | 0.66 | 5/10768 (0.0%) |
| 3   | C     | 0.52 | 3/7851 (0.0%) | 0.66 | 3/10703 (0.0%) |
| 4   | O     | 0.51 | 0/955 | 0.60 | 0/1300 |
| 4   | P     | 0.51 | 0/955 | 0.60 | 0/1300 |
| 4   | U     | 0.51 | 0/955 | 0.60 | 0/1300 |
| 5   | Q     | 0.44 | 0/844 | 0.63 | 1/1146 (0.1%) |
| 5   | S     | 0.44 | 0/844 | 0.62 | 1/1146 (0.1%) |
| 5   | V     | 0.44 | 0/844 | 0.63 | 1/1146 (0.1%) |
| All | All   | 0.82 | 10/29091 (0.0%) | 0.70 | 18/39620 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 1                   | 2                   |
| 2   | B     | 0                   | 2                   |
| 4   | O     | 0                   | 1                   |
| 4   | P     | 0                   | 1                   |
| 4   | U     | 0                   | 1                   |
| 5   | Q     | 0                   | 1                   |
| 5   | S     | 0                   | 1                   |
| 5   | V     | 0                   | 1                   |
| All | All   | 1                   | 10                  |

All (10) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z   | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1   | A     | 516 | GLU  | CB-CG | 87.00 | 3.17        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z   | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1   | A     | 516 | GLU  | CA-CB | 64.02 | 2.94        | 1.53     |
| 1   | A     | 516 | GLU  | CG-CD | 15.03 | 1.74        | 1.51     |
| 3   | C     | 336 | CYS  | N-CA  | -9.02 | 1.28        | 1.46     |
| 1   | A     | 516 | GLU  | N-CA  | 8.44  | 1.63        | 1.46     |
| 3   | C     | 336 | CYS  | CA-CB | -7.49 | 1.37        | 1.53     |
| 2   | B     | 336 | CYS  | CA-CB | -7.15 | 1.38        | 1.53     |
| 3   | C     | 336 | CYS  | CB-SG | 6.85  | 1.93        | 1.82     |
| 1   | A     | 336 | CYS  | CA-CB | -5.42 | 1.42        | 1.53     |
| 1   | A     | 515 | PHE  | C-N   | 5.29  | 1.46        | 1.34     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms         | Z   | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------------|-----|-------------|----------|
| 1   | A     | 516 | GLU  | CA-CB-CG      | -47.55 | 8.80    | 113.40   |
| 1   | A     | 516 | GLU  | N-CA-CB       | 14.55  | 136.78  | 110.60   |
| 2   | B     | 30  | ASN  | C-N-CA        | 9.23   | 144.79  | 121.70   |
| 5   | V     | 80  | PRO  | CA-N-CD       | -8.89  | 99.05   | 111.50   |
| 5   | Q     | 80  | PRO  | CA-N-CD       | -8.88  | 99.07   | 111.50   |
| 5   | S     | 80  | PRO  | CA-N-CD       | -8.88  | 99.08   | 111.50   |
| 3   | C     | 703 | ASN  | CB-CA-C       | -7.92  | 94.56   | 110.40   |
| 2   | B     | 567 | ARG  | NE-CZ-NH2     | -7.30  | 116.65  | 120.30   |
| 1   | A     | 983 | ARG  | NE-CZ-NH2     | -6.45  | 117.08  | 120.30   |
| 2   | B     | 938 | LEU  | CA-CB-CG      | 6.03   | 129.18  | 115.30   |
| 1   | A     | 515 | PHE  | C-N-CA        | 5.85   | 136.32  | 121.70   |
| 1   | A     | 617 | CYS  | CA-CB-SG      | 5.67   | 124.20  | 114.00   |
| 3   | C     | 1032| CYS  | CA-CB-SG      | 5.55   | 123.99  | 114.00   |
| 1   | A     | 436 | TRP  | CA-CB-CG      | 5.33   | 123.84  | 113.70   |
| 3   | C     | 436 | TRP  | CA-CB-CG      | 5.33   | 123.83  | 113.70   |
| 2   | B     | 436 | TRP  | CA-CB-CG      | 5.31   | 123.80  | 113.70   |
| 2   | B     | 546 | LEU  | CA-CB-CG      | 5.15   | 127.15  | 115.30   |
| 1   | A     | 336 | CYS  | CB-CA-C       | 5.05   | 120.51  | 110.40   |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1   | A     | 516 | GLU  | CA   |

All (10) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 1   | A     | 513 | LEU  | Mainchain |
| 1   | A     | 983 | ARG  | Sidechain |
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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------|
| 2   | B     | 333 | THR  | Peptide |
| 2   | B     | 567 | ARG  | Sidechain |
| 4   | O     | 106 | PHE  | Peptide |
| 4   | P     | 106 | PHE  | Peptide |
| 5   | Q     | 29  | VAL  | Peptide |
| 5   | S     | 29  | VAL  | Peptide |
| 4   | U     | 106 | PHE  | Peptide |
| 5   | V     | 29  | VAL  | Peptide |

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 7761  | 7507     | 221      | 0       |
| 2   | B     | 7732  | 7480     | 238      | 0       |
| 3   | C     | 7677  | 7374     | 233      | 0       |
| 4   | O     | 928   | 869      | 57       | 0       |
| 4   | P     | 928   | 869      | 54       | 0       |
| 4   | U     | 928   | 869      | 55       | 0       |
| 5   | Q     | 824   | 801      | 39       | 0       |
| 5   | S     | 824   | 801      | 39       | 0       |
| 5   | V     | 824   | 801      | 42       | 0       |
| 6   | D     | 39    | 34       | 1        | 0       |
| 6   | E     | 39    | 34       | 1        | 0       |
| 6   | F     | 39    | 34       | 1        | 0       |
| 7   | G     | 28    | 25       | 1        | 0       |
| 7   | H     | 28    | 25       | 0        | 0       |
| 7   | I     | 28    | 25       | 0        | 0       |
| 7   | J     | 28    | 25       | 0        | 0       |
| 7   | K     | 28    | 25       | 2        | 0       |
| 7   | L     | 28    | 25       | 1        | 0       |
| 7   | M     | 28    | 25       | 2        | 0       |
| 7   | N     | 28    | 25       | 0        | 0       |
| 7   | R     | 28    | 25       | 0        | 0       |
| 7   | T     | 28    | 25       | 0        | 0       |
| 8   | A     | 98    | 91       | 3        | 0       |
| 8   | B     | 154   | 143      | 1        | 0       |
| 8   | C     | 112   | 104      | 2        | 0       |

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (867) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1       | Atom-2       | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|--------------|--------------------------|-------------------|
| 1:A:357:ARG:HH12 | 2:B:167: THR:CA | 1.12                     | 1.63              |
| 2:B:363:ALA:CB    | 2:B:524:VAL:HG22 | 1.27                     | 1.55              |
| 3:C:363:ALA:HB2    | 3:C:524:VAL:CG1  | 1.30                     | 1.53              |
| 1:A:395:VAL:HG23   | 1:A:524:VAL:CG1  | 1.39                     | 1.53              |
| 1:A:516:GLU:CD     | 1:A:516:GLU:CG1  | 1.74                     | 1.53              |
| 3:C:363:ALA:CB     | 3:C:524:VAL:CG1  | 1.92                     | 1.46              |
| 2:B:363:ALA:CB     | 2:B:524:VAL:CG2  | 1.85                     | 1.41              |
| 2:B:391:CYS:SG     | 2:B:544:ASN:CA   | 2.11                     | 1.39              |
| 2:B:363:ALA:HB2    | 2:B:524:VAL:CG2  | 0.89                     | 1.35              |
| 2:B:391:CYS:SG     | 2:B:544:ASN:HB2  | 1.66                     | 1.34              |
| 2:B:391:CYS:SG     | 2:B:544:ASN:CB   | 2.17                     | 1.33              |
| 2:B:386:LYS:HD2    | 3:C:983:ARG:C    | 1.47                     | 1.32              |
| 2:B:391:CYS:HB2    | 2:B:544:ASN:O    | 1.31                     | 1.30              |
| 2:B:382:VAL:HG13   | 3:C:983:ARG:CD   | 1.62                     | 1.29              |
| 1:A:357:ARG:NH1    | 2:B:167:THR:CA   | 1.90                     | 1.28              |
| 2:B:383:SER:CB     | 3:C:984:LEU:HA   | 1.62                     | 1.27              |
| 1:A:362:VAL:CG1    | 1:A:527:PRO:HA   | 1.66                     | 1.25              |
| 1:A:357:ARG:NH1    | 2:B:167:THR:HA   | 1.44                     | 1.23              |
| 2:B:357:ARG:NE     | 3:C:230:PRO:CG   | 1.95                     | 1.23              |
| 2:B:393:THR:HB     | 2:B:520:ALA:O    | 1.40                     | 1.22              |
| 1:A:394:ASN:ND2    | 1:A:516:GLU:CB   | 2.03                     | 1.21              |
| 2:B:361:CYS:O      | 2:B:524:VAL:HA   | 1.38                     | 1.19              |
| 3:C:391:CYS:HB2     | 3:C:544:ASN:O    | 1.37                     | 1.19              |
| 1:A:357:ARG:HH12   | 2:B:167:THR:CB   | 1.55                     | 1.19              |
| 1:A:394:ASN:NH     | 1:A:516:GLU:CG   | 1.57                     | 1.18              |
| 2:B:383:SER:HB3    | 3:C:983:ARG:O    | 1.02                     | 1.17              |
| 2:B:391:CYS:SG     | 2:B:544:ASN:C    | 2.23                     | 1.16              |
| 2:B:391:CYS:CB     | 2:B:544:ASN:O    | 1.92                     | 1.16              |
| 2:B:357:ARG:NE     | 3:C:230:PRO:HG3  | 1.55                     | 1.16              |
| 2:B:386:CYS:SG     | 2:B:524:VAL:HG23 | 1.85                     | 1.15              |
| 1:A:362:VAL:CG1    | 1:A:527:PRO:CA   | 2.24                     | 1.15              |
| 3:C:363:ALA:HB3    | 3:C:524:VAL:HG12 | 1.25                     | 1.14              |
| 2:B:383:SER:CB     | 3:C:983:ARG:O    | 1.95                     | 1.12              |
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| Atom-1      | Atom-2      | Interatomic distance (Å) | Clash overlap (Å) |
|-------------|-------------|--------------------------|-------------------|
| 1:A:393:THR:C | 1:A:516:GLU:CB | 2.18                     | 1.12              |
| 1:A:395:VAL:HG23 | 1:A:524:VAL:HG13 | 1.29                     | 1.11              |
| 2:B:391:CYS:SG | 2:B:544:ASN:HA | 1.90                     | 1.11              |
| 2:B:361:CYS:N | 2:B:523:THR:O  | 1.80                     | 1.11              |
| 1:A:362:VAL:HG13 | 1:A:527:PRO:HA | 1.35                     | 1.08              |
| 2:B:383:SER:HB2 | 3:C:984:LEU:HG23 | 1.31                     | 1.08              |
| 3:C:363:ALA:HB2 | 3:C:524:VAL:HG11 | 1.26                     | 1.08              |
| 3:C:363:ALA:CB | 3:C:524:VAL:HG12 | 1.80                     | 1.08              |
| 2:B:382:VAL:CG1 | 3:C:983:ARG:HG2 | 1.85                     | 1.06              |
| 2:B:383:SER:CB | 3:C:984:LEU:HG23 | 1.83                     | 1.06              |
| 2:B:334:ASN:HD22 | 2:B:361:CYS:HA | 1.20                     | 1.06              |
| 1:A:395:VAL:CG2 | 1:A:524:VAL:CG1 | 2.32                     | 1.06              |
| 2:B:363:ALA:HB2 | 2:B:524:VAL:HG23 | 1.14                     | 1.06              |
| 1:A:394:ASN:H  | 1:A:516:GLU:HA | 1.03                     | 1.05              |
| 2:B:357:ARG:HE | 3:C:230:PRO:CG  | 1.60                     | 1.05              |
| 1:A:395:VAL:HG23 | 1:A:524:VAL:HG11 | 1.08                     | 1.05              |
| 1:A:394:ASN:H  | 1:A:516:GLU:HG2 | 1.13                     | 1.05              |
| 2:B:363:ALA:HB2 | 2:B:524:VAL:HG21 | 1.38                     | 1.05              |
| 2:B:383:SER:HB2 | 3:C:984:LEU:CA  | 1.86                     | 1.04              |
| 2:B:383:SER:HB2 | 3:C:984:LEU:CD2 | 1.88                     | 1.04              |
| 3:C:363:ALA:HB2 | 3:C:524:VAL:HG13 | 1.08                     | 1.03              |
| 2:B:359:SER:CA | 2:B:523:THR:HG2 | 1.86                     | 1.03              |
| 2:B:363:ALA:N  | 2:B:525:CYS:O  | 1.92                     | 1.03              |
| 2:B:382:VAL:HG13 | 3:C:983:ARG:HG2 | 1.04                     | 1.02              |
| 1:A:395:VAL:CG2 | 1:A:524:VAL:HG11 | 1.90                     | 1.01              |
| 1:A:393:THR:OG1 | 1:A:516:GLU:CB | 2.08                     | 1.01              |
| 2:B:357:ARG:HE | 3:C:230:PRO:HG2 | 1.23                     | 1.01              |
| 2:B:334:ASN:ND2 | 2:B:361:CYS:HA | 1.74                     | 1.01              |
| 2:B:363:ALA:O  | 2:B:526:GLY:HA2 | 1.59                     | 1.00              |
| 2:B:382:VAL:HG12 | 3:C:983:ARG:HB2 | 1.44                     | 1.00              |
| 1:A:395:VAL:HG21 | 1:A:524:VAL:CG2 | 1.91                     | 1.00              |
| 2:B:363:ALA:HB3 | 2:B:524:VAL:HG22 | 1.41                     | 1.00              |
| 3:C:393:THR:CG2 | 3:C:520:ALA:O  | 2.10                     | 1.00              |
| 2:B:336:CYSG | 2:B:524:VAL:CG2 | 2.50                     | 0.99              |
| 2:B:359:SER:HA | 2:B:523:THR:CG2 | 1.91                     | 0.99              |
| 1:A:394:ASN:HD22 | 1:A:516:GLU:CB | 1.66                     | 0.99              |
| 3:C:391:CYSG | 3:C:544:ASN:HA | 2.03                     | 0.98              |
| 4:U:12:LYS:H3 | 4:U:18:VAL:HG11 | 1.45                     | 0.98              |
| 4:O:12:LYS:H3 | 4:O:18:VAL:HG11 | 1.45                     | 0.98              |
| 1:A:393:THR:HA | 1:A:522:ALA:HA | 1.43                     | 0.98              |
| 1:A:394:ASN:N  | 1:A:516:GLU:HA | 1.78                     | 0.98              |

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| Atom-1  | Atom-2      | Interatomic distance (Å) | Clash overlap (Å) |
|---------|-------------|--------------------------|-------------------|
| 1:A:393:THR:OG1 | 1:A:516:GLU:CA | 2.11                     | 0.98              |
| 4:U:13:LYS:HD3  | 4:U:14:PRO:HD2 | 1.46                     | 0.98              |
| 2:B:391:CYS:SG   | 2:B:544:ASN:O  | 2.22                     | 0.97              |
| 4:P:12:LYS:HG3   | 4:P:18:VAL:HG11| 1.45                     | 0.97              |
| 4:O:13:LYS:HD3   | 4:O:14:PRO:HD2 | 1.46                     | 0.96              |
| 2:B:359:SER:CA   | 2:B:523:THR:CG2| 2.42                     | 0.96              |
| 4:P:13:LYS:HD3   | 4:P:14:PRO:HD2 | 1.46                     | 0.96              |
| 3:C:360:ASN:H    | 3:C:523:THR:HB | 1.30                     | 0.95              |
| 1:A:362:VAL:HG11| 1:A:527:PRO:HA | 1.49                     | 0.95              |
| 1:A:394:ASN:H    | 1:A:516:GLU:CA | 1.75                     | 0.94              |
| 2:B:396:TYR:HE2  | 3:C:200:TYR:HH  | 0.96                     | 0.94              |
| 2:B:393:THR:CB   | 2:B:520:ALA:O  | 2.15                     | 0.94              |
| 1:A:357:ARG:NH1  | 2:B:167:THR:O  | 2.02                     | 0.93              |
| 1:A:393:THR:CB   | 1:A:516:GLU:CB | 2.46                     | 0.93              |
| 1:A:393:THR:OG1  | 1:A:516:GLU:CG | 2.16                     | 0.92              |
| 2:B:382:VAL:CG1  | 3:C:983:ARG:CD | 2.46                     | 0.92              |
| 2:B:382:VAL:C    | 3:C:984:LEU:HD2| 1.90                     | 0.92              |
| 3:C:391:CYS:SG   | 3:C:544:ASN:CA | 2.58                     | 0.92              |
| 1:A:357:ARG:NH1  | 2:B:167:THR:C  | 2.22                     | 0.92              |
| 2:B:383:SER:HB2  | 3:C:984:LEU:HA | 0.93                     | 0.92              |
| 3:C:393:THR:HA   | 3:C:522:ALA:HA | 1.49                     | 0.92              |
| 1:A:391:CYS:HA   | 1:A:525:CYS:SG | 2.09                     | 0.92              |
| 1:A:364:ASP:OD1  | 1:A:527:PRO:HD2| 1.69                     | 0.92              |
| 2:B:357:ARG:NE   | 3:C:230:PRO:HG2| 1.81                     | 0.92              |
| 1:A:394:ASN:CG   | 1:A:516:GLU:CA | 2.39                     | 0.91              |
| 3:C:364:ASP:OD2  | 3:C:527:PRO:HD3| 1.71                     | 0.91              |
| 3:C:393:THR:HG21 | 3:C:520:ALA:O  | 1.71                     | 0.90              |
| 2:B:396:TYR:HE2  | 3:C:200:TYR:OH | 1.53                     | 0.90              |
| 1:A:883:THR:HG23 | 3:C:707:TYR:HB2| 1.54                     | 0.89              |
| 1:A:394:ASN:N    | 1:A:516:GLU:CG | 2.30                     | 0.89              |
| 2:B:396:TYR:CE2  | 3:C:200:TYR:OH | 2.23                     | 0.89              |
| 1:A:395:VAL:HG21 | 1:A:524:VAL:HG22| 1.55                    | 0.89              |
| 3:C:650:LEU:HD21 | 3:C:653:ALA:HB3| 1.55                     | 0.89              |
| 2:B:355:ARG:NH2  | 3:C:230:PRO:O  | 2.04                     | 0.89              |
| 1:A:394:ASN:OD1  | 1:A:516:GLU:CA | 2.22                     | 0.88              |
| 2:B:396:TYR:OH   | 3:C:200:TYR:HE1| 1.55                     | 0.88              |
| 1:A:357:ARG:CZ   | 2:B:167:THR:HA | 2.03                     | 0.87              |
| 1:A:395:VAL:CG2  | 1:A:524:VAL:CG2| 2.51                     | 0.87              |
| 3:C:360:ASN:H    | 3:C:523:THR:CB | 1.87                     | 0.87              |
| 2:B:396:TYR:OH   | 3:C:200:TYR:CE1| 2.27                     | 0.86              |
| 4:U:109:TRP:HE1  | 4:U:108:TRP:HE1| 1.40                     | 0.86              |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|-------------------------|------------------|
| 1:A:200:TYR:CE2 | 3:C:396:TYR:OH | 2.28 | 0.86 |
| 3:C:193:VAL:HG23 | 3:C:223:LEU:HD12 | 1.56 | 0.86 |
| 2:B:386:LYS:CD | 3:C:983:ARG:C | 2.42 | 0.85 |
| 1:A:357:ARG:HH12 | 2:B:167:THR:C | 1.79 | 0.85 |
| 4:O:4:LEU:HD13 | 4:O:109:TRP:HE1 | 1.40 | 0.85 |
| 2:B:382:VAL:HG13 | 3:C:983:ARG:HD3 | 1.58 | 0.84 |
| 3:C:391:CYS:CB | 3:C:544:ASN:O | 2.22 | 0.84 |
| 4:P:4:LEU:HD13 | 4:P:109:TRP:HE1 | 1.40 | 0.84 |
| 1:A:394:ASN:N | 1:A:516:GLU:CA | 2.37 | 0.84 |
| 2:B:334:ASN:HD22 | 2:B:361:CYS:CA | 1.91 | 0.83 |
| 2:B:361:CYS:O | 2:B:524:VAL:CA | 2.26 | 0.83 |
| 1:A:357:ARG:NH1 | 2:B:167:THR:CB | 2.31 | 0.83 |
| 3:C:360:ASN:N | 3:C:523:THR:HB | 1.93 | 0.82 |
| 1:A:362:VAL:HG11 | 1:A:527:PRO:CA | 2.06 | 0.81 |
| 3:C:363:ALA:CB | 3:C:524:VAL:HG13 | 1.82 | 0.81 |
| 3:C:393:THR:HB | 3:C:520:ALA:O | 1.80 | 0.80 |
| 2:B:336:CYS:SG | 2:B:524:VAL:CB | 2.70 | 0.80 |
| 1:A:395:VAL:CG2 | 1:A:524:VAL:HG21 | 2.12 | 0.80 |
| 2:B:383:SER:HB3 | 3:C:983:ARG:C | 2.02 | 0.80 |
| 2:B:383:SER:CA | 3:C:984:LEU:HD23 | 2.12 | 0.80 |
| 1:A:395:VAL:HG21 | 1:A:524:VAL:HG21 | 1.64 | 0.79 |
| 1:A:393:THR:H | 1:A:516:GLU:CD | 1.85 | 0.79 |
| 1:A:357:ARG:NH1 | 2:B:167:THR:OG1 | 2.16 | 0.79 |
| 1:A:364:ASP:OD1 | 1:A:527:PRO:CD | 2.31 | 0.79 |
| 2:B:363:ALA:H | 2:B:525:CYS:N | 1.80 | 0.79 |
| 2:B:383:SER:N | 3:C:984:LEU:HD23 | 1.98 | 0.78 |
| 3:C:393:THR:CB | 3:C:520:ALA:O | 2.30 | 0.78 |
| 2:B:383:SER:N | 3:C:984:LEU:CD2 | 2.46 | 0.78 |
| 2:B:355:ARG:HH21 | 3:C:230:PRO:HB2 | 1.47 | 0.78 |
| 2:B:391:CYS:CB | 2:B:544:ASN:HB2 | 2.13 | 0.78 |
| 3:C:391:CYS:HB3 | 3:C:522:ALA:CB | 2.14 | 0.77 |
| 2:B:359:SER:HA | 2:B:523:THR:HG23 | 1.65 | 0.77 |
| 2:B:359:SER:CB | 2:B:523:THR:HG21 | 2.14 | 0.77 |
| 2:B:361:CYS:O | 2:B:523:THR:O | 2.03 | 0.77 |
| 1:A:394:ASN:N | 1:A:516:GLU:CB | 2.48 | 0.76 |
| 3:C:388:ASN:O | 3:C:526:GLY:HA3 | 1.85 | 0.76 |
| 2:B:336:CYS:SG | 2:B:524:VAL:HB | 2.25 | 0.76 |
| 3:C:391:CYS:SG | 3:C:544:ASN:C | 2.64 | 0.76 |
| 2:B:363:ALA:O | 2:B:526:GLY:CA | 2.33 | 0.76 |
| 2:B:386:LYS:HD2 | 3:C:983:ARG:O | 1.84 | 0.76 |
| 2:B:383:SER:CB | 3:C:984:LEU:CD2 | 2.57 | 0.75 |

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| Atom-1       | Atom-2       | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|--------------|--------------------------|-------------------|
| 2:B:383:SER:CA | 3:C:984:LEU:CD2 | 2.65                     | 0.75              |
| 1:A:362:VAL:CG1 | 1:A:527:PRO:CB  | 2.64                     | 0.75              |
| 3:C:108:THR:OG1 | 3:C:234:ASN:O   | 2.03                     | 0.75              |
| 2:B:383:SER:CB | 3:C:984:LEU:CA  | 2.56                     | 0.74              |
| 1:A:362:VAL:HG11 | 1:A:527:PRO:CB | 2.16                     | 0.74              |
| 4:U:51:ILE:HD12 | 4:U:72:LEU:HB2  | 1.70                     | 0.74              |
| 3:C:391:CYS:HB3 | 3:C:522:ALA:HB1 | 1.70                     | 0.73              |
| 1:A:516:GLU:CD | 1:A:516:GLU:N   | 2.42                     | 0.73              |
| 1:A:983:ARG:O | 3:C:383:SER:HB3 | 1.88                     | 0.73              |
| 2:B:386:LYS:HD2 | 3:C:983:ARG:CA  | 2.19                     | 0.73              |
| 3:C:361:CYS:O | 3:C:524:VAL:HA  | 1.89                     | 0.72              |
| 2:B:386:LYS:HD2 | 3:C:984:LEU:N   | 2.01                     | 0.72              |
| 3:C:1106:GLN:HE21 | 3:C:1109:PHE:HB3 | 1.54                     | 0.72              |
| 3:C:363:ALA:CB | 3:C:524:VAL:HG11 | 1.91                     | 0.72              |
| 4:O:51:ILE:HD12 | 4:O:72:LEU:HB2  | 1.70                     | 0.72              |
| 2:B:701:VAL:HG13 | 3:C:787:GLN:HG2 | 1.70                     | 0.72              |
| 2:B:393:THR:CG2 | 2:B:520:ALA:O   | 2.36                     | 0.72              |
| 2:B:393:THR:HA | 2:B:522:ALA:HA  | 1.71                     | 0.72              |
| 3:C:335:LEU:HG | 3:C:362:VAL:O   | 1.89                     | 0.72              |
| 1:A:391:CYS:CA | 1:A:525:CYS:SG  | 2.79                     | 0.71              |
| 4:P:51:ILE:HD12 | 4:P:72:LEU:HB2  | 1.70                     | 0.71              |
| 1:A:394:ASN:O | 1:A:516:GLU:N   | 2.23                     | 0.71              |
| 2:B:395:VAL:HG21 | 2:B:524:VAL:HG11 | 1.73                     | 0.71              |
| 1:A:364:ASP:CG | 1:A:527:PRO:CG  | 2.59                     | 0.70              |
| 1:A:394:ASN:N | 1:A:516:GLU:HG2 | 1.96                     | 0.70              |
| 1:A:362:VAL:HG11 | 1:A:527:PRO:HB3 | 1.73                     | 0.70              |
| 2:B:364:ASP:OD2 | 2:B:527:PRO:HG3 | 1.92                     | 0.69              |
| 1:A:362:VAL:CG1 | 1:A:527:PRO:HB3 | 2.21                     | 0.69              |
| 4:P:4:LEU:HB2  | 4:P:109:TRP:CD1 | 2.27                     | 0.69              |
| 1:A:395:VAL:N | 1:A:524:VAL:HG11 | 2.07                     | 0.69              |
| 8:A:1302:NAG:H83 | 3:C:558:LYS:HZ1 | 1.57                     | 0.69              |
| 2:B:656:VAL:HG11 | 2:B:693:ILE:HD12 | 1.74                     | 0.69              |
| 4:U:4:LEU:HB2  | 4:U:109:TRP:CD1 | 2.27                     | 0.69              |
| 1:A:362:VAL:HG13 | 1:A:527:PRO:CA  | 2.07                     | 0.69              |
| 2:B:363:ALA:HB2 | 2:B:524:VAL:HG22 | 0.71                     | 0.69              |
| 1:A:395:VAL:CG2 | 1:A:524:VAL:HG13 | 2.12                     | 0.68              |
| 2:B:362:VAL:C  | 2:B:525:CYS:O   | 2.32                     | 0.68              |
| 4:O:4:LEU:HB2  | 4:O:109:TRP:CD1 | 2.27                     | 0.68              |
| 1:A:787:GLN:HB3 | 3:C:701:VAL:HG13 | 1.75                     | 0.68              |
| 4:U:13:LYS:HD3 | 4:U:14:PRO:CD   | 2.23                     | 0.68              |
| 1:A:46:SER:HA  | 1:A:279:TYR:O   | 1.94                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:382:VAL:C    | 3:C:984:LEU:CD2  | 2.63                     | 0.68              |
| 2:B:355:ARG:NH2  | 3:C:230:PRO:HB2  | 2.08                     | 0.67              |
| 2:B:905:ARG:NH1  | 2:B:1049:LEU:O   | 2.27                     | 0.67              |
| 4:P:72:LEU:HD21  | 4:P:74:THR:HB    | 1.77                     | 0.67              |
| 2:B:37:TYR:OH    | 2:B:53:ASP:OD2   | 2.11                     | 0.67              |
| 1:A:722:VAL:HG2  | 1:A:1065:VAL:HG22| 1.77                     | 0.66              |
| 4:U:83:ILE:HG23  | 4:U:86:LEU:HD11  | 1.77                     | 0.66              |
| 4:U:72:LEU:HD21  | 4:U:74:THR:HB    | 1.77                     | 0.66              |
| 1:A:363:ALA:HB3   | 1:A:525:CYC:C    | 2.15                     | 0.66              |
| 3:C:656:VAL:HG11 | 3:C:693:ILE:CD12 | 1.77                     | 0.66              |
| 2:B:359:SER:C    | 2:B:523:THR:HG21 | 1.87                     | 0.66              |
| 3:C:360:ASN:CA   | 3:C:523:THR:HB   | 2.24                     | 0.66              |
| 4:O:83:ILE:HG23  | 4:O:86:LEU:HD11  | 1.78                     | 0.66              |
| 4:P:13:LYS:HD3   | 4:P:14:PRO:CD    | 2.23                     | 0.66              |
| 1:A:364:ASP:CA   | 1:A:527:PRO:CD   | 2.25                     | 0.66              |
| 4:P:83:ILE:HG23  | 4:U:86:LEU:HD11  | 1.78                     | 0.66              |
| 3:C:516:GLU:HG2  | 3:C:519:HIS:H    | 1.60                     | 0.66              |
| 2:B:176:LEU:HD23 | 2:B:190:ARG:HD2  | 1.78                     | 0.65              |
| 1:A:394:ASN:CG   | 1:A:516:GLU:CB   | 2.65                     | 0.65              |
| 2:B:404:GLY:HA2  | 2:B:508:THR:CD   | 1.62                     | 0.65              |
| 3:C:364:ASP:OD2  | 3:C:527:PRO:CD   | 2.43                     | 0.65              |
| 4:O:13:LYS:HD3   | 4:O:14:PRO:CD    | 2.23                     | 0.65              |
| 1:A:404:GLY:HA2  | 1:A:508:THR:CD   | 1.62                     | 0.65              |
| 1:A:725:GLU:OE1  | 1:A:1028:LYS:NZ  | 2.28                     | 0.65              |
| 3:C:35:GLY:HA3   | 3:C:56:LEU:HB3   | 1.77                     | 0.65              |
| 4:O:72:LEU:HD21  | 4:O:74:THR:HB    | 1.77                     | 0.65              |
| 2:B:773:GLU:OE2  | 2:B:1019:ARG:NH2 | 2.30                     | 0.64              |
| 5:V:8:PRO:HG2    | 5:V:11:LEU:HB3   | 1.80                     | 0.64              |
| 3:C:905:ARG:NH1  | 3:C:1049:LEU:O   | 2.28                     | 0.64              |
| 1:A:360:ASN:N    | 1:A:523:THR:OG1  | 2.30                     | 0.64              |
| 3:C:91:TYR:OH    | 3:C:191:GLU:OE2  | 2.15                     | 0.63              |
| 2:B:330:PRO:C    | 2:B:332:ILE:CD   | 2.00                     | 0.63              |
| 3:C:360:ASN:HA   | 3:C:523:THR:CD   | 1.80                     | 0.63              |
| 5:Q:8:PRO:HG2    | 5:Q:11:LEU:HB3   | 1.80                     | 0.63              |
| 2:B:382:VAL:CG1  | 3:C:983:ARG:HB2  | 2.25                     | 0.63              |
| 2:B:395:VAL:CG2  | 2:B:524:VAL:HG11 | 2.28                     | 0.63              |
| 1:A:393:THR:O    | 1:A:516:GLU:CB   | 2.47                     | 0.63              |
| 1:A:567:ARG:HD3  | 1:A:571:ASP:HA   | 1.80                     | 0.62              |
| 1:A:364:ASP:HA   | 1:A:527:PRO:CD   | 1.82                     | 0.62              |
| 5:S:8:PRO:HG2    | 5:S:11:LEU:HB3   | 1.80                     | 0.62              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:364:ASP:CG  | 1:A:527:PRO:HG3 | 2.20                     | 0.62              |
| 4:P:106:PHE:O   | 4:P:107:ASP:HB2 | 2.00                     | 0.62              |
| 2:B:393:THR:HB  | 2:B:520:ALA:C   | 2.16                     | 0.62              |
| 2:B:743:CYS:SG  | 2:B:750:SER:N   | 2.73                     | 0.62              |
| 5:Q:15:VAL:HG13 | 5:Q:80:PRO:HD2 | 1.82                     | 0.62              |
| 1:A:983:ARG:O   | 3:C:383:SER:CB  | 2.48                     | 0.61              |
| 2:B:363:ALA:CA  | 2:B:524:VAL:HG23| 2.29                     | 0.61              |
| 1:A:64:TRP:HE1  | 1:A:264:ALA:HB1 | 1.65                     | 0.61              |
| 1:A:82:PRO:HG2  | 1:A:84:LEU:HD21 | 1.82                     | 0.61              |
| 1:A:362:VAL:HG12| 1:A:527:PRO:CA  | 2.24                     | 0.61              |
| 5:S:15:VAL:HG13 | 5:S:80:PRO:HD2  | 1.82                     | 0.61              |
| 5:V:15:VAL:HG13 | 5:V:80:PRO:HD2  | 1.82                     | 0.61              |
| 2:B:425:LEU:HD12| 2:B:426:PRO:HD2 | 1.83                     | 0.61              |
| 4:U:106:PHE:O   | 4:U:107:ASP:HB2 | 2.00                     | 0.61              |
| 1:A:393:THR:CA  | 1:A:516:GLU:CB  | 2.78                     | 0.61              |
| 1:A:425:LEU:HD12| 1:A:426:PRO:HD2 | 1.83                     | 0.61              |
| 3:C:323:THR:OG1 | 3:C:324:GLU:OE2  | 2.19                     | 0.61              |
| 5:Q:36:TYR:HD1  | 5:Q:46:LEU:HA   | 1.66                     | 0.61              |
| 1:A:360:ASN:CA  | 1:A:523:THR:OG1 | 2.49                     | 0.61              |
| 1:A:364:ASP:HA  | 1:A:527:PRO:CD  | 2.31                     | 0.60              |
| 4:O:106:PHE:O   | 4:O:107:ASP:HB2 | 2.00                     | 0.60              |
| 1:A:984:LEU:HD21| 3:C:381:GLY:O   | 2.01                     | 0.60              |
| 4:U:27:TYR:CZ   | 4:U:98:ARG:HD3  | 2.37                     | 0.60              |
| 5:V:36:TYR:HD1  | 5:V:46:LEU:HA   | 1.66                     | 0.60              |
| 1:A:905:ARG:NH1 | 1:A:1049:LEU:O  | 2.34                     | 0.60              |
| 1:A:984:LEU:HA  | 3:C:383:SER:HB2 | 1.84                     | 0.60              |
| 3:C:546:LEU:HD21| 3:C:573:THR:HG21| 1.81                     | 0.60              |
| 3:C:393:THR:HB  | 3:C:520:ALA:C   | 2.21                     | 0.60              |
| 1:A:393:THR:CB  | 1:A:516:GLU:CB  | 2.32                     | 0.60              |
| 1:A:701:VAL:HG13| 2:B:787:GLN:HG2 | 1.82                     | 0.60              |
| 1:A:364:ASP:OD1 | 1:A:527:PRO:CG  | 2.49                     | 0.60              |
| 1:A:364:ASP:CG  | 1:A:527:PRO:CD  | 2.70                     | 0.60              |
| 1:A:364:ASP:CB  | 1:A:527:PRO:HD3 | 2.31                     | 0.60              |
| 1:A:393:THR:C   | 1:A:516:GLU:HB3 | 2.20                     | 0.60              |
| 1:A:401:VAL:HG22| 1:A:509:ARG:HG2 | 1.84                     | 0.60              |
| 2:B:401:VAL:HG22| 2:B:509:ARG:HG2 | 1.84                     | 0.60              |
| 1:A:983:ARG:HB3 | 3:C:390:LEU:HD21| 1.82                     | 0.59              |
| 3:C:425:LEU:HD12| 3:C:426:PRO:HD2 | 1.83                     | 0.59              |
| 5:V:33:LEU:HD13 | 5:V:71:PHE:CD2  | 2.37                     | 0.59              |
| 5:Q:33:LEU:HD13 | 5:Q:71:PHE:CD2  | 2.37                     | 0.59              |
| 4:P:27:TYR:CZ   | 4:P:98:ARG:HD3  | 2.37                     | 0.59              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|-------------------------|------------------|
| 1:A:362:VAL:CG1 | 1:A:527:PRO:N  | 2.65                    | 0.59             |
| 2:B:391:CYS:HB3 | 2:B:522:ALA:CB | 2.32                    | 0.59             |
| 5:S:33:LEU:HD13 | 5:S:71:PHE:CD1 | 2.37                    | 0.59             |
| 5:S:36:TYR:HD2  | 5:S:46:LEU:HA  | 1.66                    | 0.59             |
| 2:B:355:ARG:HH2 | 3:C:230:PRO:C  | 2.05                    | 0.59             |
| 3:C:811:LYS:HG3 | 3:C:812:PRO:HD2| 1.85                    | 0.59             |
| 4:O:27:TYR:CG   | 4:O:98:ARG:HD3 | 2.37                    | 0.59             |
| 1:A:395:VAL:H   | 1:A:524:VAL:HG11 | 1.66                  | 0.59             |
| 1:A:789:TYR:HA  | 3:C:703:ASN:O  | 2.02                    | 0.59             |
| 3:C:985:ASP:OD1 | 3:C:985:ASP:N  | 2.30                    | 0.59             |
| 2:B:359:SER:HB3 | 2:B:523:THR:HG21| 1.84                  | 0.59             |
| 3:C:821:LEU:O   | 3:C:825:LYS:HG2 | 2.03                    | 0.59             |
| 3:C:280:ASN:HD21| 8:C:1301:NAG:HG2 | 1.68                   | 0.58             |
| 3:C:743:CYS:SG  | 3:C:750:SER:O  | 2.76                    | 0.58             |
| 2:B:383:SER:HB2 | 3:C:984:LEU:HG22| 1.82                  | 0.58             |
| 2:B:390:LEU:HD21| 3:C:983:ARG:HB3 | 1.86                    | 0.58             |
| 1:A:393:THR:O   | 1:A:516:GLU:HB3 | 2.03                    | 0.58             |
| 3:C:401:VAL:HG22| 3:C:509:ARG:HG2 | 1.84                    | 0.58             |
| 4:U:97:ALA:HB2  | 4:U:108:VAL:HG23| 1.86                   | 0.58             |
| 4:O:105:TYR:HB3 | 5:Q:34:HIS:CE1 | 2.39                    | 0.58             |
| 7:K:1:NAG:HG3   | 7:K:1:NAG:H3   | 1.85                    | 0.58             |
| 3:C:273:ARG:HD3 | 3:C:292:ALA:HB3 | 1.86                    | 0.58             |
| 3:C:299:THR:HG22| 3:C:315:THR:HG21| 1.84                   | 0.58             |
| 4:O:97:ALA:HB2  | 4:O:108:VAL:HG23| 1.86                   | 0.58             |
| 1:A:707:TYR:HB2 | 2:B:883:THR:HG23| 1.86                   | 0.58             |
| 4:P:105:TYR:HB3 | 5:S:34:HIS:CE1 | 2.39                    | 0.58             |
| 1:A:555:SER:HB3 | 1:A:586:ASP:HB2 | 1.85                    | 0.58             |
| 2:B:362:VAL:CG1 | 2:B:525:CYS:O  | 2.52                    | 0.58             |
| 1:A:703:ASN:O   | 2:B:789:TYR:HA | 2.04                    | 0.58             |
| 3:C:36:VAL:HG11 | 3:C:220:PHE:HC | 2.39                    | 0.58             |
| 5:V:6:GLN:NE2  | 5:V:88:CYS:SG  | 2.77                    | 0.58             |
| 4:O:51:ILE:HG21 | 4:O:70:PHE:HB2 | 1.86                    | 0.58             |
| 4:P:58:PRO:HB2  | 4:P:60:TYR:CG  | 2.39                    | 0.58             |
| 1:A:763:LEU:HD22| 1:A:1008:VAL:HG21| 1.86                  | 0.57             |
| 5:Q:46:LEU:HD21| 5:Q:49:TYR:HB3 | 1.86                    | 0.57             |
| 5:S:46:LEU:HD21| 5:S:49:TYR:HB3 | 1.86                    | 0.57             |
| 1:A:883:THR:HG23| 3:C:707:TYR:CB  | 2.32                    | 0.57             |
| 2:B:746:SER:HB2 | 2:B:749:CYS:SG | 2.44                    | 0.57             |
| 4:P:51:ILE:HG21 | 4:P:70:PHE:HB2 | 1.86                    | 0.57             |
| 2:B:722:VAL:HG22| 2:B:930:ALA:HB1 | 1.86                   | 0.57             |
| 1:A:393:THR:O   | 1:A:523:THR:HG22| 2.03                   | 0.57             |

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| Atom-1      | Atom-2      | Interatomic distance (Å) | Clash overlap (Å) |
|-------------|-------------|--------------------------|------------------|
| 4:U:34:MET:HG2 | 4:U:79:ALA:HB1 | 1.86                     | 0.57             |
| 4:O:58:PRO:HB2 | 4:O:60:TYR:CZ  | 2.39                     | 0.57             |
| 5:S:6:GLN:NE2 | 5:S:88:CYS:SG  | 2.77                     | 0.57             |
| 1:A:364:ASP:CB | 1:A:527:PRO:CD | 2.82                     | 0.57             |
| 4:U:105:TYR:HB3 | 5:V:34:HIS:CE1 | 2.39                     | 0.57             |
| 5:Q:6:GLN:NE2 | 5:Q:88:CYS:SG  | 2.77                     | 0.57             |
| 7:K:2:NAG:H3  | 7:K:2:NAG:H83  | 1.87                     | 0.57             |
| 5:V:46:LEU:HD21 | 5:V:49:TYR:HB3 | 1.86                     | 0.57             |
| 1:A:702:GLU:HA  | 2:B:788:ILE:HB | 1.87                     | 0.57             |
| 2:B:363:ALA:CB | 2:B:524:VAL:HG23 | 1.93                     | 0.57             |
| 2:B:1106:GLN:HE21 | 2:B:1109:PHE:HB3 | 1.70                     | 0.57             |
| 4:U:51:ILE:HG21 | 4:U:70:PHE:HB2  | 1.86                     | 0.57             |
| 4:U:58:PRO:HB2 | 4:U:60:TYR:CZ  | 2.39                     | 0.57             |
| 1:A:91:TYR:OH  | 1:A:191:GLU:OE1 | 2.17                     | 0.56             |
| 2:B:294:ASP:OD2 | 2:B:294:ASP:N   | 2.38                     | 0.56             |
| 1:A:394:ASN:H  | 1:A:516:GLU:H   | 1.51                     | 0.56             |
| 4:0:34:MET:HG2 | 4:O:79:ALA:HB1  | 1.86                     | 0.56             |
| 4:4:34:MET:HG2 | 1:A:362:VAL:HD12 | 2.37                     | 0.55             |
| 2:B:170:TYR:CE1 | 2:B:172:SER:HB2 | 2.47                     | 0.56             |
| 2:B:382:VAL:HA  | 3:C:983:ARG:CB  | 2.29                     | 0.56             |
| 2:B:386:LYS:HD3 | 3:C:982:SER:C    | 2.26                     | 0.56             |
| 4:4:34:MET:HG2 | 4:O:79:ALA:HB1  | 1.86                     | 0.56             |
| 8:A:1306:NAG:H3 | 8:A:1306:NAG:H83 | 1.87                     | 0.56             |
| 2:B:386:LYS:CD  | 3:C:983:ARG:CA  | 2.83                     | 0.56             |
| 5:S:34:HIS:HE1  | 5:S:50:TYR:CD2  | 2.24                     | 0.56             |
| 1:A:362:VAL:HG12 | 1:A:527:PRO:N    | 2.21                     | 0.56             |
| 4:O:12:LYS:HG3  | 4:O:18:VAL:CG1  | 2.30                     | 0.56             |
| 5:Q:33:LEU:HA   | 5:Q:89:GLN:O    | 2.06                     | 0.56             |
| 2:B:330:PRO:C   | 2:B:332:ILE:N   | 2.59                     | 0.55             |
| 5:S:38:GLN:HG3  | 5:S:44:PRO:HD3  | 1.88                     | 0.55             |
| 3:C:472:ILE:HD11 | 3:C:488:CYS:HB3 | 1.88                     | 0.55             |
| 3:C:738:CYS:SG  | 3:C:739:THR:N   | 2.80                     | 0.55             |
| 5:V:38:GLN:HG3  | 5:V:44:PRO:HD3  | 1.88                     | 0.55             |
| 5:S:33:LEU:HA   | 5:S:89:GLN:O    | 2.06                     | 0.55             |
| 1:A:379:CYS:HA  | 1:A:432:CYS:HA  | 1.89                     | 0.55             |
| 1:A:395:VAL:CB  | 1:A:524:VAL:HG11 | 2.37                     | 0.55             |
| 1:A:1141:LEU:HG | 1:A:1145:LEU:HD13 | 1.88                    | 0.55             |
| 2:B:391:CYS:HB3 | 2:B:522:ALA:HB3 | 1.89                     | 0.55             |
| 5:Q:64:GLY:HA2  | 5:Q:73:LEU:HA   | 1.89                     | 0.55             |
| 3:C:822:LEU:HD21 | 3:C:938:LEU:HD13 | 1.89                    | 0.55             |

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| Atom-1   | Atom-2   | Interatomic distance (Å) | Clash overlap (Å) |
|----------|----------|--------------------------|-------------------|
| 5:V:64:GLY:HA2 | 5:V:73:LEU:HA | 1.89                     | 0.55              |
| 1:A:560:LEU:H | 1:A:563:GLN:NE2 | 2.05                     | 0.55              |
| 2:B:359:SER:CA | 2:B:523:THR:HG23 | 2.25                     | 0.55              |
| 3:C:379:CYS:HA | 3:C:432:CYS:HA | 1.89                     | 0.55              |
| 5:V:33:LEU:HA | 5:V:89:GLN:O | 2.06                     | 0.55              |
| 5:V:34:HIS:HE1 | 5:V:50:TYR:CD1 | 2.24                     | 0.55              |
| 1:A:516:GLU:CD | 1:A:516:GLU:C | 2.65                     | 0.55              |
| 2:B:170:TYR:HE1 | 2:B:172:SER:HB2 | 1.72                     | 0.55              |
| 2:B:821:LEU:HD21 | 2:B:939:SER:HB2 | 1.87                     | 0.55              |
| 4:O:107:ASP:HB3 | 4:O:109:TRP:CZ3 | 2.42                     | 0.55              |
| 5:Q:38:GLN:HG3 | 5:Q:44:PRO:HD3 | 1.88                     | 0.55              |
| 4:P:107:ASP:HB3 | 4:P:109:TRP:CZ3 | 2.42                     | 0.55              |
| 3:C:364:ASP:OD2 | 3:C:527:PRO:HG3 | 2.06                     | 0.55              |
| 4:O:98:ARG:NH2 | 4:O:109:TRP:HH2 | 2.05                     | 0.55              |
| 2:B:706:ALA:HB1 | 7:M:2:NAG:O7 | 2.07                     | 0.54              |
| 4:P:12:LYS:HG3 | 4:P:18:VAL:CG1 | 2.30                     | 0.54              |
| 3:C:391:CYS:O | 3:C:522:ALA:HB2 | 2.06                     | 0.54              |
| 4:P:98:ARG:NH2 | 4:P:109:TRP:HH2 | 2.05                     | 0.54              |
| 1:A:364:ASP:CA | 1:A:527:PRO:CD | 2.86                     | 0.54              |
| 4:U:98:ARG:NH2 | 4:U:109:TRP:HH2 | 2.05                     | 0.54              |
| 5:Q:34:HIS:HE1 | 5:Q:50:TYR:CD1 | 2.24                     | 0.54              |
| 5:S:6:GLN:HE22 | 5:S:88:CYS:H | 1.56                     | 0.54              |
| 2:B:472:ILE:HD11 | 2:B:488:CYS:HB3 | 1.88                     | 0.54              |
| 4:U:33:GLY:H | 4:U:100:GLY:HA2 | 1.73                     | 0.54              |
| 4:O:33:GLY:H | 4:O:100:GLY:HA2 | 1.73                     | 0.54              |
| 2:B:390:LEU:HD11 | 3:C:983:ARG:HB3 | 1.89                     | 0.54              |
| 1:A:393:THR:CA | 1:A:522:ALA:HA | 2.30                     | 0.54              |
| 4:P:33:GLY:H | 4:P:100:GLY:HA2 | 1.73                     | 0.54              |
| 4:U:107:ASP:HB3 | 4:U:109:TRP:CZ3 | 2.42                     | 0.54              |
| 1:A:200:TYR:HE2 | 3:C:396: TYR:OH | 1.88                     | 0.53              |
| 2:B:604:THR:HG21 | 2:B:687:VAL:HG11 | 1.89                     | 0.53              |
| 2:B:707:TYR:HB2 | 3:C:883:THR:HG23 | 1.90                     | 0.53              |
| 3:C:662:CYS:HB2 | 3:C:697:MET:HG2 | 1.90                     | 0.53              |
| 2:B:127:VAL:HG21 | 8:B:1301:NAG:H5 | 1.90                     | 0.53              |
| 2:B:1039:ARG:NE | 3:C:1031:GLU:OE1 | 2.41                     | 0.53              |
| 3:C:52:GLN:OE1 | 3:C:52:GLN:N | 2.39                     | 0.53              |
| 2:B:134:GLN:HG2 | 2:B:162:SER:HB3 | 1.90                     | 0.53              |
| 2:B:276:LEU:O | 2:B:288:ALA:HA | 2.08                     | 0.53              |
| 2:B:379:CYS:HA | 2:B:432:CYS:HA | 1.89                     | 0.53              |
| 5:S:64:GLY:HA2 | 5:S:73:LEU:HA | 1.89                     | 0.53              |
| 5:Q:34:HIS:HE1 | 5:Q:50:TYR:CE1 | 2.27                     | 0.53              |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|------------------|
| 3:C:472:ILE:HD13 | 3:C:484:LYS:HG3 | 1.91 | 0.53 |
| 1:A:105:ILE:HD12 | 1:A:239:GLN:HE21 | 1.73 | 0.53 |
| 1:A:121:ASN:HD21 | 1:A:174:PRO:HB3 | 1.73 | 0.53 |
| 1:A:228:ASP:OD2 | 1:A:228:ASP:N | 2.42 | 0.53 |
| 1:A:472:ILE:HD11 | 1:A:488:CYS:HB3 | 1.88 | 0.53 |
| 2:B:303:LEU:HD12 | 2:B:308:VAL:HG12 | 1.90 | 0.53 |
| 7:G:2:NAG:H83 | 7:G:2:NAG:H3 | 1.89 | 0.53 |
| 3:C:336:CYS:SG | 3:C:524:VAL:HG22 | 2.49 | 0.53 |
| 3:C:870:ILE:O | 3:C:874:THR:HG23 | 2.09 | 0.53 |
| 1:A:1139:ASP:OD1 | 1:A:1139:ASP:N | 2.39 | 0.52 |
| 3:C:565:PHE:HB3 | 3:C:576:VAL:HG23 | 1.91 | 0.52 |
| 4:P:45:LEU:HD11 | 5:S:44:PRO:HG2 | 1.92 | 0.52 |
| 3:C:193:VAL:HB | 3:C:204:TYR:HB2 | 1.92 | 0.52 |
| 3:C:364:ASP:OD2 | 3:C:527:PRO:CG | 2.58 | 0.52 |
| 1:A:328:ARG:HD3 | 1:A:578:ASP:OD1 | 2.09 | 0.52 |
| 2:B:309:GLU:HG2 | 2:B:313:TYR:OH | 2.10 | 0.52 |
| 2:B:400:PHE:HE2 | 2:B:410:ILE:HD12 | 1.75 | 0.52 |
| 3:C:295:PRO:O | 3:C:299:THR:HG23 | 2.09 | 0.52 |
| 5:Q:6:GLN:HE22 | 5:Q:88:CYS:H | 1.56 | 0.52 |
| 5:S:34:GLY:HE1 | 5:S:50:TYR:CE2 | 2.27 | 0.52 |
| 3:C:388:ASN:O | 3:C:526:GLY:CA | 2.57 | 0.52 |
| 4:P:93:VAL:HG12 | 4:P:114:LEU:HD23 | 1.91 | 0.52 |
| 1:A:362:VAL:HG12 | 1:A:527:PRO:CB | 2.39 | 0.52 |
| 1:A:395:VAL:CB | 1:A:524:VAL:HG21 | 2.39 | 0.52 |
| 1:A:472:ILE:HD13 | 1:A:484:LYS:HG3 | 1.91 | 0.52 |
| 2:B:567:ARG:HH21 | 2:B:571:ASP:HA | 1.74 | 0.52 |
| 5:V:6:GLN:HE22 | 5:V:88:CYS:H | 1.56 | 0.52 |
| 1:A:973:ILE:HG23 | 1:A:992:GLN:OE1 | 2.10 | 0.52 |
| 2:B:391:CYS:O | 2:B:522:ALA:HB2 | 2.10 | 0.52 |
| 3:C:532:ASN:OD1 | 3:C:533:LEU:N | 2.42 | 0.52 |
| 4:U:93:VAL:HG12 | 4:U:114:LEU:HD23 | 1.91 | 0.52 |
| 2:B:334:ASN:ND2 | 2:B:360:ASN:O | 2.43 | 0.51 |
| 3:C:856:ASN:ND2 | 3:C:856:ASN:O | 2.43 | 0.51 |
| 5:V:34:HIS:HE1 | 5:V:50:TYR:CE1 | 2.27 | 0.51 |
| 1:A:393:THR:HB | 1:A:516:GLU:HB2 | 1.91 | 0.51 |
| 3:C:560:LEU:N | 3:C:563:GLN:OE1 | 2.43 | 0.51 |
| 4:U:50:TRP:CD2 | 4:U:104:TRP:HH2 | 2.28 | 0.51 |
| 1:A:393:THR:CB | 1:A:516:GLU:HB2 | 2.37 | 0.51 |
| 2:B:472:ILE:HD13 | 2:B:484:LYS:HG3 | 1.91 | 0.51 |
| 4:U:37:VAL:CG2 | 4:U:95:TYR:HB2 | 2.40 | 0.51 |
| 4:O:48:MET:HG2 | 4:O:64:PHE:CD1 | 2.46 | 0.51 |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|------------------|
| 2:B:564:GLN:HG3 | 2:B:565:PHE:N   | 2.26                     | 0.51             |
| 4:O:45:LEU:HD11 | 5:Q:44:PRO:HG2  | 1.92                     | 0.51             |
| 4:O:93:VAL:HG12 | 4:O:114:LEU:HD23| 1.91                     | 0.51             |
| 4:P:48:MET:HG2  | 4:P:64:PHE:CD1  | 2.46                     | 0.51             |
| 4:P:50:TRP:CD2  | 4:P:104:TRP:HH2 | 2.28                     | 0.51             |
| 1:A:983:ARG:HD2 | 3:C:387:VAL:HG13| 1.92                     | 0.51             |
| 3:C:746:SER:HB3 | 3:C:749:CYS:SG  | 2.51                     | 0.51             |
| 4:U:45:LEU:HD11| 5:V:44:PRO:HG2  | 1.92                     | 0.51             |
| 4:O:37:VAL:CG2  | 4:O:95:TYR:HB2  | 2.40                     | 0.51             |
| 4:P:37:VAL:CG2  | 4:P:95:TYR:HB2  | 2.40                     | 0.51             |
| 1:A:986:PRO:O   | 1:A:990:GLU:HG3 | 2.11                     | 0.51             |
| 4:U:37:VAL:HD22 | 4:U:95:TYR:HB2  | 1.93                     | 0.51             |
| 4:O:50:TRP:CD2  | 4:O:104:TRP:HH2 | 2.28                     | 0.51             |
| 2:B:316:SER:OG  | 2:B:317:ASN:N   | 2.43                     | 0.51             |
| 2:B:390:LEU:HD22| 3:C:983:ARG:HD3 | 1.92                     | 0.51             |
| 3:C:189:LEU:HD23| 3:C:208:THR:O   | 2.11                     | 0.51             |
| 1:A:217:PRO:C   | 1:A:219:GLY:H   | 2.14                     | 0.51             |
| 1:A:787:GLN:OE1 | 3:C:703:ASN:HB2 | 2.11                     | 0.51             |
| 3:C:400:PHE:HE2 | 3:C:410:ILE:HD12| 1.75                     | 0.51             |
| 4:P:35:ASN:OD1  | 4:P:47:TRP:NE1  | 2.43                     | 0.51             |
| 5:Q:84:ALA:HB3  | 5:Q:86:TYR:CE1  | 2.46                     | 0.51             |
| 1:A:400:PHE:HE2 | 1:A:410:ILE:HD12| 1.75                     | 0.51             |
| 1:A:722:VAL:HG22| 1:A:930:ALA:HB1 | 1.91                     | 0.51             |
| 2:B:395:VAL:HG21| 2:B:524:VAL:CG1 | 2.41                     | 0.51             |
| 4:U:48:MET:HG2  | 4:U:64:PHE:CD1  | 2.46                     | 0.51             |
| 2:B:200:TYR:HE1 | 2:B:230:PRO:HB3 | 1.77                     | 0.50             |
| 2:B:715:PRO:HA  | 2:B:4072:GLU:HA | 1.93                     | 0.50             |
| 3:C:298:GLU:OE2 | 3:C:316:SER:OG  | 2.29                     | 0.50             |
| 4:O:35:ASN:OD1  | 4:O:47:TRP:NE1  | 2.43                     | 0.50             |
| 3:C:200:TYR:CE1 | 3:C:230:PRO:HB3 | 2.46                     | 0.50             |
| 5:V:2:ILE:HD13 | 5:V:27:GLN:HB2  | 1.93                     | 0.50             |
| 4:O:37:VAL:HG22 | 4:O:95:TYR:HB2  | 1.93                     | 0.50             |
| 5:Q:2:ILE:HD13 | 5:Q:27:GLN:HB2  | 1.94                     | 0.50             |
| 1:A:132:GLU:HG2 | 1:A:165:ASN:HB2 | 1.94                     | 0.50             |
| 1:A:362:VAL:HG12| 1:A:527:PRO:HB3 | 1.94                     | 0.50             |
| 8:A:1302:NAG:HZ3| 3:C:558:LYS:NZ  | 2.26                     | 0.50             |
| 3:C:34:ARG:NH1  | 3:C:191:GLU:OE1 | 2.44                     | 0.50             |
| 4:U:35:ASN:OD1  | 4:U:47:TRP:NE1  | 2.43                     | 0.50             |
| 5:V:84:ALA:HB3  | 5:V:86:TYR:CE1  | 2.46                     | 0.50             |
| 3:C:391:CYS:SG  | 3:C:544:ASN:CB  | 3.00                     | 0.50             |
| 4:P:37:VAL:HG22 | 4:P:95:TYR:HB2  | 1.93                     | 0.50             |
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| Atom-1       | Atom-2       | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|--------------|--------------------------|-------------------|
| 2:B:362:VAL:HA | 2:B:525:CYS:H | 1.76                     | 0.50              |
| 3:C:105:ILE:HG12 | 3:C:241:LEU:HD21 | 1.93                     | 0.50              |
| 3:C:470:THR:HG22 | 3:C:492:LEU:HD12 | 1.94                     | 0.50              |
| 4:O:38:ARG:HD3  | 4:O:64:PHE:CE2  | 2.47                     | 0.50              |
| 5:S:2:ILE:HD13  | 5:S:27:GLN:HB2  | 1.93                     | 0.50              |
| 3:C:330:PRO:C   | 3:C:332:ILE:N   | 2.61                     | 0.50              |
| 5:Q:36:TYR:CD1  | 5:Q:46:LEU:HA   | 2.47                     | 0.50              |
| 1:A:869:MET:HG2  | 3:C:699:LEU:HD21 | 1.94                     | 0.49              |
| 1:A:359:SER:HA  | 1:A:523:THR:HG23 | 1.95                     | 0.49              |
| 1:A:391:CYS:CB  | 1:A:525:CYS:SG  | 3.00                     | 0.49              |
| 1:A:746:SER:HB3  | 1:A:749:CYS:SG  | 2.52                     | 0.49              |
| 5:V:21:ILE:O    | 5:V:72:THR:OG1  | 2.19                     | 0.49              |
| 1:A:360:ASN:HA  | 1:A:523:THR:OG1  | 2.12                     | 0.49              |
| 1:A:963:VAL:HG12 | 3:C:570:ALA:HB2  | 1.93                     | 0.49              |
| 3:C:391:CYS:SG  | 3:C:544:ASN:HB3  | 2.52                     | 0.49              |
| 4:P:38:ARG:HD3  | 4:P:64:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:473:TYR:CE2  | 1:A:475:ALA:HB2  | 2.48                     | 0.49              |
| 3:C:206:LYS:HB2  | 3:C:223:LEU:HD22 | 1.93                     | 0.49              |
| 4:U:34:MET:HG2  | 4:U:79:ALA:CB   | 2.42                     | 0.49              |
| 4:U:38:ARG:HD3  | 4:U:64:PHE:CE2  | 2.47                     | 0.49              |
| 1:A:470:THR:HG22 | 1:A:492:LEU:HD12 | 1.94                     | 0.49              |
| 2:B:386:LYS:HE2  | 3:C:981:LEU:O    | 2.12                     | 0.49              |
| 2:B:390:LEU:CD2  | 3:C:983:ARG:HD3  | 2.42                     | 0.49              |
| 3:C:170:TYR:CE2  | 3:C:172:SER:HB2  | 2.48                     | 0.49              |
| 3:C:280:ASN:ND2  | 8:C:1301:NAG:HS2  | 2.27                     | 0.49              |
| 3:C:429:PHE:HE1  | 3:C:514:SER:HA   | 1.77                     | 0.49              |
| 4:O:34:MET:HG2  | 4:O:79:ALA:CB   | 2.42                     | 0.49              |
| 1:A:578:ASP:OD2  | 1:A:581:THR:HG22 | 2.13                     | 0.49              |
| 1:A:858:LEU:HD23 | 1:A:959:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:870:ILE:O    | 1:A:874:THR:HG23 | 2.12                     | 0.49              |
| 4:P:34:MET:HG2  | 4:P:79:ALA:CB    | 2.42                     | 0.49              |
| 5:S:84:ALA:HB3   | 5:S:86:TYR:CE2   | 2.46                     | 0.49              |
| 1:A:331:ASN:HB2  | 1:A:580:GLN:HG2  | 1.93                     | 0.49              |
| 2:B:97:LYS:H2    | 2:B:187:LYS:N    | 2.11                     | 0.49              |
| 3:C:391:CYS:O    | 3:C:522:ALA:CB   | 2.61                     | 0.49              |
| 3:C:472:ILE:HG21 | 3:C:482:GLY:H    | 1.78                     | 0.48              |
| 5:S:35:TRP:CD2   | 5:S:73:LEU:HD22  | 2.48                     | 0.48              |
| 2:B:473:TYR:CE2  | 2:B:475:ALA:HB2  | 2.48                     | 0.48              |
| 5:Q:35:TRP:CD2   | 5:Q:73:LEU:HD22  | 2.48                     | 0.48              |
| 2:B:470:THR:HG22 | 2:B:492:LEU:HD12 | 1.94                     | 0.48              |
| 4:O:107:ASP:HB3  | 4:O:109:TRP:CE3  | 2.49                     | 0.48              |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 3:C:124:THR:HG22 | 3:C:174:PRO:HG3 | 1.95 | 0.48 |
| 3:C:391:CYSHB2 | 3:C:544:ASN:C | 2.27 | 0.48 |
| 3:C:473:TYR:CE2 | 3:C:475:ALA:HB2 | 2.48 | 0.48 |
| 1:A:46:SER:CA | 1:A:279:TYR:O | 2.61 | 0.48 |
| 1:A:472:ILE:HG21 | 1:A:482:GLY:H | 1.78 | 0.48 |
| 3:C:567:ARG:ZH1 | 3:C:571:ASP:OD1 | 2.47 | 0.48 |
| 1:A:976:VAL:HB | 1:A:979:ASP:OD2 | 2.14 | 0.48 |
| 2:B:472:ILE:HG21 | 2:B:482:GLY:H | 1.78 | 0.48 |
| 6:E:1:NAG:H4 | 6:E:2:NAG:H2 | 1.63 | 0.48 |
| 2:B:359:SER:C | 2:B:523:THR:HG23 | 2.15 | 0.48 |
| 4:P:107:ASP:HB3 | 4:P:109:TRP:CE3 | 2.49 | 0.48 |
| 1:A:357:ARG:ZH2 | 2:B:167:THR:HA | 2.28 | 0.48 |
| 2:B:395:VAL:CG2 | 2:B:524:VAL:CG1 | 2.92 | 0.48 |
| 4:U:4:LEU:HB2 | 4:U:109:TRP:HD1 | 1.76 | 0.48 |
| 2:B:334:ASN:HD22 | 2:B:361:CYSHB2 | 2.27 | 0.48 |
| 3:C:725:GLU:OE1 | 3:C:1028:LYS:NZ | 2.22 | 0.48 |
| 4:U:2:VAL:HG23 | 4:U:2:VAL:O | 2.13 | 0.48 |
| 5:V:35:TRP:CD2 | 5:V:73:LEU:HD22 | 2.48 | 0.48 |
| 3:C:170:TYR:CE2 | 3:C:172:SER:HB2 | 2.49 | 0.48 |
| 4:O:2:LEU:HG23 | 4:O:2:VAL:O | 2.14 | 0.48 |
| 4:P:4:LEU:HD23 | 4:P:22:CYSHG | 2.54 | 0.48 |
| 1:A:395:VAL:HB | 1:A:524:VAL:HG21 | 1.95 | 0.47 |
| 1:A:1031:GLU:N | 1:A:1031:GLU:OE1 | 2.47 | 0.47 |
| 4:U:107:ASP:HB3 | 4:U:109:TRP:CE3 | 2.49 | 0.47 |
| 1:A:1105:THR:HG22 | 1:A:1112:PRO:HA | 1.96 | 0.47 |
| 4:P:2:VAL:HG23 | 4:P:2:VAL:O | 2.13 | 0.47 |
| 3:C:200:TYR:HE1 | 3:C:230:PRO:HB3 | 1.80 | 0.47 |
| 3:C:206:LYH:HG3 | 3:C:223:LEU:HA | 1.95 | 0.47 |
| 4:O:4:LEU:HD23 | 4:O:22:CYSHG | 2.54 | 0.47 |
| 1:A:331:ASN:CB | 1:A:580:GLN:HG2 | 2.45 | 0.47 |
| 1:A:1102:TRP:HB2 | 1:A:1135:ASN:ND2 | 2.30 | 0.47 |
| 5:V:36:TYR:CD1 | 5:V:46:LEU:HA | 2.47 | 0.47 |
| 1:A:200:TYR:OH | 3:C:396:TYR:OH | 2.68 | 0.47 |
| 3:C:331:ASN:O | 3:C:332:ILE:C | 2.52 | 0.47 |
| 4:U:109:TRP:CD1 | 4:U:109:TRP:O | 2.68 | 0.47 |
| 6:D:1:NAG:H4 | 6:D:2:NAG:H2 | 1.63 | 0.47 |
| 2:B:324:GLU:OE1 | 2:B:325:SER:O | 2.40 | 0.47 |
| 5:V:4:MET:HE3 | 5:V:90:GLN:HB3 | 1.97 | 0.47 |
| 6:F:1:NAG:H4 | 6:F:2:NAG:H2 | 1.63 | 0.47 |
| 1:A:395:VAL:HG23 | 1:A:524:VAL:CB | 2.31 | 0.47 |
| 2:B:386:LYS:CD | 3:C:984:LEU:N | 2.75 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 2:B:786:LYS:HG3 | 2:B:787:GLN:HG3 | 1.97 | 0.47 |
| 3:C:715:PRO:HA | 3:C:1071:GLN:O | 2.13 | 0.47 |
| 5:V:61:ARG:NE | 5:V:79:GLN:OE1 | 2.48 | 0.47 |
| 4:P:4:LEU:HD2 | 4:P:109:TRP:HD1 | 1.77 | 0.47 |
| 1:A:99:ASN:CG | 1:A:102:ARG:HE | 2.19 | 0.47 |
| 5:Q:61:ARG:NE | 5:Q:79:GLN:OE1 | 2.48 | 0.47 |
| 1:A:394:ASN:CB | 1:A:516:GLU:CB | 2.93 | 0.46 |
| 1:A:1037:SER:OG | 1:A:1039:ARG:HG2 | 2.14 | 0.46 |
| 2:B:452:LEU:HD22 | 2:B:494:SER:HA | 1.98 | 0.46 |
| 4:U:59:THR:HG23 | 4:U:59:THR:O | 2.15 | 0.46 |
| 5:Q:55:ILE:HG23 | 5:Q:58:VAL:HB | 1.97 | 0.46 |
| 1:A:611:LEU:HG22 | 1:A:666:ILE:HG23 | 1.97 | 0.46 |
| 1:A:726:ILE:HG12 | 1:A:1061:VAL:HG22 | 1.97 | 0.46 |
| 2:B:363:ALA:O | 2:B:526:GLY:N | 2.49 | 0.46 |
| 4:O:109:TRP:CD1 | 4:O:109:TRP:O | 2.68 | 0.46 |
| 1:A:770:ILE:O | 1:A:774:GLN:HG2 | 2.15 | 0.46 |
| 2:B:363:ALA:O | 2:B:526:GLY:N | 2.49 | 0.46 |
| 2:B:418:ILE:HA | 2:B:422:ASN:HB2 | 1.98 | 0.46 |
| 4:U:37:VAL:O | 4:U:95:TYR:N | 2.45 | 0.46 |
| 5:Q:4:MET:HE3 | 5:Q:90:GLN:HB3 | 1.97 | 0.46 |
| 4:P:14:PRO:HG3 | 4:P:117:VAL:HG22 | 1.97 | 0.46 |
| 4:U:4:LEU:HD23 | 4:U:22:CYSSG | 2.54 | 0.46 |
| 4:U:67:ARG:HD2 | 4:U:84:CYSS | 2.15 | 0.46 |
| 4:O:95:TYR:HE2 | 5:Q:44:PRO:HD2 | 1.81 | 0.46 |
| 2:B:280:ASN:OD1 | 2:B:281:GLU:N | 2.42 | 0.46 |
| 4:O:67:ARG:HD2 | 4:O:84:CYSS | 2.15 | 0.46 |
| 5:S:61:ARG:NE | 5:S:79:GLN:OE1 | 2.48 | 0.46 |
| 2:B:722:VAL:HA | 2:B:1064:HIS:O | 2.14 | 0.46 |
| 3:C:418:ILE:HA | 3:C:422:ASN:HB2 | 1.98 | 0.46 |
| 1:A:282:ASN:HB2 | 1:A:284:THR:HG22 | 1.98 | 0.46 |
| 4:U:12:LYS:HG3 | 4:U:18:VAL:CG1 | 2.30 | 0.46 |
| 4:O:37:VAL:O | 4:O:95:TYR:N | 2.45 | 0.46 |
| 4:P:67:ARG:HD2 | 4:P:84:CYSS | 2.15 | 0.46 |
| 1:A:418:ILE:HA | 1:A:422:ASN:HB2 | 1.98 | 0.46 |
| 3:C:454:ARG:HE | 3:C:454:ARG:HB3 | 1.59 | 0.46 |
| 5:V:55:ILE:HG23 | 5:V:58:VAL:HB | 1.98 | 0.46 |
| 4:P:109:TRP:CD1 | 4:P:109:TRP:O | 2.68 | 0.46 |
| 5:S:55:ILE:HG23 | 5:S:58:VAL:HB | 1.98 | 0.46 |
| 1:A:320:VAL:HG22 | 1:A:591:SER:O | 2.16 | 0.46 |
| 1:A:394:ASN:ND2 | 1:A:516:GLU:CA | 2.79 | 0.46 |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:516:GLU:CB  | 1:A:516:GLU:CA  | 2.94                     | 0.46              |
| 1:A:542:ASN:OD1 | 1:A:547:THR:HG22| 2.16                     | 0.46              |
| 4:P:59:THR:HG23 | 4:P:59:THR:O    | 2.15                     | 0.46              |
| 2:B:53:ASP:HB3  | 2:B:55:PHE:CE1  | 2.51                     | 0.45              |
| 2:B:734:THR:HG21| 2:B:1007:TYR:OH | 2.16                     | 0.45              |
| 5:S:36:TYR:CD2  | 5:S:46:LEU:HA   | 2.47                     | 0.45              |
| 4:O:59:THR:HG23 | 4:O:59:THR:O    | 2.15                     | 0.45              |
| 2:B:390:LEU:HD11| 3:C:983:ARG:CB  | 2.46                     | 0.45              |
| 4:U:20:VAL:HG12 | 4:U:113:THR:HG21| 1.98                     | 0.45              |
| 1:A:957:GLN:HE21| 2:B:765:ARG:NH2 | 2.14                     | 0.45              |
| 3:C:126:VAL:CG2 | 3:C:172:SER:HB3 | 2.46                     | 0.45              |
| 3:C:725:GLU:CD  | 3:C:1028:LYS:HZ3| 2.15                     | 0.45              |
| 4:O:20:VAL:HG12 | 4:O:113:THR:HG21| 1.98                     | 0.45              |
| 1:A:359:SER:HB3 | 1:A:323:THR:HG21| 1.98                     | 0.45              |
| 2:B:362:VAL:CA  | 2:B:525:CYS:O   | 2.64                     | 0.45              |
| 2:B:362:VAL:HG13| 2:B:525:CYS:O   | 2.16                     | 0.45              |
| 3:C:973:ILE:HG23| 3:C:992:GLN:OE1 | 2.17                     | 0.45              |
| 4:U:14:PRO:HG3  | 4:U:117:VAL:HG22| 1.97                     | 0.45              |
| 4:U:95:TYR:HE2  | 5:V:44:PRO:HD2  | 1.81                     | 0.45              |
| 1:A:458:LYS:HA  | 1:A:458:LYS:HD2 | 1.41                     | 0.45              |
| 1:A:452:LEU:HD22| 1:A:494:SER:HA  | 1.98                     | 0.45              |
| 3:C:452:LEU:HD22| 3:C:494:SER:HA  | 1.98                     | 0.45              |
| 1:A:707:TYR:HB2 | 2:B:883:THR:CG2 | 2.46                     | 0.45              |
| 3:C:271:GLN:OE1 | 3:C:272:PRO:HD2 | 2.17                     | 0.45              |
| 3:C:977:LEU:HD11| 3:C:993:ILE:HG12| 1.97                     | 0.45              |
| 4:U:51:ILE:O   | 4:U:51:ILE:HG13 | 2.17                     | 0.45              |
| 4:O:4:LEU:HD13 | 4:O:109:TRP:NE1 | 2.21                     | 0.45              |
| 4:P:20:VAL:HG12 | 4:P:113:THR:HG21| 1.98                     | 0.45              |
| 2:B:934:ILE:HD13| 2:B:1063:LEU:HD13| 1.99                     | 0.45              |
| 3:C:106:PHE:HD2 | 3:C:235:ILE:HD11| 1.82                     | 0.45              |
| 3:C:531:THR:HG22| 3:C:532:ASN:N   | 2.32                     | 0.45              |
| 3:C:560:LEU:HB2 | 3:C:563:GLN:NE2 | 2.32                     | 0.45              |
| 5:Q:21:ILE:O   | 5:Q:72:THR:OG1  | 2.19                     | 0.45              |
| 4:P:51:ILE:HG22 | 4:P:58:PRO:HA   | 1.99                     | 0.45              |
| 3:C:332:ILE:C  | 3:C:334:ASN:H   | 2.21                     | 0.45              |
| 3:C:914:ASN:O  | 3:C:918:GLU:HG3 | 2.16                     | 0.45              |
| 4:O:14:PRO:HG3 | 4:O:117:VAL:HG22| 1.97                     | 0.45              |
| 1:A:345:THR:HG23| 4:U:104:TRP:HD1 | 1.82                     | 0.44              |
| 1:A:736:VAL:HG12| 1:A:858:LEU:HG | 1.99                     | 0.44              |
| 3:C:345:THR:HG23| 4:P:104:TRP:HD1 | 1.83                     | 0.44              |
| 4:U:51:ILE:HG22| 4:U:58:PRO:HA   | 1.99                     | 0.44              |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|------------------|
| 4:P:95:TYR:HE2 | 5:S:44:PRO:HD2 | 1.81 | 0.44 |
| 2:B:357:ARG:HE | 3:C:230:PRO:HG3 | 1.36 | 0.44 |
| 2:B:702:GLU:O | 2:B:703:ASN:HB3 | 2.18 | 0.44 |
| 5:V:34:HIS:CE1 | 5:V:50:TYR:CD1 | 3.05 | 0.44 |
| 5:Q:90:GLN:OE1 | 5:Q:92:ASN:N | 2.44 | 0.44 |
| 1:A:364:ASP:HB2 | 1:A:527:PRO:HD3 | 1.98 | 0.44 |
| 2:B:363:ALA:O | 2:B:525:CYS:O | 2.36 | 0.44 |
| 5:Q:24:ARG:HB2 | 5:Q:24:ARG:CE2 | 2.47 | 0.44 |
| 5:Q:61:ARG:HD3 | 5:Q:77:SER:O | 2.18 | 0.44 |
| 1:A:304:ASN:O | 1:A:515:PHE:C | 2.56 | 0.44 |
| 2:B:736:VAL:HG11 | 2:B:1004:LEU:HD11 | 1.99 | 0.44 |
| 3:C:29:THR:HG22 | 3:C:62:VAL:HG23 | 2.00 | 0.44 |
| 3:C:112:SER:HB2 | 3:C:134:GLN:HG2 | 1.99 | 0.44 |
| 5:V:24:ARG:NH2 | 5:V:24:ARG:HB2 | 2.33 | 0.44 |
| 5:V:61:ARG:HD3 | 5:V:77:SER:O | 2.18 | 0.44 |
| 5:S:4:MET:HE3 | 5:S:90:GLN:HB3 | 1.99 | 0.44 |
| 5:S:24:ARG:HB2 | 5:S:24:ARG:CE2 | 2.48 | 0.44 |
| 3:C:43:ILE:HD11 | 3:C:513:LEU:HD12 | 2.00 | 0.44 |
| 4:O:51:ILE:HG13 | 4:O:51:ILE:O | 2.17 | 0.44 |
| 1:A:811:LYS:HE2 | 1:A:811:LYS:HB2 | 1.72 | 0.44 |
| 5:Q:79:GLN:HA | 5:Q:80:PRO:HD2 | 1.87 | 0.44 |
| 4:P:51:ILE:HG13 | 4:P:51:ILE:O | 2.17 | 0.44 |
| 2:B:434:ILE:HD11 | 2:B:513:LEU:HD12 | 2.00 | 0.44 |
| 2:B:492:LEU:HA | 2:B:492:LEU:HD23 | 1.85 | 0.43 |
| 3:C:105:ILE:HD12 | 3:C:118:LEU:H2 | 1.99 | 0.43 |
| 4:O:51:ILE:HG22 | 4:O:58:PRO:HA | 1.99 | 0.43 |
| 5:S:34:HIS:CE1 | 5:S:50:TYR:CD2 | 3.05 | 0.43 |
| 1:A:121:ASN:HD21 | 1:A:174:PRO:CB | 2.30 | 0.43 |
| 1:A:296:LEU:O | 1:A:300:LYS:HG3 | 2.18 | 0.43 |
| 1:A:421:TYR:HB3 | 1:A:457:ARG:HB3 | 2.00 | 0.43 |
| 1:A:492:LEU:HD23 | 1:A:492:LEU:HA | 1.85 | 0.43 |
| 4:O:47:TRP:HZ2 | 4:O:50:TRP:HD1 | 1.66 | 0.43 |
| 2:B:714:ILE:HD11 | 2:B:1096:VAL:HG11 | 2.00 | 0.43 |
| 5:Q:24:ARG:HB2 | 5:Q:24:ARG:NH2 | 2.33 | 0.43 |
| 2:B:91:TYR:OH | 2:B:191:GLU:OE1 | 2.19 | 0.43 |
| 3:C:87:ASN:OD1 | 3:C:88:ASP:N | 2.52 | 0.43 |
| 3:C:421:TYR:HB3 | 3:C:457:ARG:HB3 | 2.00 | 0.43 |
| 5:V:24:ARG:HB2 | 5:V:24:ARG:CE2 | 2.48 | 0.43 |
| 4:O:38:ARG:HB3 | 4:O:48:MET:HE1 | 2.01 | 0.43 |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:531:THR:HG22 | 1:A:532:ASN:N   | 2.33                     | 0.43              |
| 4'O:108:VAL:O   | 4'O:108:VAL:HG13| 2.19                     | 0.43              |
| 4':P:47:TRP:HZ2 | 4':P:50:TRP:HD1 | 1.66                     | 0.43              |
| 4':P:108:VAL:HG13| 4':P:108:VAL:O | 2.19                     | 0.43              |
| 1:A:434:ILE:HD11| 1:A:513:LEU:HD12| 2.00                     | 0.43              |
| 3:C:441:LEU:HD13| 3:C:441:LEU:HA  | 1.91                     | 0.43              |
| 1:A:410:ILE:H   | 1:A:410:ILE:HG12| 1.71                     | 0.43              |
| 1:A:822:LEU:HD21| 1:A:938:LEU:HD13| 2.01                     | 0.43              |
| 2:B:296:LEU:O   | 2:B:299:THR:OG1 | 2.28                     | 0.43              |
| 3:C:410:ILE:H   | 3:C:410:ILE:HG12| 1.71                     | 0.43              |
| 5:V:6:GLN:NE2   | 5:V:88:CYS:H    | 2.17                     | 0.43              |
| 2:B:421:TYR:HB3 | 2:B:457:ARG:HB3 | 2.00                     | 0.43              |
| 2:B:455:LEU:HB3 | 2:B:456:PHE:H   | 1.51                     | 0.43              |
| 3:C:391:CYS:CB  | 3:C:544:ASN:C   | 2.85                     | 0.43              |
| 5:S:61:ARG:HD3  | 5:S:77:SER:O    | 2.18                     | 0.43              |
| 1:A:299:THR:HA  | 1:A:302:THR:HG22| 2.00                     | 0.43              |
| 1:A:707:TYR:CD1 | 2:B:883:THR:HG23| 2.54                     | 0.43              |
| 1:A:912:THR:OG1 | 1:A:914:ASN:ND2 | 2.52                     | 0.43              |
| 3:C:276:LEU:O   | 3:C:288:ALA:HA  | 2.19                     | 0.43              |
| 4'O:4:LEU:HD11  | 4'O:27:TYR:OH   | 2.19                     | 0.43              |
| 5:Q:6:GLN:NE2   | 5:Q:88:CYS:H    | 2.17                     | 0.43              |
| 5:Q:6:GLN:OE1   | 5:Q:102:THR:HG23| 2.19                     | 0.43              |
| 4':P:4:LEU:HD11 | 4':P:27:TYR:OH  | 2.19                     | 0.43              |
| 1:A:394:ASN:OD1 | 1:A:516:GLU:C   | 2.56                     | 0.43              |
| 2:B:914:ASN:O   | 2:B:918:GLU:HG3 | 2.18                     | 0.43              |
| 2:B:985:ASP:OD2 | 2:B:987:PRO:HD2 | 2.18                     | 0.43              |
| 3:C:57:PRO:HB3  | 3:C:273:ARG:HH21| 1.84                     | 0.43              |
| 4'O:4:LEU:HB2   | 4'O:109:TRP:HD1 | 1.77                     | 0.43              |
| 4'O:39:GLN:HG3  | 4'O:45:LEU:HD23 | 2.01                     | 0.43              |
| 2:B:821:LEU:O   | 2:B:825:LYS:HG2 | 2.19                     | 0.42              |
| 5:S:6:GLN:OE1   | 5:S:102:THR:HG23| 2.19                     | 0.42              |
| 5:S:84:ALA:O    | 5:S:86:TYR:HD2  | 2.02                     | 0.42              |
| 2:B:129:LYS:HG2 | 2:B:169:GLU:HG2 | 2.01                     | 0.42              |
| 2:B:201:PHE:HE2 | 2:B:203:ILE:HD11| 1.84                     | 0.42              |
| 3:C:564:GLN:OE1 | 3:C:577:ARG:HD2 | 2.19                     | 0.42              |
| 5:S:34:HIS:CE1  | 5:S:50:TYR:HD2  | 2.38                     | 0.42              |
| 1:A:199:GLY:HA2 | 1:A:232:GLY:HA2 | 2.01                     | 0.42              |
| 1:A:320:VAL:HG23| 1:A:590:CYS:HB3 | 2.01                     | 0.42              |
| 1:A:328:ARG:NH1 | 1:A:578:ASP:OD2 | 2.53                     | 0.42              |
| 1:A:360:ASN:N   | 1:A:523:THR:HG23| 1.85                     | 0.42              |
| 1:A:393:THR:OG1 | 1:A:516:GLU:C   | 2.58                     | 0.42              |

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| Atom-1      | Atom-2      | Interatomic distance (Å) | Clash overlap (Å) |
|-------------|-------------|--------------------------|------------------|
| 3:C:205:SER:O | 3:C:206:LYS:HG2 | 2.20                     | 0.42             |
| 3:C:336:CYS:SG | 3:C:524:VAL:HG13 | 2.59                     | 0.42             |
| 3:C:425:LEU:HD12 | 3:C:425:LEU:HA | 1.79                     | 0.42             |
| 5:V:6:GLN:OE1 | 5:V:102:THR:HG23 | 2.19                     | 0.42             |
| 4:P:35:ASN:ND2 | 4:P:35:ASN:H | 2.18                     | 0.42             |
| 1:A:790:LYS:H | 3:C:704:SER:HA | 1.84                     | 0.42             |
| 2:B:332:ILE:O | 2:B:362:VAL:HG23 | 2.20                     | 0.42             |
| 2:B:381:GLY:O | 3:C:984:LEU:HD11 | 2.19                     | 0.42             |
| 2:B:555:SER:HB3 | 2:B:586:ASP:HB2 | 2.01                     | 0.42             |
| 2:B:856:ASN:OD1 | 2:B:856:ASN:N | 2.50                     | 0.42             |
| 4:U:35:ASN:ND2 | 4:U:35:ASN:H | 2.18                     | 0.42             |
| 4:U:108:VAL:O | 4:U:108:VAL:HG13 | 2.19                     | 0.42             |
| 5:V:79:GLN:HA | 5:V:80:PRO:HD2 | 1.86                     | 0.42             |
| 5:V:84:ALA:O | 5:V:86:TYR:HD1 | 2.02                     | 0.42             |
| 1:A:391:CYS:HB3 | 1:A:522:ALA:HB1 | 2.02                     | 0.42             |
| 2:B:39:PRO:HG3 | 2:B:51:THR:HG21 | 2.02                     | 0.42             |
| 2:B:48:LEU:CD2 | 2:B:278:LYS:HG3 | 2.50                     | 0.42             |
| 2:B:396:TYR:OH | 3:C:230:PRO:HB3 | 2.19                     | 0.42             |
| 3:C:402:ILE:HG13 | 3:C:402:ILE:HG13 | 1.77                     | 0.42             |
| 1:A:29:THR:HG22 | 1:A:30:ASN:N | 2.34                     | 0.42             |
| 2:B:382:VAL:O | 3:C:984:LEU:HD21 | 2.15                     | 0.42             |
| 2:B:916:LEU:HD12 | 2:B:923:ILE:HD12 | 2.02                     | 0.42             |
| 4:U:38:ARG:HB3 | 4:U:48:MET:HE1 | 2.02                     | 0.42             |
| 5:V:34:HIS:CE1 | 5:V:50:TYR:HD1 | 2.38                     | 0.42             |
| 5:V:62:PHE:HB3 | 5:V:75:ILE:HA | 2.02                     | 0.42             |
| 5:Q:84:ALA:O | 5:Q:86:TYR:HD1 | 2.02                     | 0.42             |
| 5:S:37:GLN:HB3 | 5:S:47:LEU:HD11 | 2.02                     | 0.42             |
| 1:A:326:ILE:O | 1:A:326:ILE:HG13 | 2.19                     | 0.42             |
| 2:B:583:GLU:HG2 | 2:B:584:ILE:HG2 | 1.84                     | 0.42             |
| 3:C:280:ASN:CG | 3:C:281:GLU:H | 2.23                     | 0.42             |
| 3:C:363:ALA:H | 3:C:525:CYS:H | 1.67                     | 0.42             |
| 3:C:558:LYS:O | 3:C:558:LYS:HG3 | 2.20                     | 0.42             |
| 3:C:33:THR:HA | 3:C:58:PHE:CD1 | 2.55                     | 0.42             |
| 3:C:105:ILE:CD1 | 3:C:118:LEU:HG | 2.50                     | 0.42             |
| 4:U:34:MET:SD | 4:U:96:CYS:SG | 3.18                     | 0.42             |
| 4:U:47:TRP:HZ2 | 4:U:50:TRP:HD1 | 1.66                     | 0.42             |
| 5:Q:34:HIS:CE1 | 5:Q:50:TYR:HD1 | 2.38                     | 0.42             |
| 4:P:37:VAL:O | 4:P:95:TYR:N | 2.45                     | 0.42             |
| 5:S:3:GLN:OE1 | 5:S:3:GLN:HA | 2.20                     | 0.42             |
| 5:S:11:LEU:HD23 | 5:S:11:LEU:HD23 | 1.85                     | 0.42             |
| 1:A:809:PRO:HA | 1:A:814:LYS:HE3 | 2.01                     | 0.42             |

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| Atom-1   | Atom-2   | Interatomic distance (Å) | Clash overlap (Å) |
|----------|----------|--------------------------|-------------------|
| 4:U:4:LEU:HD11 | 4:U:27:TYR:OH | 2.19                     | 0.42              |
| 5:V:3:GLN:HA  | 5:V:3:GLN:OE1 | 2.20                     | 0.42              |
| 4:O:104:TRP:CE2 | 5:Q:94:TRP:HH2 | 2.38                     | 0.42              |
| 5:Q:62:PHE:HB3 | 5:Q:75:ILE:HA | 2.02                     | 0.42              |
| 7:L:1:NAG:H61 | 7:L:2:NAG:H82 | 2.02                     | 0.42              |
| 2:B:368:LEU:N | 2:B:368:LEU:CD1 | 2.83                     | 0.41              |
| 1:A:402:ILE:H  | 1:A:402:ILE:HG13 | 1.77                     | 0.41              |
| 2:B:126:VAL:HG13 | 2:B:172:SER:HB3 | 2.03                     | 0.41              |
| 2:B:552:LEU:HA  | 2:B:586:ASP:O | 2.19                     | 0.41              |
| 3:C:1102:TRP:CE2 | 3:C:1133:VAL:HG21 | 2.55                     | 0.41              |
| 4:U:39:GLN:CE2 | 4:U:45:LEU:HD23 | 2.01                     | 0.41              |
| 4:O:34:MET:SD  | 4:O:96:CYS:SG | 3.18                     | 0.41              |
| 1:A:217:PRO:CE2 | 1:A:219:GLY:N | 2.73                     | 0.41              |
| 1:A:394:ASN:OE2 | 1:A:515:PHE:HA | 2.20                     | 0.41              |
| 1:A:868:GLU:OE2 | 1:A:868:GLU:N | 2.51                     | 0.41              |
| 4:U:35:ASN:ND2 | 4:U:99:GLY:O  | 2.54                     | 0.41              |
| 4:U:62:ASP:HA  | 4:U:65:ARG:HH2 | 1.85                     | 0.41              |
| 4:U:104:TRP:CE2 | 5:V:94:TRP:HH2 | 2.39                     | 0.41              |
| 4:P:34:MET:SD  | 4:P:96:CYS:SG | 3.18                     | 0.41              |
| 4:P:39:GLN:CE2 | 4:P:45:LEU:HD23 | 2.01                    | 0.41              |
| 2:B:577:ARG:HA  | 2:B:583:GLU:O | 2.20                     | 0.41              |
| 5:Q:11:LEU:HD23 | 5:Q:11:LEU:H  | 1.85                     | 0.41              |
| 1:A:975:SER:OG  | 3:C:571:ASP:OD2 | 2.38                    | 0.41              |
| 2:B:1107:ARG:HD2 | 3:C:904:TYR:CE2 | 2.55                    | 0.41              |
| 3:C:31:SER:O   | 3:C:59:PHE:HA | 2.20                     | 0.41              |
| 5:V:11:LEU:HD23 | 5:V:11:LEU:H  | 1.85                     | 0.41              |
| 4:P:35:ASN:ND2 | 4:P:99:GLY:O  | 2.54                     | 0.41              |
| 2:B:562:PHE:HB2 | 3:C:41:LYS:HE2 | 2.01                     | 0.41              |
| 2:B:733:LYS:HE3 | 2:B:771:ALA:O | 2.21                     | 0.41              |
| 3:C:114:THR:HG2 | 3:C:115:GLN:N | 2.35                     | 0.41              |
| 3:C:901:GLN:O  | 3:C:905:ARG:HG3 | 2.20                    | 0.41              |
| 2:B:382:VAL:CB  | 3:C:983:ARG:HD2 | 2.49                    | 0.41              |
| 2:B:552:LEU:CD2 | 2:B:587:ILE:HG12 | 2.51                    | 0.41              |
| 2:B:741:TYR:CE1 | 2:B:966:LEU:HD11 | 2.56                    | 0.41              |
| 2:B:1027:THR:HG2 | 2:B:1042:PHE:HZ | 1.85                    | 0.41              |
| 1:A:134:GLN:NE2 | 1:A:162:SER:OG | 2.32                     | 0.41              |
| 1:A:386:LYS:H   | 1:A:386:LYS:HG3 | 1.58                     | 0.41              |
| 2:B:363:ALA:O   | 2:B:525:CYS:C  | 2.24                     | 0.41              |
| 2:B:437:ASN:HE2 | 2:B:508:TYR:CE2 | 2.56                     | 0.41              |
| 2:B:981:ILE:HG13 | 2:B:981:ILE:N  | 2.36                     | 0.41              |
| 3:C:437:ASN:HB2 | 3:C:508:TYR:CE1 | 2.56                     | 0.41              |

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| Atom-1   | Atom-2   | Interatomic distance (Å) | Clash overlap (Å) |
|----------|----------|--------------------------|-------------------|
| 4:U:50:TRP:CG | 4:U:104:TRP:HH2 | 2.39                      | 0.41              |
| 4:O:35:ASN:H  | 4:O:35:ASN:ND2 | 2.18                      | 0.41              |
| 4:O:39:GLN:NE2 | 4:O:40:ALA:O  | 2.54                      | 0.41              |
| 4:O:60:TYR:CE1 | 4:O:69:VAL:HA | 2.56                      | 0.41              |
| 1:A:336:CY5:HA | 1:A:337:PRO:HD3 | 1.95                      | 0.41              |
| 1:A:368:LEU:N  | 1:A:368:LEU:CD1 | 2.83                      | 0.41              |
| 1:A:743:CY5:SG | 1:A:750:SER:N  | 2.93                      | 0.41              |
| 1:A:789:TYR:HD1 | 3:C:703:ASN:O | 2.04                      | 0.41              |
| 2:B:172:SER:OG | 2:B:173:GLN:N  | 2.53                      | 0.41              |
| 2:B:658:ASN:ND2 | 2:B:660:TYR:CZ | 2.89                      | 0.41              |
| 2:B:658:ASN:ND2 | 2:B:660:TYR:OH | 2.42                      | 0.41              |
| 3:C:461:LEU:HD13 | 3:C:461:LEU:HA | 1.90                      | 0.41              |
| 5:V:91:SER:HA  | 5:V:96:LEU:HD22 | 2.03                      | 0.41              |
| 4:O:50:TRP:CG  | 4:O:104:TRP:HH2 | 2.39                      | 0.41              |
| 5:Q:3:GLN:HA   | 5:Q:3:GLN:OE1  | 2.20                      | 0.41              |
| 4:P:62:ASP:HA  | 4:P:65:ARG:HH21 | 1.85                      | 0.41              |
| 4:P:104:TRP:CE2 | 5:S:94:TRP:HH2 | 2.38                      | 0.41              |
| 5:S:62:PHE:HB3  | 5:S:75:ILE:HA  | 2.02                      | 0.41              |
| 1:A:441:LEU:HD13 | 1:A:441:LEU:HA | 1.91                      | 0.41              |
| 2:B:583:GLU:HG2 | 2:B:584:ILE:N  | 2.36                      | 0.41              |
| 4:U:39:GLN:NE2 | 4:U:40:ALA:O  | 2.54                      | 0.41              |
| 5:V:37:GLN:HB3  | 5:V:47:LEU:HD11 | 2.02                     | 0.41              |
| 4:O:95:TYR:CE2  | 5:Q:44:PRO:HD2 | 2.56                      | 0.41              |
| 5:Q:34:HIS:CE1  | 5:Q:50:TYR:CD1 | 3.05                      | 0.41              |
| 5:Q:37:GLN:HB3  | 5:Q:47:LEU:HD11 | 2.02                     | 0.41              |
| 5:Q:4:LEU:HD13  | 5:P:109:TRP:NE1 | 2.21                      | 0.41              |
| 5:S:91:SER:HA   | 5:S:96:LEU:HD22 | 2.03                      | 0.41              |
| 1:A:303:LEU:HD23 | 1:A:308:VAL:HG12 | 2.03                     | 0.40              |
| 2:B:29:THR:HG22 | 2:B:30:ASN:N  | 2.37                      | 0.40              |
| 3:C:90:VAL:HG21 | 3:C:238:PHE:CE1 | 2.56                      | 0.40              |
| 5:V:104:LEU:HD23 | 5:V:104:LEU:HA | 1.91                      | 0.40              |
| 4:O:35:ASN:ND2  | 4:O:99:GLY:O   | 2.54                      | 0.40              |
| 4:P:95:TYR:CE2  | 5:S:44:PRO:HD2 | 2.56                      | 0.40              |
| 1:A:34:ARG:NH2  | 1:A:217:PRO:HB2 | 2.36                      | 0.40              |
| 1:A:643:PHE:CE2  | 1:A:645:THR:HG22 | 2.56                     | 0.40              |
| 3:C:189:LEU:HD12 | 3:C:216:LEU:HD11 | 2.03                     | 0.40              |
| 5:V:21:ILE:O    | 5:V:21:ILE:HG13 | 2.22                      | 0.40              |
| 4:O:98:ARG:HH21 | 4:O:109:TRP:HH2 | 1.69                      | 0.40              |
| 4:P:50:TRP:CG   | 4:P:104:TRP:HH2 | 2.39                      | 0.40              |
| 5:S:6:GLN:NE2   | 5:S:88:CYS:H   | 2.17                      | 0.40              |
| 2:B:326:ILE:HG13 | 2:B:326:ILE:O  | 2.21                      | 0.40              |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 3:C:90:VAL:HG23 | 3:C:267:VAL:HG13 | 2.02 | 0.40 |
| 3:C:386:LYS:H | 3:C:386:LYS:HG3 | 1.59 | 0.40 |
| 3:C:959:LEU:HD23 | 3:C:959:LEU:HA | 1.89 | 0.40 |
| 5:V:61:ARG:HG3 | 5:V:62:PHE:CD2 | 2.57 | 0.40 |
| 5:S:61:ARG:HG3 | 5:S:62:PHE:CD1 | 2.57 | 0.40 |
| 2:B:280:ASN:CG | 2:B:281:GLU:N | 2.75 | 0.40 |
| 2:B:410:ILE:H | 2:B:410:ILE:HG12 | 1.71 | 0.40 |
| 2:B:560:LEU:N | 2:B:563:GLN:OE1 | 2.55 | 0.40 |
| 4:U:95:TYR:CE2 | 5:V:44:PRO:HD2 | 2.56 | 0.40 |
| 5:S:9:SER:O | 5:S:102:THR:HA | 2.22 | 0.40 |
| 7:M:1:NAG:O4 | 7:M:2:NAG:O7 | 2.39 | 0.40 |
| 1:A:914:ASN:O | 1:A:918:GLU:HG3 | 2.22 | 0.40 |
| 2:B:805:ILE:HD11 | 2:B:931:ILE:HD12 | 2.03 | 0.40 |
| 3:C:368:LEU:N | 3:C:368:LEU:CD1 | 2.83 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|----------|----------|---------|----------|-------------|
| 1   | A     | 988/1016 (97%) | 901 (91%) | 74 (8%) | 13 (1%) | 12 47 |
| 2   | B     | 982/1000 (98%) | 891 (91%) | 80 (8%) | 11 (1%) | 14 50 |
| 3   | C     | 982/1000 (98%) | 893 (91%) | 76 (8%) | 13 (1%) | 12 47 |
| 4   | O     | 116/118 (98%) | 94 (81%) | 22 (19%) | 0 | 100 100 |
| 4   | P     | 116/118 (98%) | 94 (81%) | 22 (19%) | 0 | 100 100 |
| 4   | U     | 116/118 (98%) | 94 (81%) | 22 (19%) | 0 | 100 100 |
| 5   | Q     | 105/107 (98%) | 92 (88%) | 13 (12%) | 0 | 100 100 |
| 5   | S     | 105/107 (98%) | 92 (88%) | 13 (12%) | 0 | 100 100 |
| 5   | V     | 105/107 (98%) | 92 (88%) | 13 (12%) | 0 | 100 100 |

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| Mol | Chain | Analysed   | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|------------|----------|---------|----------|-------------|
| All | All   | 3615/3691 (98%) | 3243 (90%) | 335 (9%) | 37 (1%) | 20 51 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 378 | LYS  |
| 1   | A     | 516 | GLU  |
| 1   | A     | 613 | GLN  |
| 2   | B     | 32  | PHE  |
| 2   | B     | 378 | LYS  |
| 3   | C     | 332 | ILE  |
| 3   | C     | 378 | LYS  |
| 1   | A     | 32  | PHE  |
| 1   | A     | 110 | LEU  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 492 | LEU  |
| 2   | B     | 422 | ASN  |
| 2   | B     | 492 | LEU  |
| 2   | B     | 703 | ASN  |
| 3   | C     | 422 | ASN  |
| 3   | C     | 492 | LEU  |
| 3   | C     | 516 | GLU  |
| 3   | C     | 518 | LEU  |
| 1   | A     | 385 | THR  |
| 1   | A     | 477 | SER  |
| 1   | A     | 491 | PRO  |
| 2   | B     | 385 | THR  |
| 2   | B     | 477 | SER  |
| 2   | B     | 491 | PRO  |
| 3   | C     | 385 | THR  |
| 3   | C     | 477 | SER  |
| 3   | C     | 491 | PRO  |
| 3   | C     | 333 | THR  |
| 1   | A     | 218 | GLN  |
| 2   | B     | 518 | LEU  |
| 3   | C     | 481 | ASN  |
| 1   | A     | 463 | PRO  |
| 2   | B     | 463 | PRO  |
| 3   | C     | 463 | PRO  |
| 2   | B     | 445 | VAL  |
| 1   | A     | 445 | VAL  |
| 3   | C     | 445 | VAL  |
5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|----------|-----------|----------|-------------|
| 1   | A     | 857/880 (97%) | 783 (91%) | 74 (9%)  | 10 39       |
| 2   | B     | 858/877 (98%) | 784 (91%) | 74 (9%)  | 10 39       |
| 3   | C     | 844/875 (96%) | 764 (90%) | 80 (10%) | 8 34        |
| 4   | O     | 97/97 (100%)  | 97 (100%) | 0        | 100 100    |
| 4   | P     | 97/97 (100%)  | 97 (100%) | 0        | 100 100    |
| 4   | U     | 97/97 (100%)  | 97 (100%) | 0        | 100 100    |
| 5   | Q     | 94/94 (100%)  | 94 (100%) | 0        | 100 100    |
| 5   | S     | 94/94 (100%)  | 94 (100%) | 0        | 100 100    |
| 5   | V     | 94/94 (100%)  | 94 (100%) | 0        | 100 100    |
| All | All   | 3132/3205 (98%)| 2904 (93%)| 228 (7%) | 18 44      |

All (228) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 31  | SER  |
| 1   | A     | 33  | THR  |
| 1   | A     | 80  | ASP  |
| 1   | A     | 157 | PHE  |
| 1   | A     | 206 | LYS  |
| 1   | A     | 208 | THR  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 285 | THR  |
| 1   | A     | 331 | ASN  |
| 1   | A     | 332 | ILE  |
| 1   | A     | 333 | THR  |
| 1   | A     | 334 | ASN  |
| 1   | A     | 335 | LEU  |
| 1   | A     | 356 | LYS  |
| 1   | A     | 367 | VAL  |
| 1   | A     | 376 | THR  |
| 1   | A     | 378 | LYS  |
| 1   | A     | 382 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 386 | LYS  |
| 1   | A     | 387 | LEU  |
| 1   | A     | 389 | ASP  |
| 1   | A     | 394 | ASN  |
| 1   | A     | 398 | ASP  |
| 1   | A     | 402 | ILE  |
| 1   | A     | 405 | ASP  |
| 1   | A     | 407 | VAL  |
| 1   | A     | 408 | ARG  |
| 1   | A     | 409 | GLN  |
| 1   | A     | 410 | ILE  |
| 1   | A     | 422 | ASN  |
| 1   | A     | 424 | LYS  |
| 1   | A     | 425 | LEU  |
| 1   | A     | 428 | ASP  |
| 1   | A     | 430 | THR  |
| 1   | A     | 434 | ILE  |
| 1   | A     | 436 | TRP  |
| 1   | A     | 440 | ASN  |
| 1   | A     | 441 | LEU  |
| 1   | A     | 443 | SER  |
| 1   | A     | 444 | LYS  |
| 1   | A     | 450 | ASN  |
| 1   | A     | 452 | LEU  |
| 1   | A     | 454 | ARG  |
| 1   | A     | 455 | LEU  |
| 1   | A     | 456 | PHE  |
| 1   | A     | 458 | LYS  |
| 1   | A     | 459 | SER  |
| 1   | A     | 462 | LYS  |
| 1   | A     | 463 | PRO  |
| 1   | A     | 466 | ARG  |
| 1   | A     | 472 | ILE  |
| 1   | A     | 480 | CYS  |
| 1   | A     | 483 | VAL  |
| 1   | A     | 484 | LYS  |
| 1   | A     | 493 | GLN  |
| 1   | A     | 495 | TYR  |
| 1   | A     | 498 | GLN  |
| 1   | A     | 503 | VAL  |
| 1   | A     | 508 | TYR  |
| 1   | A     | 512 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 516 | GLU  |
| 1   | A     | 517 | LEU  |
| 1   | A     | 518 | LEU  |
| 1   | A     | 599 | THR  |
| 1   | A     | 602 | THR  |
| 1   | A     | 613 | GLN  |
| 1   | A     | 615 | VAL  |
| 1   | A     | 701 | VAL  |
| 1   | A     | 716 | THR  |
| 1   | A     | 738 | CYS  |
| 1   | A     | 747 | THR  |
| 1   | A     | 881 | THR  |
| 1   | A     | 937 | SER  |
| 1   | A     | 967 | SER  |
| 2   | B     | 34  | ARG  |
| 2   | B     | 50  | SER  |
| 2   | B     | 134 | GLN  |
| 2   | B     | 167 | THR  |
| 2   | B     | 205 | SER  |
| 2   | B     | 274 | THR  |
| 2   | B     | 331 | ASN  |
| 2   | B     | 334 | ASN  |
| 2   | B     | 356 | LYS  |
| 2   | B     | 367 | VAL  |
| 2   | B     | 374 | THR  |
| 2   | B     | 376 | THR  |
| 2   | B     | 378 | LYS  |
| 2   | B     | 382 | VAL  |
| 2   | B     | 386 | LYS  |
| 2   | B     | 387 | LEU  |
| 2   | B     | 389 | ASP  |
| 2   | B     | 394 | ASN  |
| 2   | B     | 398 | ASP  |
| 2   | B     | 402 | ILE  |
| 2   | B     | 405 | ASP  |
| 2   | B     | 407 | VAL  |
| 2   | B     | 408 | ARG  |
| 2   | B     | 409 | GLN  |
| 2   | B     | 410 | ILE  |
| 2   | B     | 422 | ASN  |
| 2   | B     | 424 | LYS  |
| 2   | B     | 425 | LEU  |
| 2   | B     | 428 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 430 | THR  |
| 2   | B     | 434 | ILE  |
| 2   | B     | 436 | TRP  |
| 2   | B     | 440 | ASN  |
| 2   | B     | 441 | LEU  |
| 2   | B     | 443 | SER  |
| 2   | B     | 444 | LYS  |
| 2   | B     | 450 | ASN  |
| 2   | B     | 452 | LEU  |
| 2   | B     | 454 | ARG  |
| 2   | B     | 455 | LEU  |
| 2   | B     | 456 | PHE  |
| 2   | B     | 458 | LYS  |
| 2   | B     | 459 | SER  |
| 2   | B     | 462 | LYS  |
| 2   | B     | 463 | PRO  |
| 2   | B     | 466 | ARG  |
| 2   | B     | 472 | ILE  |
| 2   | B     | 480 | CYS  |
| 2   | B     | 483 | VAL  |
| 2   | B     | 484 | LYS  |
| 2   | B     | 493 | GLN  |
| 2   | B     | 495 | TYR  |
| 2   | B     | 498 | GLN  |
| 2   | B     | 503 | VAL  |
| 2   | B     | 508 | TYR  |
| 2   | B     | 512 | VAL  |
| 2   | B     | 517 | LEU  |
| 2   | B     | 518 | LEU  |
| 2   | B     | 531 | THR  |
| 2   | B     | 532 | ASN  |
| 2   | B     | 546 | LEU  |
| 2   | B     | 558 | LYS  |
| 2   | B     | 567 | ARG  |
| 2   | B     | 581 | THR  |
| 2   | B     | 586 | ASP  |
| 2   | B     | 615 | VAL  |
| 2   | B     | 638 | THR  |
| 2   | B     | 701 | VAL  |
| 2   | B     | 703 | ASN  |
| 2   | B     | 738 | CYS  |
| 2   | B     | 938 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 940 | SER  |
| 2   | B     | 983 | ARG  |
| 2   | B     | 1037| SER  |
| 2   | B     | 1097| SER  |
| 3   | C     | 33  | THR  |
| 3   | C     | 63  | THR  |
| 3   | C     | 126 | VAL  |
| 3   | C     | 167 | THR  |
| 3   | C     | 175 | PHE  |
| 3   | C     | 276 | LEU  |
| 3   | C     | 284 | THR  |
| 3   | C     | 334 | ASN  |
| 3   | C     | 335 | LEU  |
| 3   | C     | 356 | LYS  |
| 3   | C     | 367 | VAL  |
| 3   | C     | 376 | THR  |
| 3   | C     | 378 | LYS  |
| 3   | C     | 382 | VAL  |
| 3   | C     | 386 | LYS  |
| 3   | C     | 387 | LEU  |
| 3   | C     | 389 | ASP  |
| 3   | C     | 394 | ASN  |
| 3   | C     | 398 | ASP  |
| 3   | C     | 402 | ILE  |
| 3   | C     | 405 | ASP  |
| 3   | C     | 407 | VAL  |
| 3   | C     | 408 | ARG  |
| 3   | C     | 409 | GLN  |
| 3   | C     | 410 | ILE  |
| 3   | C     | 422 | ASN  |
| 3   | C     | 424 | LYS  |
| 3   | C     | 425 | LEU  |
| 3   | C     | 428 | ASP  |
| 3   | C     | 430 | THR  |
| 3   | C     | 434 | ILE  |
| 3   | C     | 436 | TRP  |
| 3   | C     | 440 | ASN  |
| 3   | C     | 441 | LEU  |
| 3   | C     | 443 | SER  |
| 3   | C     | 444 | LYS  |
| 3   | C     | 450 | ASN  |
| 3   | C     | 452 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 454 | ARG  |
| 3   | C     | 455 | LEU  |
| 3   | C     | 456 | PHE  |
| 3   | C     | 458 | LYS  |
| 3   | C     | 459 | SER  |
| 3   | C     | 462 | LYS  |
| 3   | C     | 463 | PRO  |
| 3   | C     | 466 | ARG  |
| 3   | C     | 472 | ILE  |
| 3   | C     | 480 | CYS  |
| 3   | C     | 483 | VAL  |
| 3   | C     | 484 | LYS  |
| 3   | C     | 493 | GLN  |
| 3   | C     | 495 | TYR  |
| 3   | C     | 498 | GLN  |
| 3   | C     | 503 | VAL  |
| 3   | C     | 508 | TYR  |
| 3   | C     | 512 | VAL  |
| 3   | C     | 514 | SER  |
| 3   | C     | 516 | GLU  |
| 3   | C     | 518 | LEU  |
| 3   | C     | 539 | VAL  |
| 3   | C     | 568 | ASP  |
| 3   | C     | 586 | ASP  |
| 3   | C     | 591 | SER  |
| 3   | C     | 599 | THR  |
| 3   | C     | 615 | VAL  |
| 3   | C     | 701 | VAL  |
| 3   | C     | 704 | SER  |
| 3   | C     | 705 | VAL  |
| 3   | C     | 760 | CYS  |
| 3   | C     | 785 | VAL  |
| 3   | C     | 819 | GLU  |
| 3   | C     | 856 | ASN  |
| 3   | C     | 860 | VAL  |
| 3   | C     | 881 | THR  |
| 3   | C     | 887 | THR  |
| 3   | C     | 904 | TYR  |
| 3   | C     | 974 | SER  |
| 3   | C     | 980 | ILE  |
| 3   | C     | 1077| THR  |
| 3   | C     | 1136| THR  |
Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 218 | GLN  |
| 1   | A     | 239 | GLN  |
| 1   | A     | 280 | ASN  |
| 1   | A     | 474 | GLN  |
| 1   | A     | 532 | ASN  |
| 1   | A     | 563 | GLN  |
| 1   | A     | 580 | GLN  |
| 1   | A     | 613 | GLN  |
| 1   | A     | 751 | ASN  |
| 1   | A     | 914 | ASN  |
| 1   | A     | 1071| GLN  |
| 1   | A     | 1101| HIS  |
| 1   | A     | 1135| ASN  |
| 2   | B     | 52  | GLN  |
| 2   | B     | 137 | ASN  |
| 2   | B     | 207 | HIS  |
| 2   | B     | 334 | ASN  |
| 2   | B     | 474 | GLN  |
| 2   | B     | 655 | HIS  |
| 2   | B     | 762 | GLN  |
| 2   | B     | 784 | GLN  |
| 2   | B     | 804 | GLN  |
| 2   | B     | 935 | GLN  |
| 2   | B     | 1005| GLN  |
| 2   | B     | 1101| HIS  |
| 3   | C     | 61  | ASN  |
| 3   | C     | 134 | GLN  |
| 3   | C     | 280 | ASN  |
| 3   | C     | 394 | ASN  |
| 3   | C     | 474 | GLN  |
| 3   | C     | 935 | GLN  |
| 3   | C     | 1005| GLN  |
| 3   | C     | 1135| ASN  |
| 4   | U     | 82  | GLN  |
| 5   | V     | 34  | HIS  |
| 5   | V     | 89  | GLN  |
| 4   | O     | 82  | GLN  |
| 5   | Q     | 89  | GLN  |
| 4   | P     | 82  | GLN  |
| 5   | S     | 34  | HIS  |
| 5   | S     | 89  | GLN  |
5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

29 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | Bond angles |
|-----|------|-------|-----|------|--------------|-------------|
|     |      |       |     |      | Counts | RMSZ | $|Z| > 2$ | Counts | RMSZ | $|Z| > 2$ |
| 6   | NAG  | D     | 1   | 6,1  | 14,1,15 | 0.73 | 1 (7%) | 17,19,21 | 2.54 | 6 (35%) |
| 6   | NAG  | D     | 2   | 6    | 14,1,15 | 0.52 | 0 | 17,19,21 | 1.14 | 2 (11%) |
| 6   | BMA  | D     | 3   | 6    | 11,1,12 | 0.44 | 0 | 15,15,17 | 0.49 | 0 |
| 6   | NAG  | E     | 1   | 6,2  | 14,1,15 | 0.74 | 1 (7%) | 17,19,21 | 2.54 | 6 (35%) |
| 6   | NAG  | E     | 2   | 6    | 14,1,15 | 0.49 | 0 | 17,19,21 | 1.12 | 2 (11%) |
| 6   | BMA  | E     | 3   | 6    | 11,1,12 | 0.44 | 0 | 15,15,17 | 0.49 | 0 |
| 6   | NAG  | F     | 1   | 3,6  | 14,1,15 | 0.74 | 1 (7%) | 17,19,21 | 2.53 | 6 (35%) |
| 6   | NAG  | F     | 2   | 6    | 14,1,15 | 0.50 | 0 | 17,19,21 | 1.12 | 2 (11%) |
| 6   | BMA  | F     | 3   | 6    | 11,1,12 | 0.43 | 0 | 15,15,17 | 0.48 | 0 |
| 7   | NAG  | G     | 1   | 7    | 14,1,15 | 0.75 | 1 (7%) | 17,19,21 | 0.61 | 0 |
| 7   | NAG  | G     | 2   | 7    | 14,1,15 | 0.42 | 0 | 17,19,21 | 1.23 | 1 (5%) |
| 7   | NAG  | H     | 1   | 7,1  | 14,1,15 | 0.38 | 0 | 17,19,21 | 0.53 | 0 |
| 7   | NAG  | H     | 2   | 7    | 14,1,15 | 0.33 | 0 | 17,19,21 | 0.38 | 0 |
| 7   | NAG  | I     | 1   | 7,1  | 14,1,15 | 0.28 | 0 | 17,19,21 | 0.62 | 1 (5%) |
| 7   | NAG  | I     | 2   | 7    | 14,1,15 | 0.29 | 0 | 17,19,21 | 0.37 | 0 |
| 7   | NAG  | J     | 1   | 7,1  | 14,1,15 | 1.03 | 1 (7%) | 17,19,21 | 0.92 | 1 (5%) |
| 7   | NAG  | J     | 2   | 7    | 14,1,15 | 0.26 | 0 | 17,19,21 | 0.41 | 0 |
| 7   | NAG  | K     | 1   | 7,1  | 14,1,15 | 0.38 | 0 | 17,19,21 | 1.27 | 2 (11%) |
| 7   | NAG  | K     | 2   | 7    | 14,1,15 | 0.40 | 0 | 17,19,21 | 1.27 | 1 (5%) |
| 7   | NAG  | L     | 1   | 7,2  | 14,1,15 | 0.49 | 0 | 17,19,21 | 0.44 | 0 |
In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 6   | NAG  | D     | 1   | 6,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | D     | 2   | 6    | -       | 6/6/23/26 | 0/1/1/1 |
| 6   | BMA  | D     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | E     | 1   | 6,2  | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | E     | 2   | 6    | -       | 6/6/23/26 | 0/1/1/1 |
| 6   | BMA  | E     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | F     | 1   | 3,6  | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | F     | 2   | 6    | -       | 6/6/23/26 | 0/1/1/1 |
| 6   | BMA  | F     | 3   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | G     | 1   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | G     | 2   | 7    | -       | 5/6/23/26 | 0/1/1/1 |
| 7   | NAG  | H     | 1   | 7,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | H     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | I     | 1   | 7,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | I     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | J     | 1   | 7,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 7   | NAG  | J     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 1   | 7,1  | -       | 4/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 2   | 7    | -       | 5/6/23/26 | 0/1/1/1 |
| 7   | NAG  | L     | 1   | 7,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | L     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 1   | 7,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 2   | 7    | -       | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 7   | NAG  | N     | 1   | 3,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | N     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | R     | 1   | 3,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | R     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | T     | 1   | 3,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | T     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z   | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 7   | J     | 1   | NAG  | O5-C1 | -3.68 | 1.37        | 1.43     |
| 7   | M     | 1   | NAG  | O5-C1 | -2.71 | 1.39        | 1.43     |
| 7   | R     | 1   | NAG  | O5-C1 | -2.68 | 1.39        | 1.43     |
| 7   | G     | 1   | NAG  | O5-C1 | -2.62 | 1.39        | 1.43     |
| 6   | E     | 1   | NAG  | O5-C1 | -2.28 | 1.40        | 1.43     |
| 6   | F     | 1   | NAG  | O5-C1 | -2.28 | 1.40        | 1.43     |
| 6   | D     | 1   | NAG  | O5-C1 | -2.23 | 1.40        | 1.43     |
| 7   | M     | 2   | NAG  | O5-C1 | -2.04 | 1.40        | 1.43     |

All (31) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z   | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 6   | D     | 1   | NAG  | C1-O5-C5 | -7.33 | 102.27     | 112.19   |
| 6   | E     | 1   | NAG  | C1-O5-C5 | -7.31 | 102.28     | 112.19   |
| 6   | F     | 1   | NAG  | C1-O5-C5 | -7.30 | 102.30     | 112.19   |
| 7   | K     | 2   | NAG  | C2-N2-C7 | 4.33  | 129.06     | 122.90   |
| 7   | K     | 1   | NAG  | C2-N2-C7 | 4.32  | 129.06     | 122.90   |
| 7   | G     | 2   | NAG  | C2-N2-C7 | 4.23  | 128.93     | 122.90   |
| 6   | E     | 1   | NAG  | C6-C5-C4 | 3.30  | 120.73     | 113.00   |
| 6   | F     | 1   | NAG  | C6-C5-C4 | 3.29  | 120.71     | 113.00   |
| 6   | D     | 1   | NAG  | C6-C5-C4 | 3.29  | 120.70     | 113.00   |
| 6   | D     | 2   | NAG  | O5-C5-C4 | -3.27 | 102.86     | 110.83   |
| 6   | F     | 1   | NAG  | O5-C5-C4 | -3.27 | 102.87     | 110.83   |
| 6   | E     | 1   | NAG  | O5-C5-C4 | -3.26 | 102.89     | 110.83   |
| 6   | D     | 2   | NAG  | C1-O5-C5 | 3.06  | 116.34     | 112.19   |
| 6   | D     | 1   | NAG  | C4-C3-C2 | 3.03  | 115.47     | 111.02   |
| 6   | E     | 1   | NAG  | C4-C3-C2 | 3.03  | 115.45     | 111.02   |
| 6   | F     | 1   | NAG  | C4-C3-C2 | 3.02  | 115.44     | 111.02   |
| 6   | F     | 2   | NAG  | C1-O5-C5 | 3.01  | 116.27     | 112.19   |
| 6   | E     | 2   | NAG  | C1-O5-C5 | 2.99  | 116.24     | 112.19   |
| 6   | E     | 1   | NAG  | C2-N2-C7 | 2.72  | 126.77     | 122.90   |

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| Mol | Chain | Res | Type | Atoms     | Z  | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|----|-------------|----------|
| 6   | D     | 1   | NAG  | C2-N2-C7  | 2.69 | 126.73      | 122.90   |
| 6   | F     | 1   | NAG  | C2-N2-C7  | 2.68 | 126.72      | 122.90   |
| 7   | J     | 2   | NAG  | C3-C4-C5  | 2.26 | 114.28      | 110.24   |
| 6   | D     | 2   | NAG  | C3-C4-C5  | 2.24 | 114.23      | 110.24   |
| 6   | E     | 1   | NAG  | O4-C4-C5  | 2.23 | 114.85      | 109.30   |
| 6   | F     | 1   | NAG  | O4-C4-C5  | 2.23 | 114.83      | 109.30   |
| 6   | D     | 1   | NAG  | O4-C4-C5  | 2.23 | 114.83      | 109.30   |
| 6   | E     | 2   | NAG  | C3-C4-C5  | 2.20 | 114.17      | 110.24   |
| 6   | F     | 2   | NAG  | C3-C4-C5  | 2.20 | 114.17      | 110.24   |
| 7   | I     | 1   | NAG  | C1-O5-C5  | 2.12 | 115.07      | 112.19   |
| 7   | K     | 1   | NAG  | C1-C2-N2  | 2.06 | 114.00      | 110.49   |
| 7   | M     | 1   | NAG  | C1-O5-C5  | 2.02 | 114.92      | 112.19   |

There are no chirality outliers.

All (65) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms     |
|-----|-------|-----|------|-----------|
| 6   | D     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | D     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | D     | 2   | NAG  | C8-C7-N2-C2 |
| 6   | E     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | E     | 2   | NAG  | C8-C7-N2-C2 |
| 6   | F     | 1   | NAG  | C8-C7-N2-C2 |
| 6   | F     | 2   | NAG  | C8-C7-N2-C2 |
| 6   | F     | 2   | NAG  | C8-C7-N2-C2 |
| 7   | M     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | M     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | J     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | J     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | J     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | J     | 2   | NAG  | C4-C5-C6-O6 |
| 7   | T     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms            |
|-----|-------|-----|------|------------------|
| 7   | G     | 2   | NAG  | C8-C7-N2-C2     |
| 7   | G     | 2   | NAG  | O7-C7-N2-C2     |
| 7   | K     | 1   | NAG  | C8-C7-N2-C2     |
| 7   | K     | 2   | NAG  | O7-C7-N2-C2     |
| 7   | K     | 2   | NAG  | C4-C5-C6-O6     |
| 7   | R     | 1   | NAG  | C4-C5-C6-O6     |
| 6   | E     | 2   | NAG  | O5-C5-C6-O6     |
| 6   | E     | 2   | NAG  | O1-C2-N2-C7     |
| 7   | N     | 2   | NAG  | O5-C5-C6-O6     |
| 7   | N     | 2   | NAG  | C4-C5-C6-O6     |
| 6   | D     | 2   | NAG  | O5-C5-C6-O6     |
| 7   | D     | 2   | NAG  | O5-C5-C6-O6     |
| 6   | E     | 2   | NAG  | C1-C2-N2-C7     |
| 6   | F     | 2   | NAG  | C1-C2-N2-C7     |
| 7   | T     | 2   | NAG  | O5-C5-C6-O6     |
| 7   | H     | 2   | NAG  | O5-C5-C6-O6     |
| 7   | G     | 2   | NAG  | C4-C5-C6-O6     |
| 6   | D     | 2   | NAG  | C3-C2-N2-C7     |
| 6   | E     | 1   | NAG  | C3-C2-N2-C7     |
| 6   | F     | 1   | NAG  | C3-C2-N2-C7     |
| 7   | N     | 1   | NAG  | C4-C5-C6-O6     |
| 7   | J     | 1   | NAG  | C1-C2-N2-C7     |
| 7   | R     | 2   | NAG  | C4-C5-C6-O6     |
| 7   | N     | 1   | NAG  | O5-C5-C6-O6     |
| 6   | D     | 2   | NAG  | C3-C2-N2-C7     |
| 6   | E     | 2   | NAG  | C3-C2-N2-C7     |
| 6   | F     | 2   | NAG  | C3-C2-N2-C7     |
| 7   | M     | 2   | NAG  | C3-C2-N2-C7     |
| 6   | D     | 2   | NAG  | C4-C5-C6-O6     |
| 6   | E     | 2   | NAG  | C4-C5-C6-O6     |
| 6   | F     | 2   | NAG  | C4-C5-C6-O6     |
| 7   | L     | 1   | NAG  | C1-C2-N2-C7     |
| 7   | R     | 2   | NAG  | O5-C5-C6-O6     |
| 7   | K     | 1   | NAG  | C4-C5-C6-O6     |
| 7   | G     | 2   | NAG  | C3-C2-N2-C7     |
| 7   | K     | 1   | NAG  | C3-C2-N2-C7     |
| 7   | K     | 2   | NAG  | C3-C2-N2-C7     |
| 7   | I     | 2   | NAG  | C4-C5-C6-O6     |

There are no ring outliers.
13 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | F     | 2   | NAG  | 1       | 0            |
| 6   | D     | 1   | NAG  | 1       | 0            |
| 6   | E     | 2   | NAG  | 1       | 0            |
| 6   | D     | 2   | NAG  | 1       | 0            |
| 7   | L     | 1   | NAG  | 1       | 0            |
| 7   | M     | 1   | NAG  | 1       | 0            |
| 6   | E     | 1   | NAG  | 1       | 0            |
| 7   | M     | 2   | NAG  | 2       | 0            |
| 7   | K     | 2   | NAG  | 1       | 0            |
| 6   | F     | 1   | NAG  | 1       | 0            |
| 7   | L     | 2   | NAG  | 1       | 0            |
| 7   | K     | 1   | NAG  | 1       | 0            |
| 7   | G     | 2   | NAG  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.
Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings
Oligosaccharide Chain J

- Bond lengths
- Bond angles
- Torsions
- Rings
Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings
Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings
Oligosaccharide Chain N

Bond lengths

Bond angles

Torsions

Rings
### 5.6 Ligand geometry

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | Bond angles |
|-----|------|-------|-----|------|--------------|-------------|
|     |      |       |     |      | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 8   | NAG  | A     | 1304| 1    | 14,14,15 | 0.34 | 0     | 17,19,21 | 0.57 | 0     |
| 8   | NAG  | B     | 1302| 2    | 14,14,15 | 0.27 | 0     | 17,19,21 | 0.54 | 0     |
| 8   | NAG  | B     | 1303| 2    | 14,14,15 | 0.19 | 0     | 17,19,21 | 0.51 | 0     |
| 8   | NAG  | C     | 1308| 3    | 14,14,15 | 0.26 | 0     | 17,19,21 | 0.43 | 0     |
### Bond lengths

| Mol | Type | Chain | Res | Link | Bond lengths | Bond angles |
|-----|------|-------|-----|------|--------------|-------------|
|     |      |       |     |      | Counts | RMSZ | #|Z| > 2 | Counts | RMSZ | #|Z| > 2 |
| 8   | NAG  | C     | 1306| 3    | 14,14,15 | 0.18 | 0 | 17,19,21 | 0.47 | 0 |
| 8   | NAG  | B     | 1307| 2    | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.42 | 0 |
| 8   | NAG  | B     | 1304| 2    | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.54 | 0 |
| 8   | NAG  | C     | 1307| 3    | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.38 | 0 |
| 8   | NAG  | C     | 1302| 3    | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.45 | 0 |
| 8   | NAG  | C     | 1304| 3    | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.43 | 0 |
| 8   | NAG  | C     | 1305| 3    | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.42 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

### Chirals

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | NAG  | A     | 1304| 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 1302| 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 1303| 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 1308| 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 1306| 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 1307| 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 1304| 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 1307| 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 1302| 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 1304| 3    | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 8   | NAG  | B     | 1309| 2    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1305| 1    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1310| 2    | -       | 1/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1302| 1    | -       | 3/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1306| 2    | -       | 3/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1312| 2    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | C     | 1309| 3    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1307| 1    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | C     | 1301| 3    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1306| 1    | -       | 3/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1303| 1    | -       | 4/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1308| 2    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | A     | 1301| 1    | -       | 3/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1311| 2    | -       | 2/6/23/26| 0/1/1/1|
| 8   | NAG  | B     | 1301| 2    | -       | 4/6/23/26| 0/1/1/1|

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z   | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-----|-------------|----------|
| 8   | A     | 1306| NAG  | C2-N2-C7    | 4.31| 129.04      | 122.90   |
| 8   | B     | 1312| NAG  | C1-O5-C5    | 2.58| 115.69      | 112.19   |
| 8   | B     | 1310| NAG  | C1-O5-C5    | 2.39| 115.43      | 112.19   |

There are no chirality outliers.

All (61) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | B     | 1304| NAG  | C4-C5-C6-O6 |
| 8   | C     | 1301| NAG  | C4-C5-C6-O6 |
| 8   | C     | 1306| NAG  | C4-C5-C6-O6 |
| 8   | A     | 1301| NAG  | O5-C5-C6-O6 |
| 8   | A     | 1303| NAG  | O5-C5-C6-O6 |
| 8   | A     | 1305| NAG  | O5-C5-C6-O6 |
| 8   | C     | 1306| NAG  | O5-C5-C6-O6 |
| 8   | B     | 1304| NAG  | O5-C5-C6-O6 |
| 8   | C     | 1301| NAG  | O5-C5-C6-O6 |
| 8   | A     | 1307| NAG  | C4-C5-C6-O6 |

Continued on next page...
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 8   | B     | 1302| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1306| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1312| NAG  | O5-C5-C6-O6    |
| 8   | A     | 1304| NAG  | O5-C5-C6-O6    |
| 8   | A     | 1301| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1301| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1303| NAG  | O5-C5-C6-O6    |
| 8   | C     | 1309| NAG  | O5-C5-C6-O6    |
| 8   | A     | 1304| NAG  | C4-C5-C6-O6    |
| 8   | A     | 1302| NAG  | C4-C5-C6-O6    |
| 8   | A     | 1307| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1311| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1301| NAG  | C4-C5-C6-O6    |
| 8   | C     | 1309| NAG  | C4-C5-C6-O6    |
| 8   | A     | 1303| NAG  | C4-C5-C6-O6    |
| 8   | A     | 1305| NAG  | C4-C5-C6-O6    |
| 8   | C     | 1307| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1303| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1306| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1312| NAG  | C4-C5-C6-O6    |
| 8   | A     | 1303| NAG  | C8-C7-N2-C2    |
| 8   | A     | 1303| NAG  | O7-C7-N2-C2    |
| 8   | A     | 1304| NAG  | C8-C7-N2-C2    |
| 8   | A     | 1304| NAG  | O7-C7-N2-C2    |
| 8   | A     | 1306| NAG  | C8-C7-N2-C2    |
| 8   | A     | 1306| NAG  | O7-C7-N2-C2    |
| 8   | B     | 1301| NAG  | C8-C7-N2-C2    |
| 8   | B     | 1301| NAG  | O7-C7-N2-C2    |
| 8   | B     | 1303| NAG  | C8-C7-N2-C2    |
| 8   | B     | 1303| NAG  | O7-C7-N2-C2    |
| 8   | C     | 1302| NAG  | C8-C7-N2-C2    |
| 8   | C     | 1302| NAG  | O7-C7-N2-C2    |
| 8   | B     | 1302| NAG  | O5-C5-C6-O6    |
| 8   | C     | 1307| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1309| NAG  | O5-C5-C6-O6    |
| 8   | A     | 1302| NAG  | O5-C5-C6-O6    |
| 8   | C     | 1302| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1311| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1310| NAG  | O5-C5-C6-O6    |
| 8   | C     | 1302| NAG  | O5-C5-C6-O6    |
| 8   | B     | 1308| NAG  | C4-C5-C6-O6    |
| 8   | B     | 1304| NAG  | C1-C2-N2-C7    |

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| Mol | Chain | Res | Type   | Atoms          |
|-----|-------|-----|--------|----------------|
| 8   | B     | 1308| NAG    | O5-C5-C6-O6    |
| 8   | B     | 1309| NAG    | C4-C5-C6-O6    |
| 8   | A     | 1302| NAG    | C3-C2-N2-C7    |
| 8   | B     | 1302| NAG    | C3-C2-N2-C7    |
| 8   | B     | 1306| NAG    | C3-C2-N2-C7    |
| 8   | C     | 1304| NAG    | C4-C5-C6-O6    |
| 8   | A     | 1301| NAG    | C1-C2-N2-C7    |
| 8   | C     | 1304| NAG    | O5-C5-C6-O6    |
| 8   | A     | 1306| NAG    | C3-C2-N2-C7    |

There are no ring outliers.

4 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type   | Clashes | Symm-Clashes |
|-----|-------|-----|--------|---------|--------------|
| 8   | A     | 1302| NAG    | 2       | 0            |
| 8   | C     | 1301| NAG    | 2       | 0            |
| 8   | A     | 1306| NAG    | 1       | 0            |
| 8   | B     | 1301| NAG    | 1       | 0            |

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | C     | 8                |
| 1   | A     | 8                |
| 2   | B     | 8                |

All chain breaks are listed below:

| Model | Chain | Residue-1  | Atom-1 | Residue-2  | Atom-2 | Distance (Å) |
|-------|-------|------------|--------|------------|--------|--------------|
| 1     | C     | 241:LEU    | C      | 261:GLY    | N      | 14.44        |
| 1     | A     | 241:LEU    | C      | 261:GLY    | N      | 13.72        |
| 1     | C     | 620:VAL    | C      | 641:ASN    | N      | 12.86        |
| 1     | A     | 620:VAL    | C      | 640:SER    | N      | 12.55        |
| 1     | C     | 176:LEU    | C      | 187:LYS    | N      | 12.05        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 176:LEU   | C      | 187:LYS   | N      | 11.99        |
| 1     | B     | 176:LEU   | C      | 187:LYS   | N      | 11.91        |
| 1     | A     | 828:LEU   | C      | 853:GLN   | N      | 11.67        |
| 1     | C     | 828:LEU   | C      | 853:GLN   | N      | 10.51        |
| 1     | B     | 620:VAL   | C      | 638:THR   | N      | 9.78         |
| 1     | B     | 241:LEU   | C      | 263:ALA   | N      | 9.47         |
| 1     | B     | 209:PRO   | C      | 217:PRO   | N      | 9.42         |
| 1     | B     | 828:LEU   | C      | 853:GLN   | N      | 9.11         |
| 1     | C     | 95:THR    | C      | 99:ASN    | N      | 8.82         |
| 1     | A     | 95:THR    | C      | 99:ASN    | N      | 7.64         |
| 1     | B     | 66:HIS    | C      | 81:ASN    | N      | 7.50         |
| 1     | A     | 142:GLY   | C      | 156:GLU   | N      | 7.26         |
| 1     | C     | 66:HIS    | C      | 81:ASN    | N      | 6.61         |
| 1     | C     | 140:PHE   | C      | 157:PHE   | N      | 6.54         |
| 1     | A     | 66:HIS    | C      | 79:PHE    | N      | 6.04         |
| 1     | B     | 672:ALA   | C      | 687:VAL   | N      | 5.40         |
| 1     | A     | 672:ALA   | C      | 687:VAL   | N      | 5.33         |
| 1     | C     | 672:ALA   | C      | 687:VAL   | N      | 5.14         |
| 1     | B     | 141:LEU   | C      | 155:SER   | N      | 4.86         |
6 Map visualisation

This section contains visualisations of the EMDB entry D_1300026375. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

The images above show the map projected in three orthogonal directions.
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map

The images above show the 3D surface view of the map at the recommended contour level 0.177. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.
7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.
7.2 Volume estimate

The volume at the recommended contour level is 285 \text{ nm}^3; this corresponds to an approximate mass of 257 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.
7.3 Rotationally averaged power spectrum

*Reported resolution corresponds to spatial frequency of 0.270 Å\(^{-1}\)
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.
9  Map-model fit

This section contains information regarding the fit between EMDB map D_1300026375 and PDB model D_1300026375. Per-residue inclusion information can be found in section 3 on page 8.

9.1  Map-model overlay

The images above show the 3D surface view of the map at the recommended contour level 0.177 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.
9.2 Atom inclusion

At the recommended contour level, 73% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.