

**Tetra-\textit{n}\textendash butylammonium orotate hydrate: knowledge-based comparison of the results of accurate and lower-resolution analyses and a non-routine disorder refinement**

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**SUPPORTING INFORMATION**

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III. Results of Mogul geometry check for (\textsuperscript{\textit{n}}Bu\textsubscript{4}N)(Horot)-H\textsubscript{2}O at T = 295 K, 2 (internal code est4l).
Refinement of the disordered terminal ethyl fragment in the \(\text{Bu}_4\text{N}^+\) cation at \(T = 295\) K, 2.

For the structure of \((\text{Bu}_4\text{N})(\text{Horot})\cdot\text{H}_2\text{O}\) at \(T = 100\) K, 1, the cation presents a simple two-way disorder of the terminal methyl group at C14, Fig. S1. This type of disorder is common and is handled routinely by refining the populations of the two disorder groups such that they sum to 1.0. The two disordered congeners of C14 were observed in a difference map. The H atoms of the neighboring CH\(_2\) group at C13 were placed at calculated positions such that one pair of H atoms corresponds to the geometry required by the principal component of the disordered methyl group (pink in Fig. S1), and the other corresponds to the minor component (C14B, light blue in Fig. S1). The populations of the two pairs of CH\(_2\) H atoms were tied to those of their respective methyl-group neighbors. The refined value of the population of the major component, C14A, was 0.698 (4).

It can be seen that the displacement ellipsoids in the C11 - C14 chain become more prolate -- more extended in a transverse direction -- toward the periphery of the chain. It is possible to split C13 into two components, but the resulting geometry is no more favorable than that involving the mean position used in our refinement. Another feature of the result is relatively common, if unwelcome -- the apparent bond distances C13---C14A, 1.408 (3) Å, and C13---C14B, 1.191 (5) Å, are shorter than expected, with both affected in the well-known way by both libration and the disorder.

At \(T = 295\) K, the disorder is further developed, with C13 now sufficiently disordered to be represented naturally by two atomic sites -- observed sites, not calculated by splitting an atom. The more challenging aspect of the disorder at this temperature, however, arises with C14, which is now split into three atomic sites. Fig. S2 is a composite image of the entire disorder assembly. Here again, all non-hydrogen atomic sites were observed in a difference map.

The first task to be undertaken in such a case is to factor the overall set of atomic sites (the "disorder assembly" as per the Core CIF Dictionary) into chemically sound fragments ("disorder groups" in the Core CIF Dictionary) which populate this region of the structure but which are not simultaneously present in a given asymmetric unit. In this case, it was possible to identify four credible disorder groups:
1) C11/C12/C13A/C14A (pink in Fig. S3);
2) C11/C12/C13B/C14B (light blue in Fig. S3);
3) C11/C12/C13A/C14C (pink in Fig. S4);
4) C11/C12/C13B/C14C (light blue in Fig. S4).
The atoms of just one disorder group simultaneously populate a given asymmetric unit.

The same two principal factors must be addressed in a case such as this, as in a simpler case such as in the structure of 1: a) Populations must be assigned to all of the atomic sites in such a way that the overall stoichiometry is correct for the known chemical fragment that comprises the disorder assembly and is correct also for each of the individual disorder groups. b) Those hydrogen atoms whose positions can be calculated reliably on the basis of the locations of the heavier atoms, should be thus placed. In the
present case this is complicated by the fact that the two congeners of C13 are bonded not only to methyl groups that can be identified individually with each of them -- namely C14A bonded to C13A and C14B to C13B -- but both are also bonded to a third methyl site common to both of them, namely C14C.

Our approach to the first item -- assigning populations to the disordered atomic sites, relied in the first instance on constrained refinement of populations. For example, the occupancies of C13A and C13B must sum to 1.0, as must the occupancies of C14A, C14B and C14C. We carried out a refinement dividing the atoms involved into the four groups defined above, refining their populations but with a strong restraint to a total population of 1.0. The final assignment of site occupancies was based on the result of this refinement; the only arbitrary assignment involved the common methyl group C14C, whose occupancy was divided equally between the two groups to which it belongs. The final occupancies of the four groups defined above are 1) 0.35; 2) 0.25; 3) 0.20; 4) 0.20. Atomic site occupancy factors were set on this basis, keeping in mind that some of the atoms belong to more than one disorder group. So for example, the occupancy of C13A was fixed at 0.55, the total for the two disorder groups, 1) and 3) above, to which it belongs.

As for the calculation of H-atom positions, it is necessary to invoke some program-specific terminology in order to describe how this was done. The refinement was conducted with ShelXL2018/1 (Sheldrick, 2015), which has a facility for assigning atoms to different "parts" whose geometries are calculated independently of each other. In a case of simple disorder such as that found for the structure at T = 100 K, 1, a simple division of the disordered methyl groups and the correspondingly affected H atoms bonded to C13 into "PART 1" and "PART 2" permits the calculation of the H-atom positions, for which C13 must initially be bonded to exactly two other atoms. So when the positions of the pink H atoms are being calculated, Fig. S3, the program only considers C13 to be bonded to C12 and C14A.

For the more complex disorder at T = 295 K, 2, the situation is more involved. One can assign C13A to "PART 1" and C13B to "PART 2" (Fig. S3, pink and blue, respectively); but C14C is also bonded to C13A and C13B, so each of them has bonds to three neighbors rather than the two required to permit the calculation of positions for two methylene H atoms on each of C13A and C13B.

A simple construct permits the calculation of all of the affected H atoms in the disorder assembly. There are five carbon atom sites, methylene C13A and C13B and methyl C14A, C14B and C14C. These were all assigned to different part numbers, namely C13A to PART 1, C13B to PART 2, C14A to PART 4, C14B to PART 5 and C14C to PART 3. In this way it is possible to exert individual control over which C---C bonds are considered relevant when generating H-atom positions, by using the instruction "BIND m n" which permits atoms from PART m to be considered bonded to atoms from PART n. The details can be found by examining the embedded instruction file within the CIF. As an example, C13A, in PART 1, needs two H atoms whose geometry is consistent with the presence of a methyl group at C14A (pink in Fig. S3). An AFIX instruction can be inserted with the two H atoms belonging to PART 4, with a "BIND 1 4" instruction having been included earlier in the input. The other atoms bonded to C13A do not interfere with the generation
of the two H atoms. Similarly, C13A needs two adjoined H atoms consistent with the presence of a methyl group at C14C. With a "BIND 1 3" instruction having been introduced earlier, C13A can be followed by an additional "AFIX 23" instruction with the two H atoms included in PART 3 (pink in Fig. S4).

Other approaches to modelling this disorder assembly will also work. The conceptually simple model described here was intended to model the average electron density in this region of the structure while still employing an atomic model. If it had become more complex, then other solutions, possibly including a non-atomic model (i.e., Squeeze; Spek, 2015) could have been considered. In the actual event, while the overall geometrical results are typical of refinements of n-butyl groups, all of the C—C bond distances involving methyl groups are observed with the foreshortened distances [in the range 1.321 (12) - 1.425 (15) Å] commonly associated with disorder and/or libration. These "apparent" distances (a term that is invoked for disorder and especially for dynamic processes, Stebler & Bürgi, 1987) cannot be used as representative distances for C—C single bonds.

REFERENCES

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FIGURE CAPTIONS

Figure S1. "Bu4N⁺ cation from the structure of (Bu4N)(Horot)·H2O at T = 100 K, 1. The disorder component shown in pink has a fractional population of 0.698 (4). Non-hydrogen atoms are represented by their 50% probability ellipsoids.

Figure S2. Composite image of the "Bu4N⁺ cation from the structure of (Bu4N)(Horot)·H2O at T = 295 K, 2, showing the positions of all of the atoms in the disorder assembly at the distal end of the C11 - C14 n-butyl group. Non-hydrogen atoms are represented by their 50% probability ellipsoids.
**Figure S3.** Composite image of the disorder assembly at C12/C13/C14 in the structure of ("Bu₄N)(Horot)-H₂O at T = 295 K, 2. Two of the disorder groups are identified by color, namely C12/C13A/C14A in pink and C12/C13B/C14B in light blue. Other than C12, which is represented by its 50% ellipsoid, the C atoms are shown as circles of arbitrary radius. H atoms are represented by smaller circles. Atoms and bonds not belonging to the fragments represented in pink and light blue, are shown in gray.

**Figure S4.** Composite image of the disorder assembly at C12/C13/C14 in the structure of ("Bu₄N)(Horot)-H₂O at T = 295 K, 2, now with the remaining two disorder groups identified by color. C12/C13A/C14C is drawn mostly in pink (C12 in gray), and C12/C13BC14C mostly in light blue. C14C belongs to both disorder groups and is drawn in pink with blue divisions.
FIGURES

Figure S1.

Figure S2.
| Type    | Molecule | Fragment | Classification                  | No. of hits | Query value | Mean | Std. dev. | z-score | x - mean | Minimum | Maximum | Median | d(min) | Local density |
|---------|----------|----------|---------------------------------|-------------|-------------|------|-----------|---------|----------|---------|---------|-------|---------|----------------|
| bond    | iai12p-l₁₁ | C2 N1    | Not unusual (enough hits)       | 1428        | 1.374       | 1.371| 0.012     | 0.326   | 0.004   | 1.299   | 1.452   | 1.370 | 0.000 | --        |
| bond    | iai12p-l₁₁ | C6 N1    | Not unusual (enough hits)       | 18          | 1.369       | 1.359| 0.011     | 0.897   | 0.010   | 1.342   | 1.383   | 1.356 | 0.001 | --        |
| bond    | iai12p-l₁₁ | O2 C2    | Not unusual (enough hits)       | 2995        | 1.222       | 1.228| 0.015     | 0.374   | 0.006   | 1.166   | 1.520   | 1.227 | 0.000 | --        |
| bond    | iai12p-l₁₁ | C2 N3    | Not unusual (enough hits)       | 1428        | 1.375       | 1.371| 0.012     | 0.387   | 0.005   | 1.299   | 1.452   | 1.370 | 0.000 | --        |
| bond    | iai12p-l₁₁ | C4 N3    | Not unusual (enough hits)       | 708         | 1.385       | 1.381| 0.013     | 0.324   | 0.004   | 1.256   | 1.419   | 1.380 | 0.000 | --        |
| bond    | iai12p-l₁₁ | O4 C4    | Not unusual (enough hits)       | 1300        | 1.227       | 1.241| 0.016     | 0.894   | 0.014   | 1.196   | 1.355   | 1.240 | 0.000 | --        |
| bond    | iai12p-l₁₁ | C5 C4    | Not unusual (enough hits)       | 491         | 1.448       | 1.423| 0.019     | 1.346   | 0.025   | 1.352   | 1.464   | 1.426 | 0.000 | --        |
| bond    | iai12p-l₁₁ | C5 C6    | Not unusual (enough hits)       | 24          | 1.345       | 1.360| 0.011     | 1.411   | 0.015   | 1.339   | 1.375   | 1.363 | 0.002 | --        |
| bond    | iai12p-l₁₁ | C7 C6    | Not unusual (enough hits)       | 16          | 1.530       | 1.481| 0.025     | 1.985   | 0.049   | 1.438   | 1.542   | 1.483 | 0.012 | --        |
| bond    | iai12p-l₁₁ | O7 C7    | Not unusual (enough hits)       | 32          | 1.250       | 1.254| 0.006     | 0.734   | 0.005   | 1.242   | 1.275   | 1.253 | 0.001 | --        |
| bond    | iai12p-l₁₁ | O8 C7    | Not unusual (enough hits)       | 32          | 1.244       | 1.254| 0.006     | 1.620   | 0.010   | 1.242   | 1.275   | 1.253 | 0.002 | --        |
| bond    | iai12p-l₁₂ | C11 N10  | Not unusual (enough hits)       | 4078        | 1.516       | 1.521| 0.024     | 0.234   | 0.006   | 1.246   | 1.915   | 1.521 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C15 N10  | Not unusual (enough hits)       | 4078        | 1.524       | 1.521| 0.024     | 0.118   | 0.003   | 1.246   | 1.915   | 1.521 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C19 N10  | Not unusual (enough hits)       | 4078        | 1.525       | 1.521| 0.024     | 0.164   | 0.004   | 1.246   | 1.915   | 1.521 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C23 N10  | Not unusual (enough hits)       | 4078        | 1.524       | 1.521| 0.024     | 0.122   | 0.003   | 1.246   | 1.915   | 1.521 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C11 C12  | Not unusual (enough hits)       | 4114        | 1.518       | 1.512| 0.038     | 0.149   | 0.006   | 0.989   | 1.778   | 1.516 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C13 C12  | Not unusual (enough hits)       | 4212        | 1.538       | 1.512| 0.057     | 0.450   | 0.026   | 0.951   | 2.000   | 1.520 | 0.000 | --        |
| bond    | iai12p-l₁₂ | C14A C13 | Not unusual (enough hits)       | 4446        | 1.408       | 1.499| 0.069     | 1.329   | 0.091   | 0.743   | 2.085   | 1.514 | 0.000 | --        |
| bond          | C15 C16 | Not unusual (enough hits) | 4114 | 1.524 | 1.512 | 0.038 | 0.312 | 0.012 | 0.989 | 1.778 | 1.516 | 0.000 | --     |
| bond          | C17 C16 | Not unusual (enough hits) | 4212 | 1.522 | 1.512 | 0.057 | 0.169 | 0.010 | 0.951 | 2.000 | 1.520 | 0.000 | --     |
| bond          | C18 C17 | Not unusual (enough hits) | 4446 | 1.520 | 1.499 | 0.069 | 0.307 | 0.021 | 0.743 | 2.085 | 1.514 | 0.000 | --     |
| bond          | C19 C20 | Not unusual (enough hits) | 4114 | 1.517 | 1.512 | 0.038 | 0.133 | 0.005 | 0.989 | 1.778 | 1.516 | 0.000 | --     |
| bond          | C21 C20 | Not unusual (enough hits) | 4212 | 1.518 | 1.512 | 0.057 | 0.103 | 0.006 | 0.951 | 2.000 | 1.520 | 0.000 | --     |
| bond          | C22 C20 | Not unusual (enough hits) | 4446 | 1.520 | 1.499 | 0.069 | 0.307 | 0.021 | 0.743 | 2.085 | 1.514 | 0.000 | --     |
| bond          | C23 C24 | Not unusual (enough hits) | 4114 | 1.518 | 1.512 | 0.038 | 0.145 | 0.006 | 0.989 | 1.778 | 1.516 | 0.000 | --     |
| bond          | C25 C24 | Not unusual (enough hits) | 4212 | 1.527 | 1.512 | 0.057 | 0.264 | 0.015 | 0.951 | 2.000 | 1.520 | 0.000 | --     |
| bond          | C26 C25 | Not unusual (enough hits) | 4446 | 1.524 | 1.499 | 0.069 | 0.363 | 0.025 | 0.743 | 2.085 | 1.514 | 0.000 | --     |
| angle         | O7 C7 C6 | No hits                       | 0    | 116.543 | -- | -- | -- | -- | -- | -- | -- | -- | -- |
| angle         | O8 C7 C6 | No hits                       | 0    | 115.525 | -- | -- | -- | -- | -- | -- | -- | -- |
| angle         | C6 N1 C2 | Not unusual (enough hits) | 37   | 122.843 | 122.592 | 0.225 | 0.251 | 119.430 | 126.873 | 122.686 | 0.011 | -- |
| angle         | O2 C2 N1 | Not unusual (enough hits) | 1430 | 123.055 | 121.890 | 1.372 | 0.850 | 1.166 | 114.623 | 129.397 | 122.097 | 0.002 | -- |
| angle         | N3 C2 N1 | Not unusual (enough hits) | 546  | 115.073 | 115.584 | 1.146 | 0.445 | 0.510 | 111.680 | 120.111 | 115.557 | 0.004 | -- |
| angle         | O2 C2 N3 | Not unusual (enough hits) | 1430 | 121.869 | 121.890 | 1.372 | 0.015 | 0.021 | 114.623 | 129.397 | 122.097 | 0.000 | -- |
| angle         | C4 N3 C2 | Not unusual (enough hits) | 80   | 126.061 | 125.819 | 0.906 | 0.268 | 0.243 | 123.775 | 127.201 | 126.077 | 0.006 | -- |
| angle         | O4 C4 N3 | Not unusual (enough hits) | 708  | 119.911 | 119.363 | 1.239 | 0.443 | 0.548 | 114.543 | 125.340 | 119.479 | 0.000 | -- |
| angle         | C5 C4 N3 | Not unusual (enough hits) | 411  | 114.702 | 115.159 | 1.080 | 0.423 | 0.457 | 111.751 | 118.350 | 114.989 | 0.005 | -- |
| angle         | O4 C4 C5 | Not unusual (enough hits) | 491  | 125.386 | 125.544 | 1.120 | 0.141 | 0.158 | 120.918 | 128.433 | 125.635 | 0.002 | -- |
| angle         | C6 C5 C4 | Not unusual (enough hits) | 39   | 120.017 | 120.080 | 1.157 | 0.054 | 0.063 | 118.559 | 123.568 | 119.831 | 0.030 | -- |
angle iall2p-l_1 C5 C6 N1 Not unusual (enough hits) 15 120.998 120.844 0.865 0.178 0.154 119.785 123.023 120.575 0.014 --
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angle iall2p-l_1 C7 C6 C5 Not unusual (enough hits) 15 123.499 123.416 1.147 0.072 0.083 121.820 125.803 123.279 0.115 --
angle iall2p-l_1 O8 C7 O7 Unusual (enough hits) 16 127.931 124.896 0.744 4.083 3.036 123.030 125.770 125.092 2.161 --
angle iall2p-l_2 C15 N10 C11 Not unusual (enough hits) 4236 110.828 109.501 3.057 0.434 1.328 71.683 156.520 110.339 0.000 --
angle iall2p-l_2 C19 N10 C11 Not unusual (enough hits) 4236 106.335 109.501 3.057 1.036 3.166 71.683 156.520 110.339 0.002 --
angle iall2p-l_2 C23 N10 C11 Not unusual (enough hits) 4236 110.998 109.501 3.057 0.490 1.498 71.683 156.520 110.339 0.000 --
angle iall2p-l_2 C19 N10 C15 Not unusual (enough hits) 4236 110.025 109.501 3.057 0.172 0.524 71.683 156.520 110.339 0.001 --
angle iall2p-l_2 C23 N10 C15 Not unusual (enough hits) 4236 107.796 109.501 3.057 0.557 1.704 71.683 156.520 110.339 0.002 --
angle iall2p-l_2 C12 C11 N10 Not unusual (enough hits) 4005 114.968 115.932 3.049 0.316 0.964 87.318 160.053 115.821 0.000 --
angle iall2p-l_2 C11 C12 C13 Not unusual (enough hits) 4050 109.226 110.660 3.728 0.385 1.434 82.441 169.508 110.390 0.000 --
angle iall2p-l_2 C14A C13 C12 Not unusual (enough hits) 4246 116.234 113.580 5.905 0.449 2.654 70.885 172.726 113.126 0.007 --
angle iall2p-l_2 C16 C15 N10 Not unusual (enough hits) 4005 115.361 115.932 3.049 0.187 0.571 87.318 160.053 115.821 0.000 --
angle iall2p-l_2 C15 C16 C17 Not unusual (enough hits) 4050 110.718 110.660 3.728 0.016 0.058 82.441 169.508 110.390 0.000 --
angle iall2p-l_2 C18 C17 C16 Not unusual (enough hits) 4246 112.720 113.580 5.905 0.146 0.860 70.885 172.726 113.126 0.000 --
angle iall2p-l_2 C20 C19 N10 Not unusual (enough hits) 4005 115.267 115.932 3.049 0.218 0.665 87.318 160.053 115.821 0.000 --
angle iall2p-l_2 C19 C20 C21 Not unusual (enough hits) 4050 110.575 110.660 3.728 0.230 0.085 82.441 169.508 110.390 0.000 --
angle iall2p-l_2 C22 C21 C20 Not unusual (enough hits) 4246 112.279 113.580 5.905 0.220 1.301 70.885 172.726 113.126 0.000 --
angle iall2p-l_2 C24 C23 N10 Not unusual (enough hits) 4005 114.513 115.932 3.049 0.465 1.419 87.318 160.053 115.821 0.000 --

file:///E:/falvello/0-pub/00-2019-ActaE-NBu4Horot/send/figures-SuppInf/T100K-Mogul-1.html
| angle  | torsion  | l_2  | g | C23 C24 C25 | C26 C25 C24 | O7 C7 C6 N1 | C26 C25 C24 | O7 C7 C6 C5 | C26 C25 C24 | O8 C7 C6 C5 | C12 C11 N10 C15 | C12 C11 N10 C19 | C12 C11 N10 C23 | C16 C15 N10 C11 | C16 C15 N10 C19 | C16 C15 N10 C23 | C20 C19 N10 C11 | C20 C19 N10 C15 | C20 C19 N10 C23 | C24 C23 N10 C11 | C24 C23 N10 C15 | C24 C23 N10 C19 | C13 C12 C11 N10 |
|--------|----------|------|---|-------------|-------------|------------|-------------|------------|-------------|------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| C23 C24 C25 | Not unusual (enough hits) | 4050 | 111.289 | 110.660 | 3.728 | 0.169 | 0.629 | 82.441 | 169.508 | 110.390 | 0.000 | -- | 110.390 | 0.000 | -- | 110.390 | 0.000 | -- | 110.390 | 0.000 | -- | 110.390 | 0.000 | -- |
| C26 C25 C24 | Not unusual (enough hits) | 4246 | 111.658 | 113.580 | 5.905 | 0.325 | 1.922 | 70.885 | 172.726 | 113.126 | 0.000 | -- | 113.126 | 0.000 | -- | 113.126 | 0.000 | -- | 113.126 | 0.000 | -- | 113.126 | 0.000 | -- |
| O7 C7 C6 N1 | Not unusual (enough hits) | 40 | 158.554 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| O8 C7 C6 N1 | Not unusual (enough hits) | 40 | -21.132 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| O7 C7 C6 C5 | Not unusual (enough hits) | 36 | -22.683 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| O8 C7 C6 C5 | Not unusual (enough hits) | 36 | 157.631 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C12 C11 N10 C15 | Not unusual (enough hits) | 4732 | -60.826 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C12 C11 N10 C19 | Not unusual (enough hits) | 4732 | 179.618 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C12 C11 N10 C23 | Not unusual (enough hits) | 4732 | 58.928 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C16 C15 N10 C11 | Not unusual (enough hits) | 4732 | -52.028 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C16 C15 N10 C19 | Not unusual (enough hits) | 4732 | 65.290 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C16 C15 N10 C23 | Not unusual (enough hits) | 4732 | -173.682 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C20 C19 N10 C11 | Not unusual (enough hits) | 4732 | -176.325 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C20 C19 N10 C15 | Not unusual (enough hits) | 4732 | 63.597 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C20 C19 N10 C23 | Not unusual (enough hits) | 4732 | -55.562 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C24 C23 N10 C11 | Not unusual (enough hits) | 4732 | 55.882 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C24 C23 N10 C15 | Not unusual (enough hits) | 4732 | 177.430 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C24 C23 N10 C19 | Not unusual (enough hits) | 4732 | -62.080 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| C13 C12 C11 N10 | Not unusual (enough hits) | 3984 | 173.303 | -- | -- | -- | -- | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | -- | 813 | 0.350 | -- | -- | -- | 813 | 0.350 |
| Torsion ial12p-l_2 | C11 C12 C13 C14A | Not unusual (enough hits) | 4215 | 59.052 | -- | -- | -- | -- | -- | 0.007 | 0.110 |
|-------------------|------------------|---------------------------|------|--------|---|---|---|---|---|--------|--------|
| C17 C16 C15 N10   | Not unusual (enough hits) | 3984 | -167.647 | -- | -- | -- | -- | -- | 0.001 | 0.755 |
| C15 C16 C17 C18   | Not unusual (enough hits) | 4215 | -176.639 | -- | -- | -- | -- | -- | 0.001 | 0.697 |
| C21 C20 C19 N10   | Not unusual (enough hits) | 3984 | -173.009 | -- | -- | -- | -- | -- | 0.000 | 0.919 |
| C19 C20 C21 C22   | Not unusual (enough hits) | 4215 | 177.663 | -- | -- | -- | -- | -- | 0.000 | 0.688 |
| C25 C24 C23 N10   | Not unusual (enough hits) | 3984 | 170.921 | -- | -- | -- | -- | -- | 0.000 | 0.943 |
| C23 C24 C25 C26   | Not unusual (enough hits) | 4215 | -178.309 | -- | -- | -- | -- | -- | 0.002 | 0.682 |
| Type | Molecule | Fragment | Classification                  | No. of hits | Query value | Mean    | Std. dev. | | z-score | | x - mean | Minimum | Maximum | Median | | d(min) | | Local density |
|------|----------|----------|----------------------------------|-------------|-------------|---------|-----------|-------------|-----------|-------------|-----------|-------------|-----------|-------------|
| bond | est4l_1  | C2 N1    | Not unusual (enough hits)        | 1428        | 1.365       | 1.371   | 0.012     | 0.483       | 0.006     | 1.299       | 1.452     | 1.370       | 0.000     | --          |
| bond | est4l_1  | C6 N1    | Not unusual (enough hits)        | 18          | 1.367       | 1.359   | 0.011     | 0.711       | 0.008     | 1.342       | 1.383     | 1.356       | 0.001     | --          |
| bond | est4l_1  | O2 C2    | Not unusual (enough hits)        | 2995        | 1.215       | 1.228   | 0.015     | 0.846       | 0.013     | 1.166       | 1.520     | 1.227       | 0.000     | --          |
| bond | est4l_1  | C2 N3    | Not unusual (enough hits)        | 1428        | 1.369       | 1.371   | 0.012     | 0.124       | 0.001     | 1.299       | 1.452     | 1.370       | 0.000     | --          |
| bond | est4l_1  | C4 N3    | Not unusual (enough hits)        | 708         | 1.383       | 1.381   | 0.013     | 0.199       | 0.003     | 1.256       | 1.419     | 1.380       | 0.000     | --          |
| bond | est4l_1  | O4 C4    | Not unusual (enough hits)        | 1300        | 1.225       | 1.241   | 0.016     | 1.016       | 0.016     | 1.196       | 1.355     | 1.240       | 0.000     | --          |
| bond | est4l_1  | C5 C4    | Not unusual (enough hits)        | 491         | 1.431       | 1.423   | 0.019     | 0.405       | 0.008     | 1.352       | 1.464     | 1.426       | 0.000     | --          |
| bond | est4l_1  | C7 C6    | Not unusual (enough hits)        | 16          | 1.522       | 1.481   | 0.025     | 1.665       | 0.041     | 1.438       | 1.542     | 1.483       | 0.010     | --          |
| bond | est4l_1  | C5 C6    | Unusual (enough hits)            | 24          | 1.327       | 1.360   | 0.011     | 3.065       | 0.034     | 1.339       | 1.375     | 1.363       | 0.012     | --          |
| bond | est4l_1  | O7 C7    | Unusual (enough hits)            | 32          | 1.235       | 1.254   | 0.006     | 3.047       | 0.019     | 1.242       | 1.275     | 1.253       | 0.007     | --          |
| bond | est4l_1  | O8 C7    | Unusual (enough hits)            | 32          | 1.224       | 1.254   | 0.006     | 4.820       | 0.031     | 1.242       | 1.275     | 1.253       | 0.019     | --          |
| bond | est4l_2  | C15 N10  | Not unusual (enough hits)        | 4078        | 1.519       | 1.521   | 0.024     | 0.098       | 0.002     | 1.246       | 1.915     | 1.521       | 0.000     | --          |
| bond | est4l_2  | C19 N10  | Not unusual (enough hits)        | 4078        | 1.509       | 1.521   | 0.024     | 0.524       | 0.012     | 1.246       | 1.915     | 1.521       | 0.000     | --          |
| bond | est4l_2  | C23 N10  | Not unusual (enough hits)        | 4078        | 1.525       | 1.521   | 0.024     | 0.168       | 0.004     | 1.246       | 1.915     | 1.521       | 0.000     | --          |
| bond | est4l_2  | C15 C16  | Not unusual (enough hits)        | 4114        | 1.521       | 1.512   | 0.038     | 0.227       | 0.009     | 0.989       | 1.778     | 1.516       | 0.000     | --          |
| bond | est4l_2  | C17 C16  | Not unusual (enough hits)        | 4212        | 1.444       | 1.512   | 0.057     | 1.209       | 0.069     | 0.951       | 2.000     | 1.520       | 0.000     | --          |
| bond | est4l_2  | C18 C17  | Not unusual (enough hits)        | 4446        | 1.485       | 1.499   | 0.069     | 0.197       | 0.014     | 0.743       | 2.085     | 1.514       | 0.000     | --          |
| bond | est4l_2  | C19 C20  | Not unusual (enough hits)        | 4114        | 1.504       | 1.512   | 0.038     | 0.221       | 0.008     | 0.989       | 1.778     | 1.516       | 0.000     | --          |
| bond | est4l_2  | C21 C20  | Not unusual (enough hits)        | 4212        | 1.489       | 1.512   | 0.057     | 0.410       | 0.023     | 0.951       | 2.000     | 1.520       | 0.000     | --          |
| bond | est4l_2  | C22 C21  | Not unusual (enough hits)        | 4446        | 1.504       | 1.499   | 0.069     | 0.078       | 0.005     | 0.743       | 2.085     | 1.514       | 0.000     | --          |
| bond        | est4l_2 | C23 C24  | Not unusual (enough hits) | 4114 | 1.532 | 1.512 | 0.038 | 0.515 | 0.020 | 0.989 | 1.778 | 1.516 | 0.000 -- |
| bond        | est4l_2 | C25 C24  | Not unusual (enough hits) | 4212 | 1.416 | 1.512 | 0.057 | 1.697 | 0.097 | 0.951 | 2.000 | 1.520 | 0.000 -- |
| bond        | est4l_2 | C26 C25  | Not unusual (enough hits) | 4446 | 1.504 | 1.499 | 0.069 | 0.070 | 0.005 | 0.743 | 2.085 | 1.514 | 0.000 -- |
| angle       | est4l_1 | O7 C7 C6 | No hits                  | 0    | 116.313 | -- | -- | -- | -- | -- | -- | -- | -- |
| angle       | est4l_1 | O8 C7 C6 | No hits                  | 0    | 116.170 | -- | -- | -- | -- | -- | -- | -- |
| angle       | est4l_1 | C6 N1 C2 | Not unusual (enough hits) | 37   | 124.008 | 122.592 | 1.270 | 1.416 | 119.430 | 126.873 | 122.686 | 0.037 -- |
| angle       | est4l_1 | O2 C2 N1 | Not unusual (enough hits) | 1430 | 124.065 | 121.890 | 1.586 | 2.176 | 114.623 | 129.397 | 122.097 | 0.010 -- |
| angle       | est4l_1 | N3 C2 N1 | Not unusual (enough hits) | 546  | 113.971 | 115.584 | 1.146 | 1.612 | 111.680 | 120.111 | 115.557 | 0.001 -- |
| angle       | est4l_1 | O2 C2 N3 | Not unusual (enough hits) | 1430 | 121.961 | 121.890 | 0.052 | 0.071 | 114.623 | 129.397 | 122.097 | 0.002 -- |
| angle       | est4l_1 | C4 N3 C2 | Not unusual (enough hits) | 80   | 126.241 | 125.819 | 0.906 | 0.465 | 0.422 | 123.775 | 127.201 | 126.077 | 0.002 -- |
| angle       | est4l_1 | O4 C4 N3 | Not unusual (enough hits) | 708  | 119.441 | 119.363 | 1.239 | 0.052 | 0.071 | 114.543 | 125.340 | 119.479 | 0.000 -- |
| angle       | est4l_1 | C5 C4 N3 | Not unusual (enough hits) | 80   | 126.241 | 125.819 | 0.906 | 0.465 | 0.422 | 123.775 | 127.201 | 126.077 | 0.002 -- |
| angle       | est4l_2 | O4 C4 O7 | Unusual (enough hits)    | 16   | 127.508 | 124.896 | 1.372 | 1.586 | 118.559 | 123.568 | 119.831 | 0.088 -- |
| angle       | est4l_2 | C19 N10 C15 | Not unusual (enough hits) | 4236 | 109.834 | 109.501 | 3.057 | 0.109 | 0.333 | 71.683 | 156.520 | 110.339 | 0.000 -- |
| angle       | est4l_2 | C23 N10 C15 | Not unusual (enough hits) | 4236 | 109.834 | 109.501 | 3.057 | 0.109 | 0.333 | 71.683 | 156.520 | 110.339 | 0.000 -- |
| angle       | est4l_2 | C23 N10 C19 | Not unusual (enough hits) | 4236 | 111.217 | 109.501 | 3.057 | 0.109 | 0.333 | 71.683 | 156.520 | 110.339 | 0.000 -- |
| Angle est4l_2 | C16 C15 N10 | Not unusual (enough hits) | 4005 | 115.615 | 115.932 3.049 | 0.104 | 0.316 | 87.318 | 160.053 | 115.821 0.001 | -- |
| Angle est4l_2 | C15 C16 C17 | Not unusual (enough hits) | 4050 | 113.239 | 110.660 3.728 | 0.692 | 2.579 | 82.441 | 169.508 | 110.390 0.002 | -- |
| Angle est4l_2 | C18 C17 C16 | Not unusual (enough hits) | 4246 | 116.470 | 113.580 5.905 | 0.489 | 2.890 | 70.885 | 172.726 | 113.126 0.003 | -- |
| Angle est4l_2 | C20 C19 N10 | Not unusual (enough hits) | 4005 | 116.012 | 115.932 0.026 | 0.080 | 87.318 | 160.053 | 115.821 0.000 | -- |
| Angle est4l_2 | C19 C20 C21 | Not unusual (enough hits) | 4050 | 111.860 | 110.660 3.728 | 0.322 | 1.200 | 82.441 | 169.508 | 110.390 0.003 | -- |
| Angle est4l_2 | C22 C21 C20 | Not unusual (enough hits) | 4246 | 113.537 | 113.580 0.007 | 0.043 | 70.885 | 172.726 | 113.126 0.001 | -- |
| Angle est4l_2 | C24 C23 N10 | Not unusual (enough hits) | 4005 | 114.355 | 115.932 3.049 | 0.517 | 1.577 | 87.318 | 160.053 | 115.821 0.000 | -- |
| Angle est4l_2 | C23 C24 C25 | Not unusual (enough hits) | 4050 | 114.761 | 110.660 3.728 | 1.100 | 4.101 | 82.441 | 169.508 | 110.390 0.015 | -- |
| Angle est4l_2 | C26 C25 C24 | Not unusual (enough hits) | 4246 | 115.327 | 113.580 0.296 | 1.747 | 70.885 | 172.726 | 113.126 0.000 | -- |
| Torsion est4l_1 | O7 C7 C6 N1 | Not unusual (enough hits) | 40 | 161.730 | -- -- -- -- -- -- -- | -- | 0.040 | 0.350 |
| Torsion est4l_1 | O8 C7 C6 N1 | Not unusual (enough hits) | 40 | -19.239 | -- -- -- -- -- -- -- | -- | 1.418 | 0.350 |
| Torsion est4l_1 | O7 C7 C6 C5 | Not unusual (enough hits) | 36 | -19.222 | -- -- -- -- -- -- -- | -- | 0.018 | 0.389 |
| Torsion est4l_1 | O8 C7 C6 C5 | Not unusual (enough hits) | 36 | 159.809 | -- -- -- -- -- -- -- | -- | 0.090 | 0.333 |
| Torsion est4l_2 | C16 C15 N10 C19 | Not unusual (enough hits) | 4732 | 60.014 | -- -- -- -- -- -- -- | -- | 0.004 | 0.613 |
| Torsion est4l_2 | C16 C15 N10 C23 | Not unusual (enough hits) | 4732 | -179.201 | -- -- -- -- -- -- -- | -- | 0.000 | 0.302 |
| Torsion est4l_2 | C20 C19 N10 C15 | Not unusual (enough hits) | 4732 | 60.798 | -- -- -- -- -- -- -- | -- | 0.000 | 0.611 |
| Torsion est4l_2 | C20 C19 N10 C23 | Not unusual (enough hits) | 4732 | -57.355 | -- -- -- -- -- -- -- | -- | 0.003 | 0.604 |
| Torsion est4l_2 | C24 C23 N10 C15 | Not unusual (enough hits) | 4732 | 177.352 | -- -- -- -- -- -- -- | -- | 0.001 | 0.313 |
| Torsion est4l_2 | C24 C23 N10 C19 | Not unusual (enough hits) | 4732 | -62.748 | -- -- -- -- -- -- -- | -- | 0.000 | 0.588 |
| Torsion | C17 C16 C15 N10 | Not unusual (enough hits) | 3984 | 177.527 | -- | -- | -- | -- | -- | 0.001 | 0.825 |
|---------|------------------|----------------------------|------|---------|----|----|----|----|----|--------|--------|
| torsion est4l_2 | C15 C16 C17 C18 | Not unusual (enough hits) | 4215 | 179.726 | -- | -- | -- | -- | -- | 0.000 | 0.661 |
| torsion est4l_2 | C21 C20 C19 N10 | Not unusual (enough hits) | 3984 | -176.180 | -- | -- | -- | -- | -- | 0.002 | 0.860 |
| torsion est4l_2 | C19 C20 C21 C22 | Not unusual (enough hits) | 4215 | 179.217 | -- | -- | -- | -- | -- | 0.001 | 0.670 |
| torsion est4l_2 | C25 C24 C23 N10 | Not unusual (enough hits) | 3984 | -179.338 | -- | -- | -- | -- | -- | 0.001 | 0.762 |
| torsion est4l_2 | C23 C24 C25 C26 | Not unusual (enough hits) | 4215 | 179.249 | -- | -- | -- | -- | -- | 0.000 | 0.670 |