



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:58 AM UTC

PDB ID : 6T15 / pdb\_00006t15  
EMDB ID : EMD-10318  
Title : The III2-IV(5B)1 respiratory supercomplex from *S. cerevisiae*  
Authors : Marechal, A.; Pinotsis, N.; Hartley, A.  
Deposited on : 2019-10-03  
Resolution : 3.29 Å (reported)  
Based on initial model : 6HU9

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

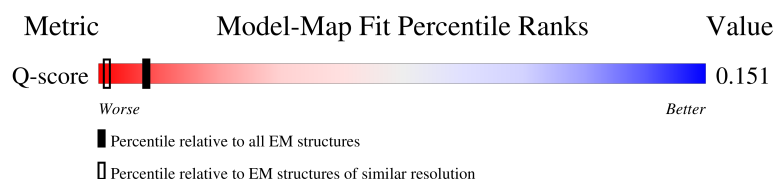
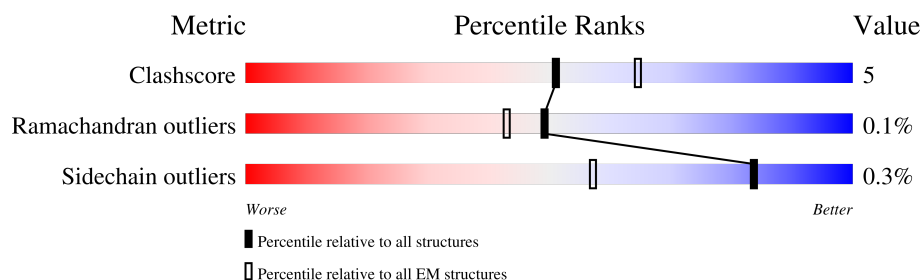
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 3.29 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<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13997 ( 2.91 - 3.91 )                                    |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 431    | <div> <div>100%</div> <div>89% 11%</div> </div> |
| 1   | L     | 431    | <div> <div>100%</div> <div>87% 13%</div> </div> |
| 2   | B     | 352    | <div> <div>100%</div> <div>87% 13%</div> </div> |
| 2   | M     | 352    | <div> <div>100%</div> <div>84% 16%</div> </div> |

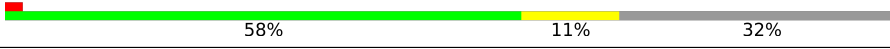
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 385    |                  |
| 3   | N     | 385    |                  |
| 4   | D     | 248    |                  |
| 4   | O     | 248    |                  |
| 5   | E     | 185    |                  |
| 5   | P     | 185    |                  |
| 6   | F     | 147    |                  |
| 6   | Q     | 147    |                  |
| 7   | G     | 127    |                  |
| 7   | R     | 127    |                  |
| 8   | H     | 94     |                  |
| 8   | S     | 94     |                  |
| 9   | I     | 66     |                  |
| 9   | T     | 66     |                  |
| 10  | J     | 77     |                  |
| 10  | U     | 77     |                  |
| 11  | a     | 534    |                  |
| 12  | b     | 236    |                  |
| 13  | c     | 269    |                  |
| 14  | d     | 130    |                  |
| 15  | e     | 134    |                  |
| 16  | f     | 108    |                  |
| 17  | g     | 59     |                  |
| 18  | h     | 51     |                  |
| 19  | i     | 55     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 20  | j     | 82     |  |
| 21  | k     | 131    |  |
| 22  | l     | 66     |  |
| 23  | m     | 224    |  |

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 48966 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 CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 431      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3345  | 2110 | 576 | 653 | 6 |         |       |
| 1   | L     | 431      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3345  | 2110 | 576 | 653 | 6 |         |       |

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 352      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2735  | 1747 | 453 | 534 | 1 |         |       |
| 2   | M     | 352      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2735  | 1747 | 453 | 534 | 1 |         |       |

- Molecule 3 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3090  | 2082 | 484 | 503 | 21 |         |       |
| 3   | N     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3090  | 2082 | 484 | 503 | 21 |         |       |

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | D     | 247      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1951  | 1243 | 338 | 361 | 9 |         |       |
| 4   | O     | 247      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1951  | 1243 | 338 | 361 | 9 |         |       |

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | E     | 185      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1411  | 893 | 242 | 266 | 10 |         |       |
| 5   | P     | 185      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1411  | 893 | 242 | 266 | 10 |         |       |

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6, COMPLEX III SUBUNIT VI, CYTOCHROME C1 NON-HEME 17 KDA PROTEIN, MITOCHONDRIAL HINGE PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | F     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 396 | 109 | 126 | 2 |         |       |
| 6   | Q     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 633   | 396 | 109 | 126 | 2 |         |       |

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 653 | 173 | 191 | 2 |         |       |
| 7   | R     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 653 | 173 | 191 | 2 |         |       |

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 510 | 131 | 130 | 2 |         |       |
| 8   | S     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 510 | 131 | 130 | 2 |         |       |

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 9   | I     | 57       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 465   | 310 | 77 | 78 |  |         |       |
| 9   | T     | 57       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 465   | 310 | 77 | 78 |  |         |       |

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 10  | J     | 76       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 599   | 391 | 98 | 108 | 2 |         |       |
| 10  | U     | 76       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 599   | 391 | 98 | 108 | 2 |         |       |

- Molecule 11 is a protein called CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | a     | 534      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4162  | 2778 | 649 | 713 | 22 |         |       |

- Molecule 12 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | b     | 236      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1889  | 1242 | 286 | 351 | 10 |         |       |

- Molecule 13 is a protein called CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | c     | 269      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2146  | 1430 | 344 | 357 | 15 |         |       |

- Molecule 14 is a protein called CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | d     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 576 | 151 | 181 | 5 |         |       |

- Molecule 15 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | e     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1083  | 694 | 188 | 199 | 2 |         |       |

- Molecule 16 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | f     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 866   | 554 | 141 | 170 | 1 |         |       |

- Molecule 17 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | g     | 59       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 484   | 328 | 83 | 73 |         |       |

- Molecule 18 is a protein called Cytochrome c oxidase polypeptide VIII, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | h     | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 409   | 278 | 66 | 64 | 1 |         |       |

- Molecule 19 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7A; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VIIA, COX9.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | i     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 456   | 300 | 79 | 74 | 3 |         |       |

- Molecule 20 is a protein called Cytochrome c oxidase subunit 6B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | j     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 410 | 109 | 118 | 5 |         |       |

- Molecule 21 is a protein called CYTOCHROME C OXIDASE SUBUNIT 6A, MITOCHONDRIAL; CYTOCHROME C OXIDASE POLYPEPTIDE VIA, COX13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | k     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 626 | 167 | 171 | 3 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| k     | 130     | GLY      | -      | expression tag | UNP P32799 |
| k     | 131     | ALA      | -      | expression tag | UNP P32799 |
| k     | 132     | ARG      | -      | expression tag | UNP P32799 |
| k     | 133     | GLY      | -      | expression tag | UNP P32799 |
| k     | 134     | SER      | -      | expression tag | UNP P32799 |
| k     | 135     | HIS      | -      | expression tag | UNP P32799 |
| k     | 136     | HIS      | -      | expression tag | UNP P32799 |
| k     | 137     | HIS      | -      | expression tag | UNP P32799 |
| k     | 138     | HIS      | -      | expression tag | UNP P32799 |
| k     | 139     | HIS      | -      | expression tag | UNP P32799 |
| k     | 140     | HIS      | -      | expression tag | UNP P32799 |

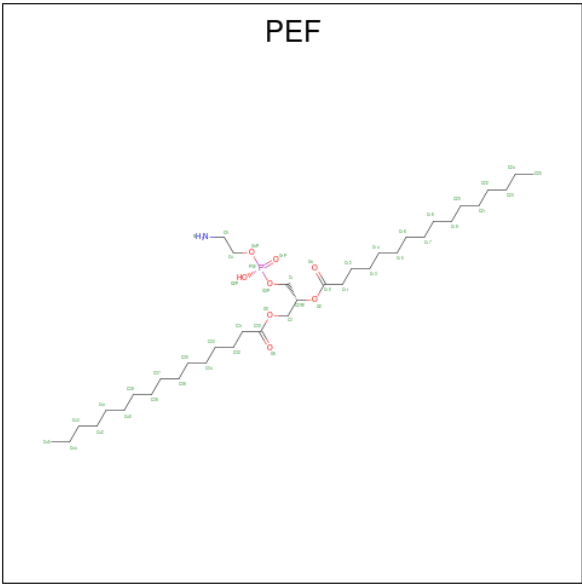
- Molecule 22 is a protein called COX26; SYNONYM: Uncharacterized protein YDR119W-A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | l     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 361   | 238 | 63 | 59 | 1 |         |       |

- Molecule 23 is a protein called RCF2; SYNONYM: Respiratory supercomplex factor 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | m     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 799   | 511 | 140 | 144 | 4 |         |       |

- Molecule 24 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 24  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 24  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 24  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 24  | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 24  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 24  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 24  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 24  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 24  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 24  | P     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 24  | S     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 24  | U     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |

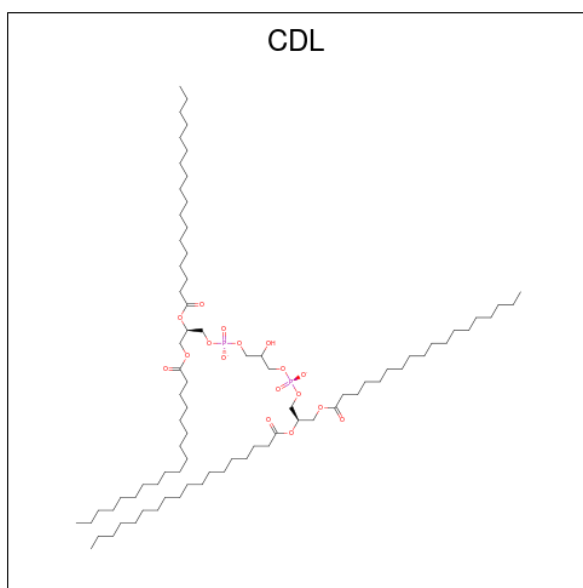
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| Mol | Chain | Residues | Atoms       |         |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 24  | a     | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 24  | b     | 1        | Total<br>40 | C<br>30 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 24  | b     | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 24  | c     | 1        | Total<br>36 | C<br>26 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 24  | c     | 1        | Total<br>41 | C<br>31 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 24  | e     | 1        | Total<br>42 | C<br>32 | N<br>1 | O<br>8 | P<br>1 | 0       |

- # HEM

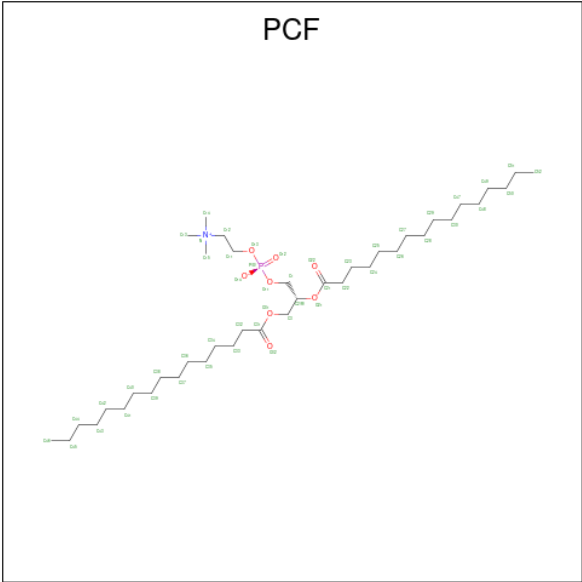
- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand

of Interest" by depositor).



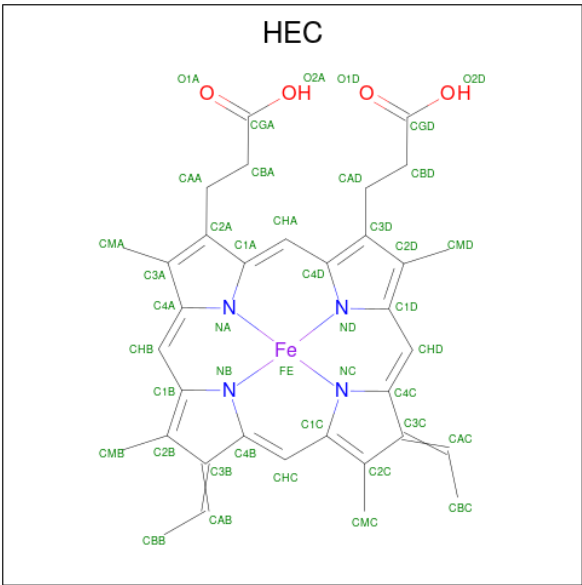
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 26  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 55    | 36 | 17 | 2 |         |
| 26  | D     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 67    | 48 | 17 | 2 |         |
| 26  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |
| 26  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 58    | 39 | 17 | 2 |         |
| 26  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 66    | 47 | 17 | 2 |         |
| 26  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 71    | 52 | 17 | 2 |         |
| 26  | S     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 53    | 34 | 17 | 2 |         |

- Molecule 27 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



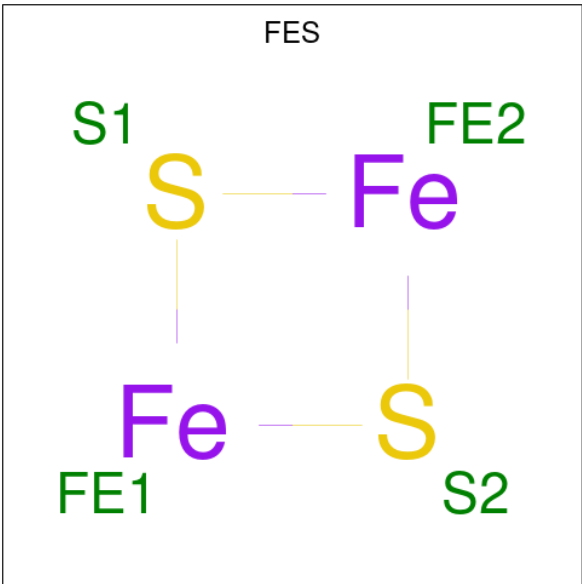
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 27  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 27  | I     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 27  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 27  | S     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 27  | T     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 27  | e     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |

- Molecule 28 is HEME C (CCD ID: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 28  | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 28  | O     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 29 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

Continued on next page...

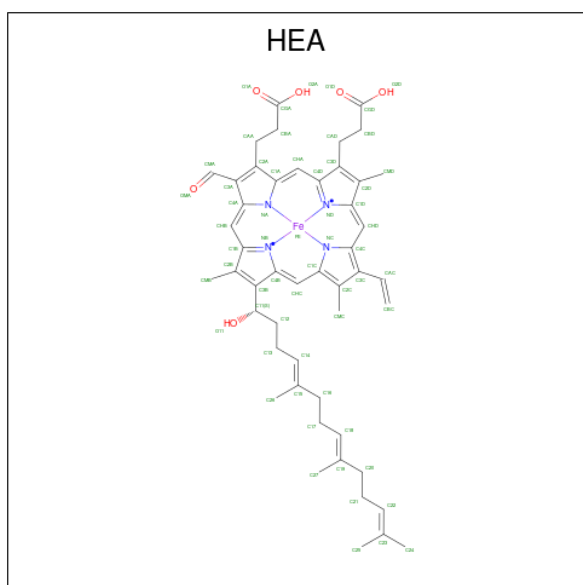
Continued from previous page...

| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 29  | P     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 30 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | a     | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 31 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

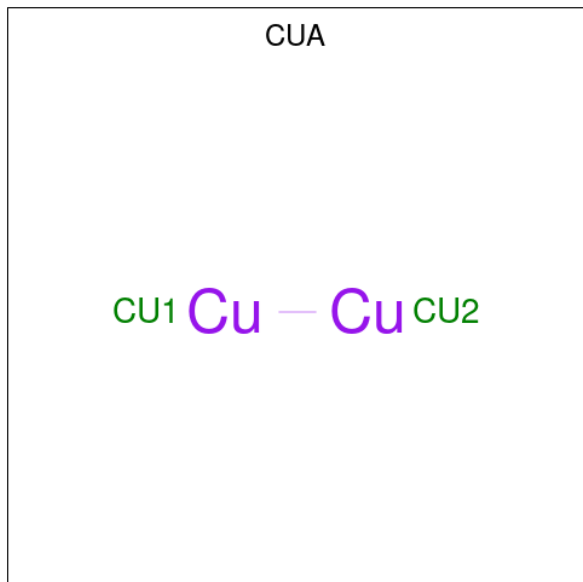


| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 31  | a     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |
| 31  | a     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 32  | a     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 33 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula:  $\text{Cu}_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 33  | b     | 1        | Total | Cu | 0       |
|     |       |          | 2     | 2  |         |

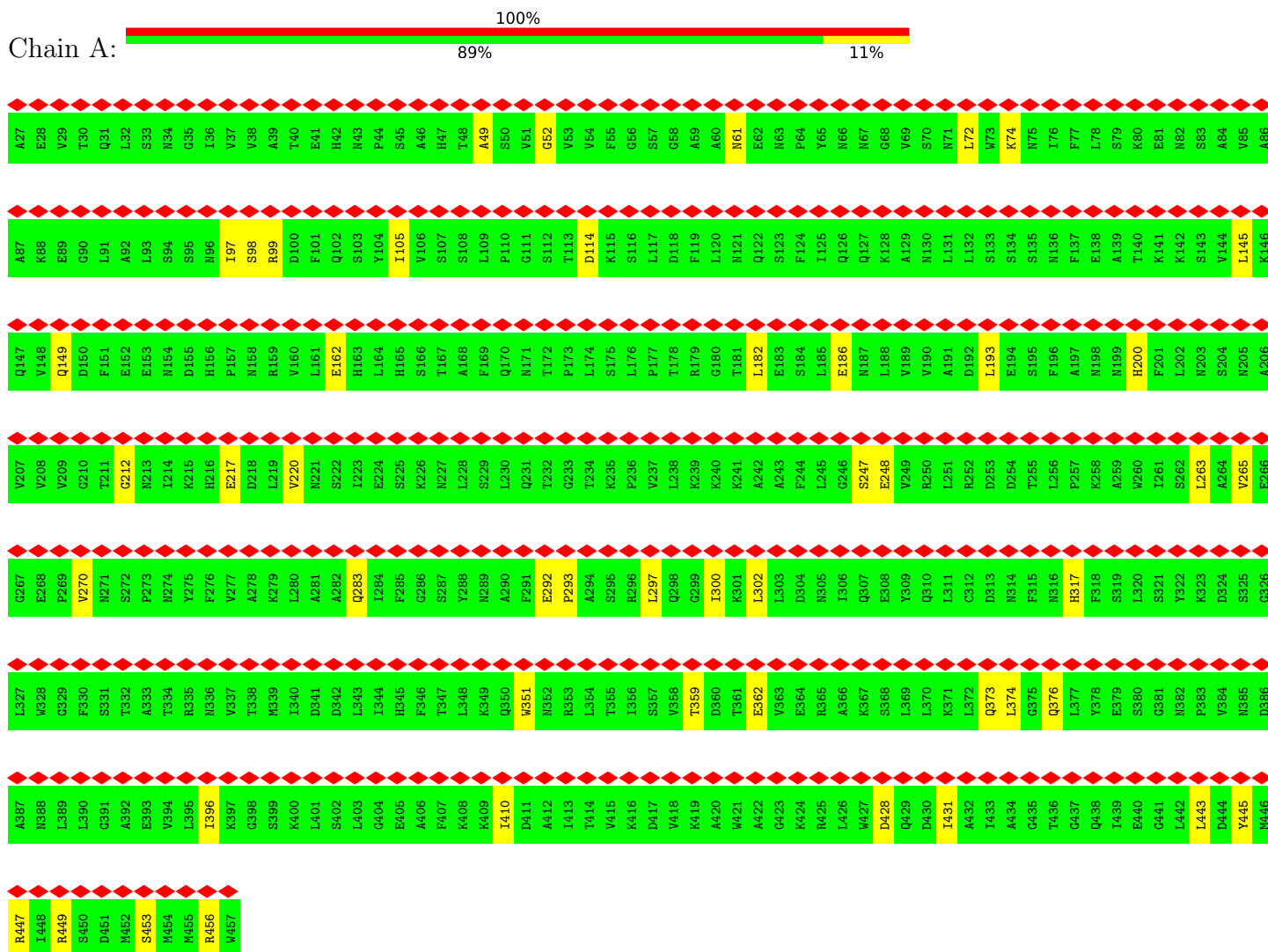
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 34  | d     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

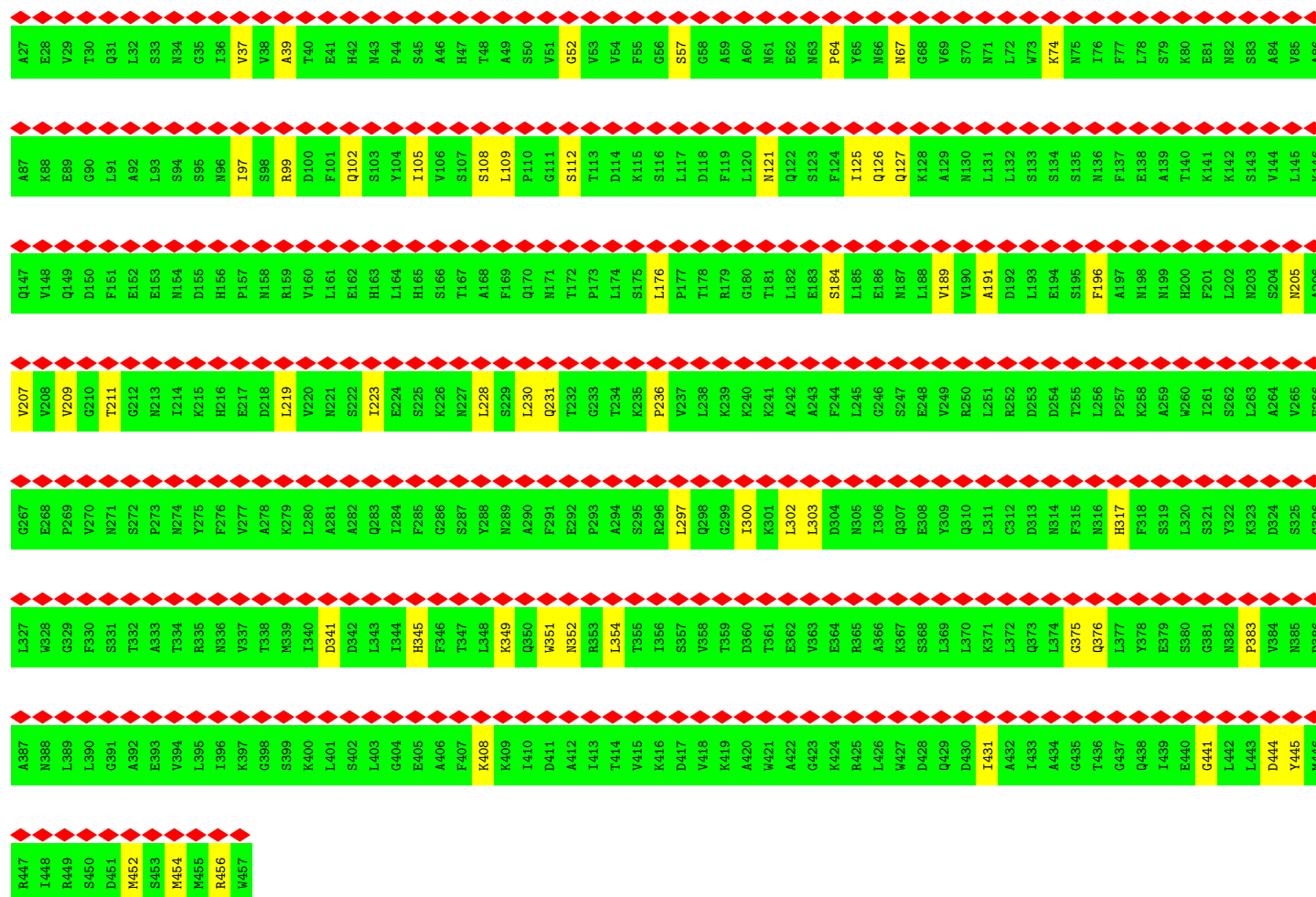
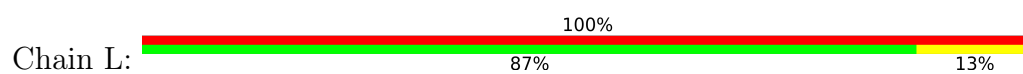
### 3 Residue-property plots

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.

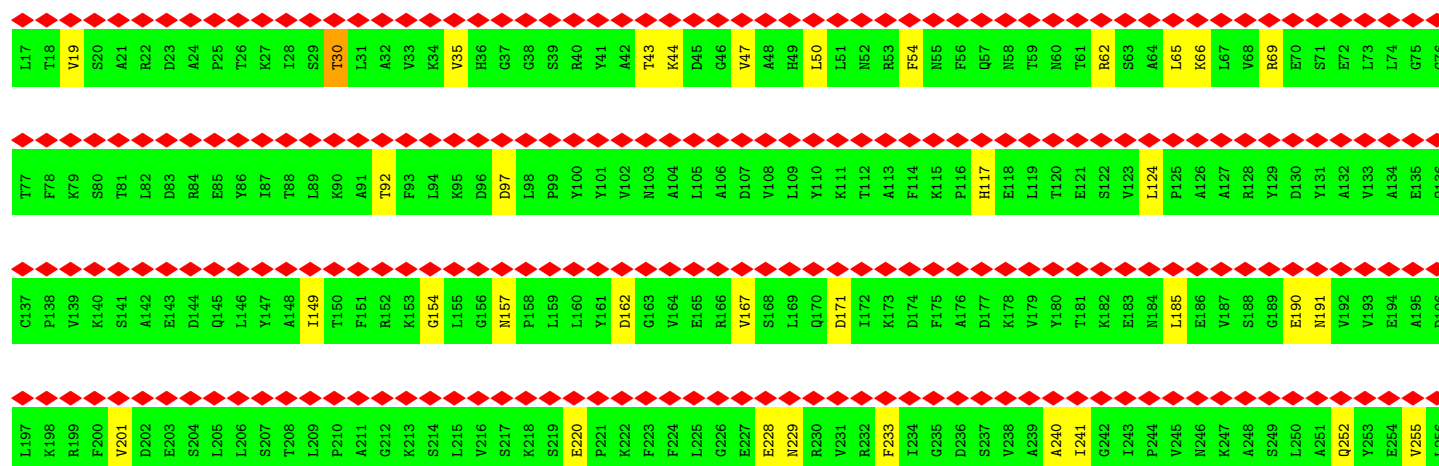
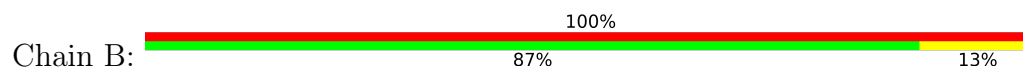
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

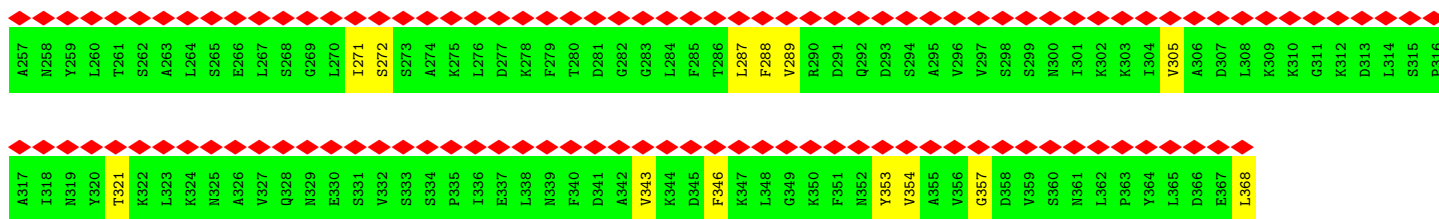


- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 1, CORE PROTEIN I, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 1

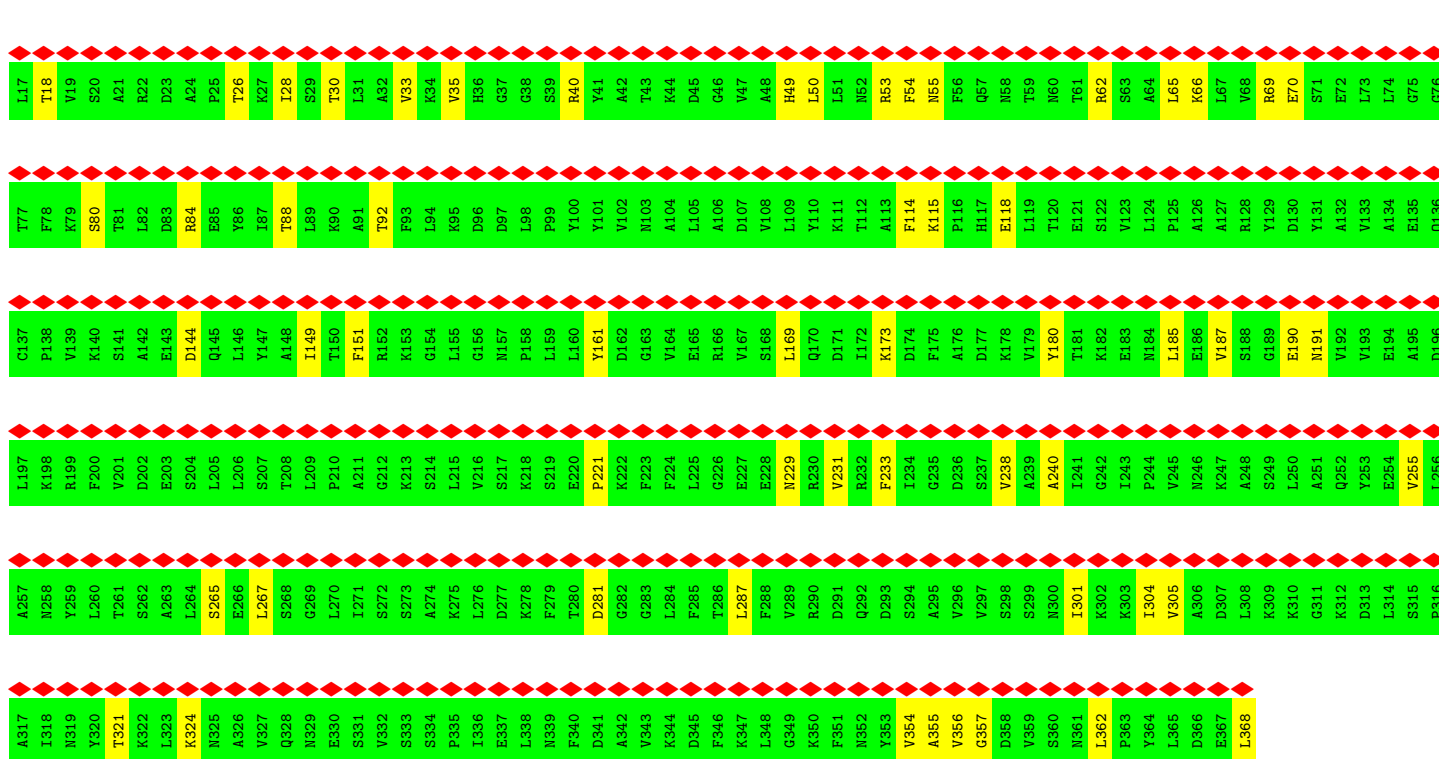
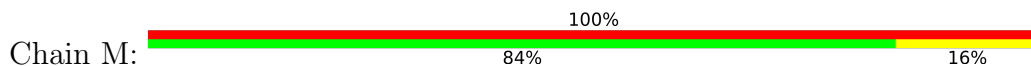


● Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

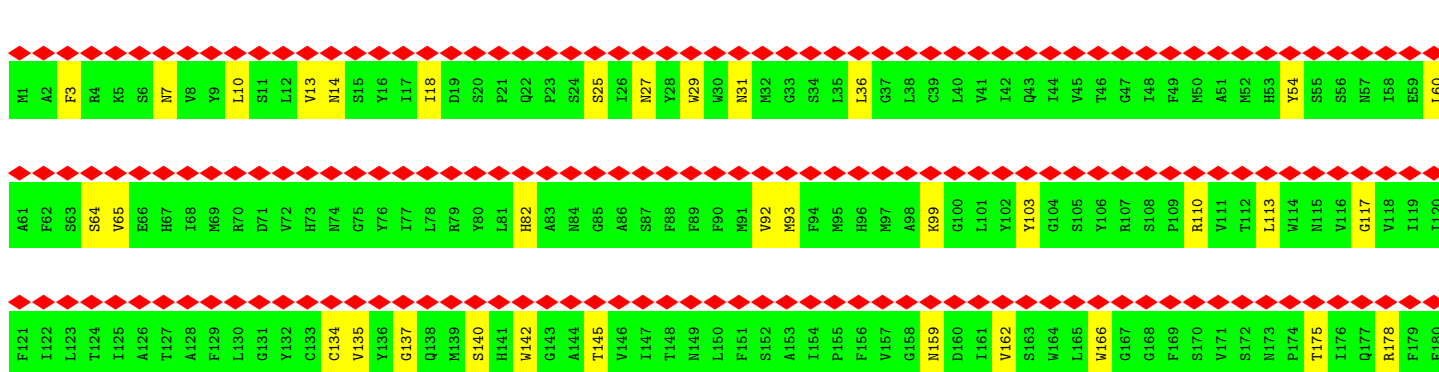
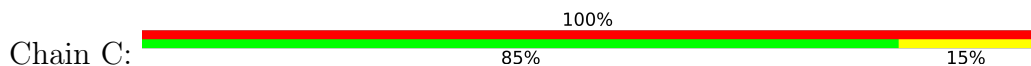


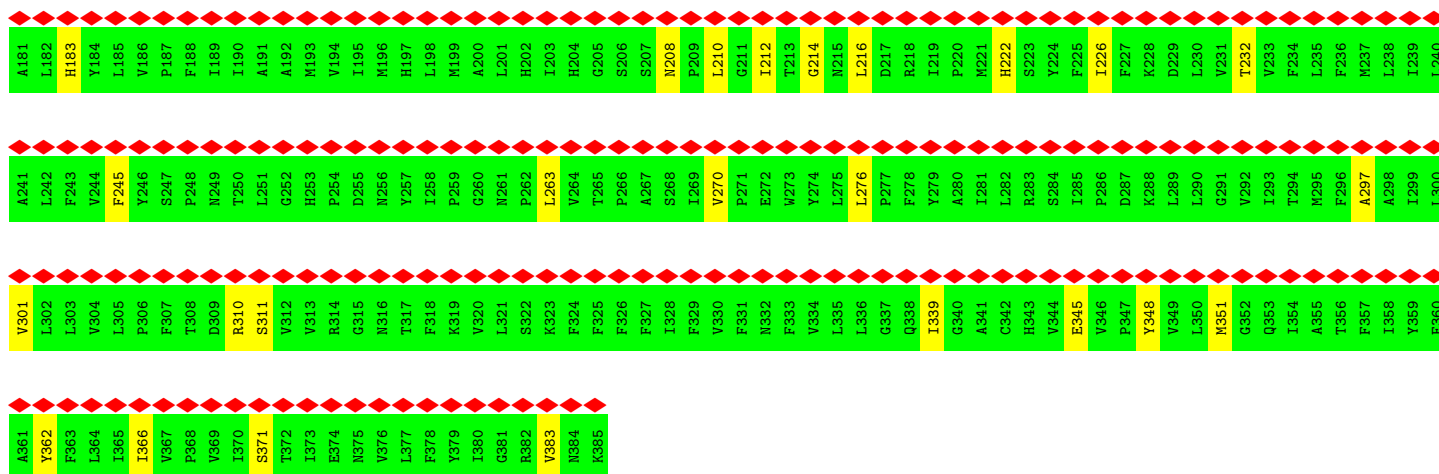


● Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

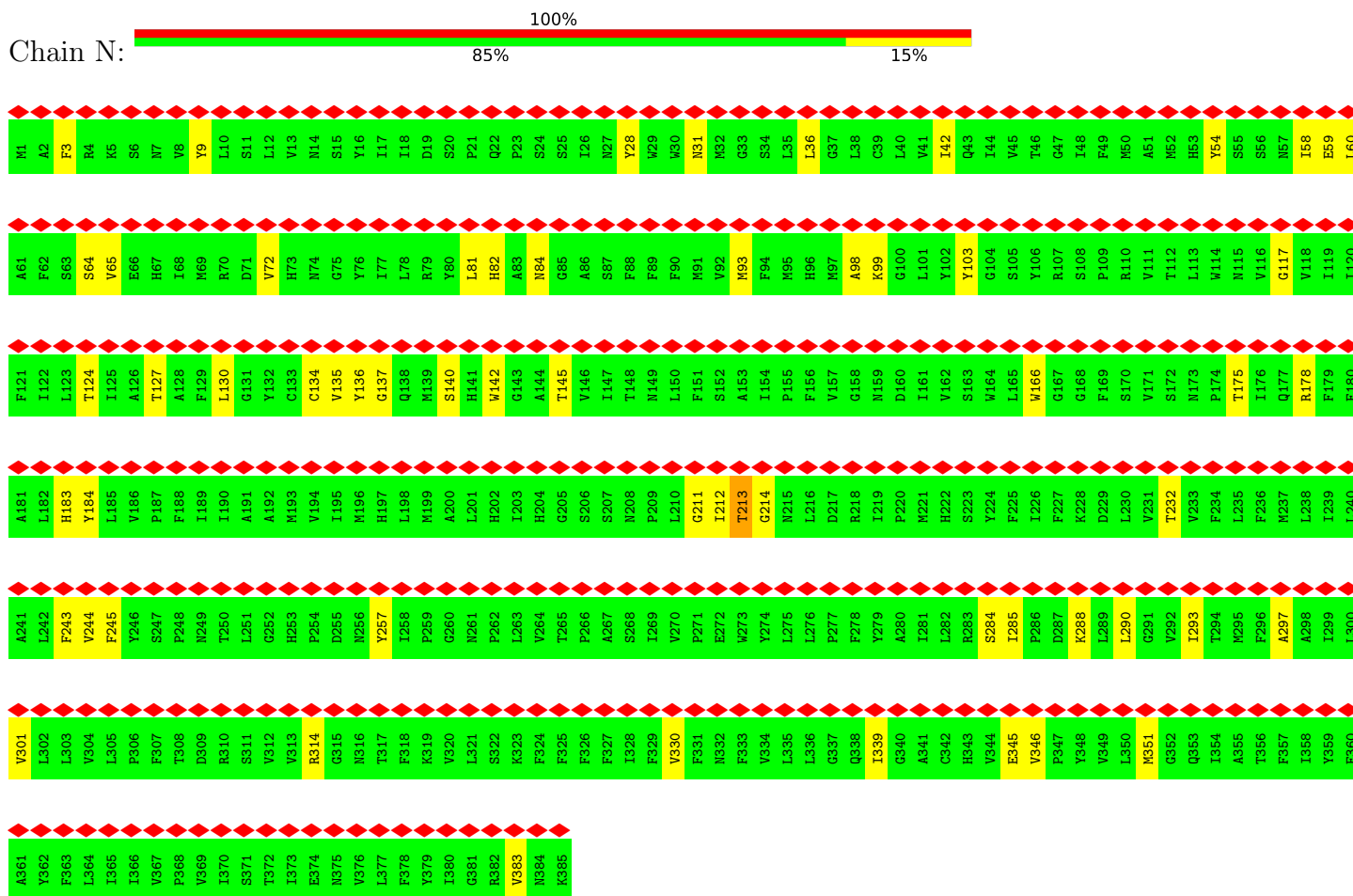


● Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2

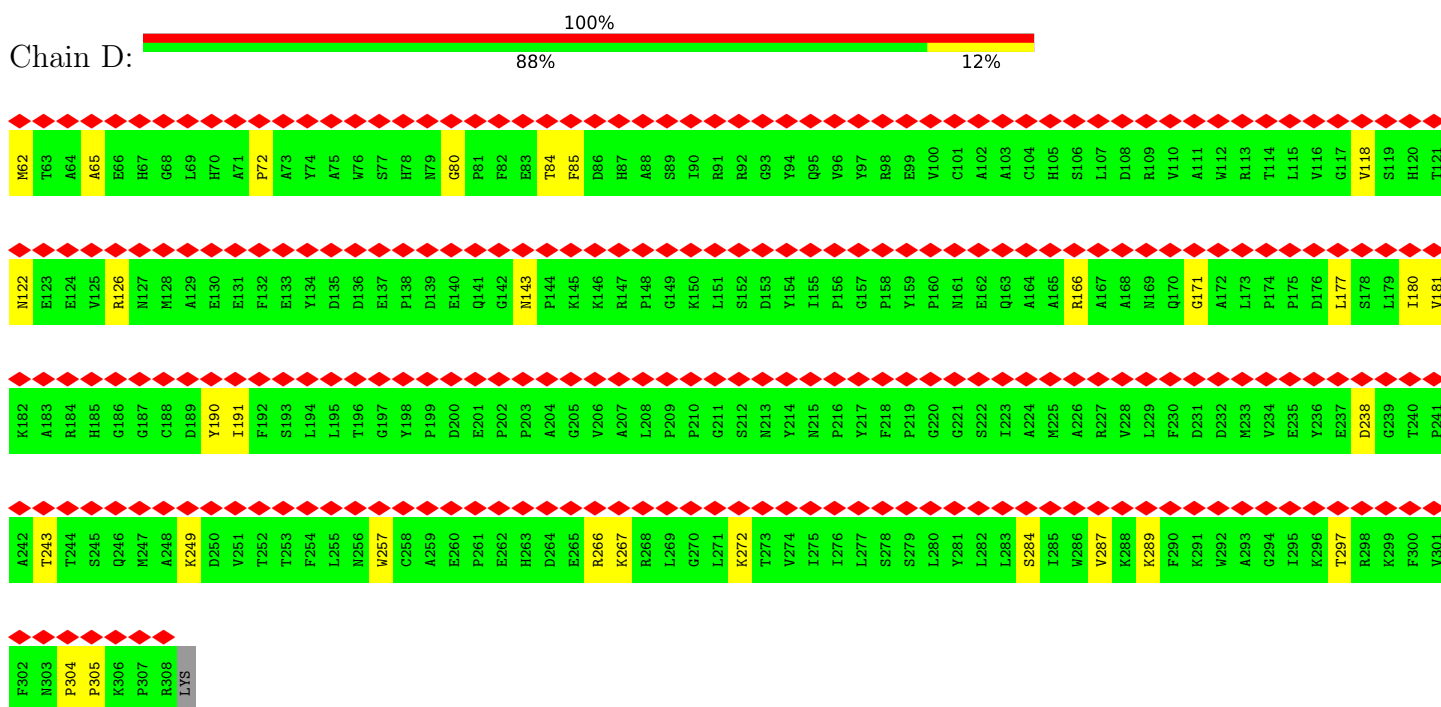




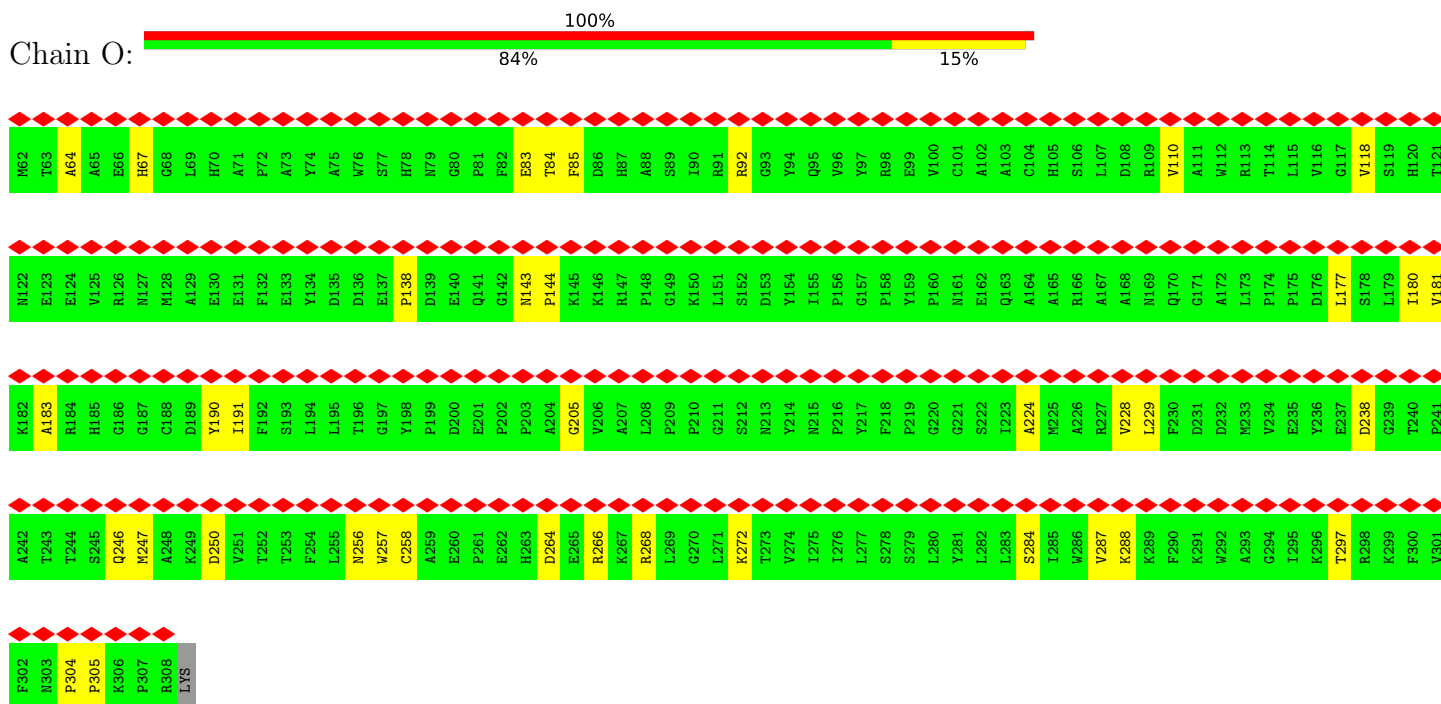
- Molecule 3: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 2, CORE PROTEIN II, UBIQUINOL-CYTOCHROME-C COMPLEX CORE PROTEIN 2



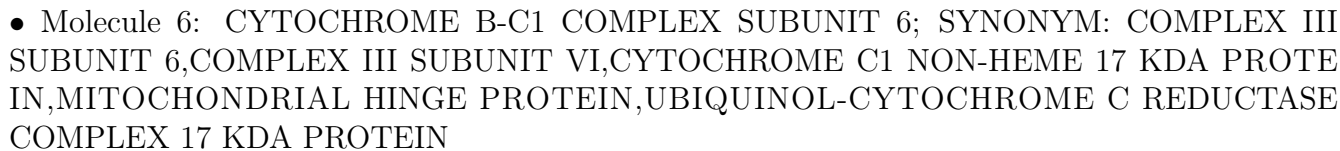
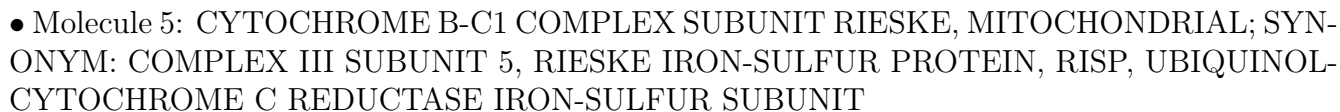
- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1



- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 4, COMPLEX III SUBUNIT IV, CYTOCHROME B-C1 COMPLEX SUBUNIT 4, UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CYTOCHROME C1 SUBUNIT, CYTOCHROME C-1

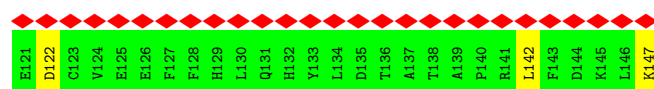
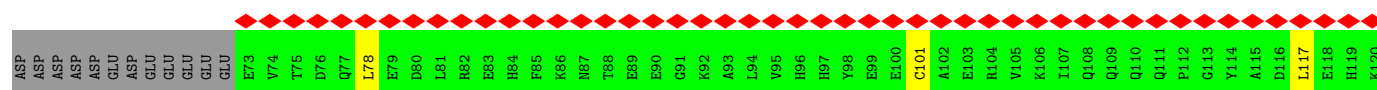
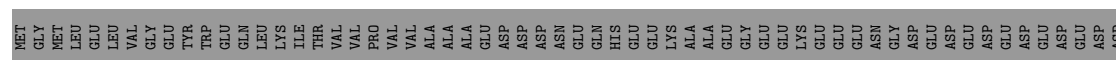


- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL; SYNONYM: COMPLEX III SUBUNIT 5, RIESKE IRON-SULFUR PROTEIN, RISP, UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

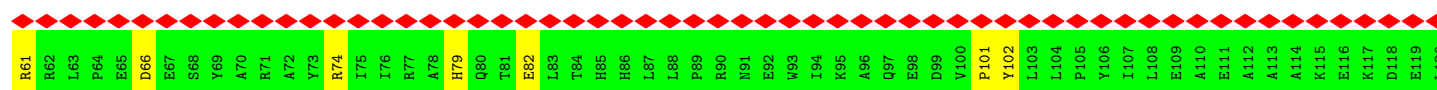
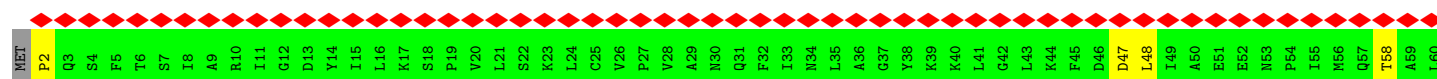
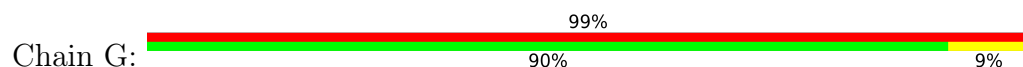




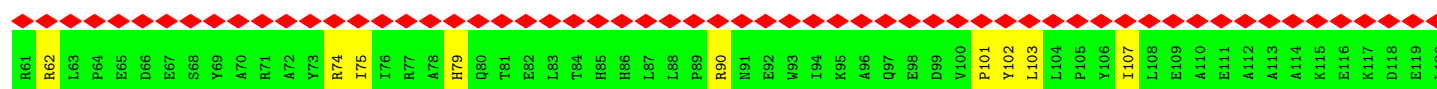
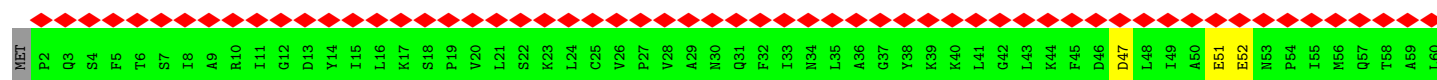
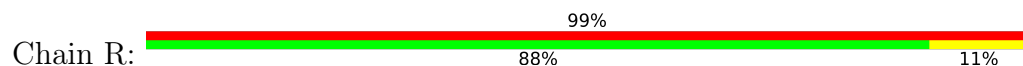
- Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 6; SYNONYM: COMPLEX III SUBUNIT 6,COMPLEX III SUBUNIT VI,CYTOCHROME C1 NON-HEME 17 KDA PROTEIN,MITOCHONDRIAL HINGE PROTEIN,UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KDA PROTEIN



- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

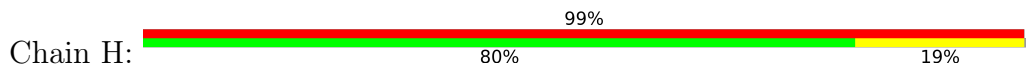


- Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 7; SYNONYM: COMPLEX III SUBUNIT 7,COMPLEX III SUBUNIT VII,UBIQUINOL-CYTOCHROME C REDUCTASE C REDUCTASE COMPLEX 14 KDA PROTEIN

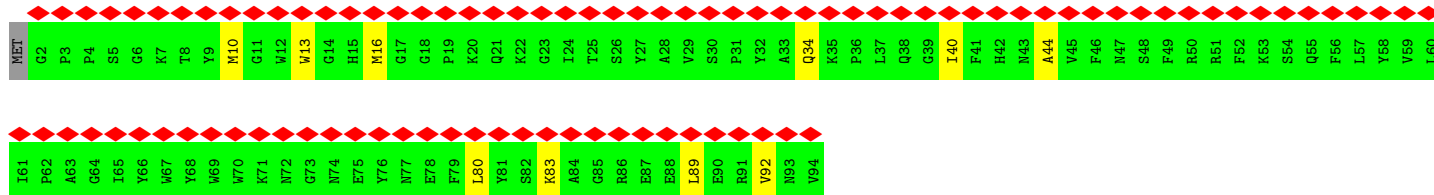
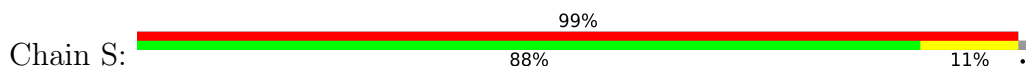




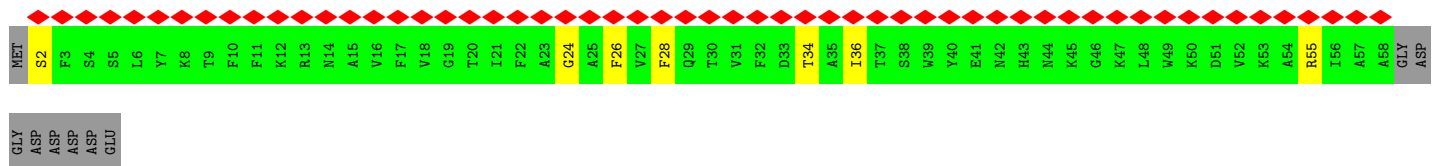
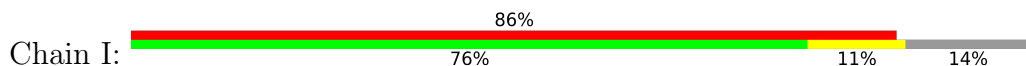
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



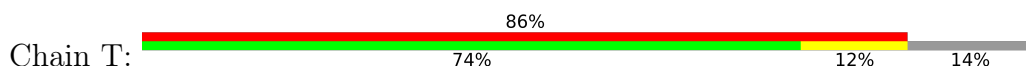
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 8; SYNONYM: COMPLEX III SUBUNIT 8, COMPLEX III SUBUNIT VII, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

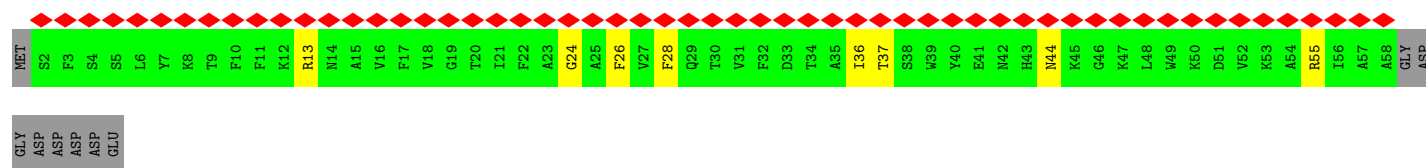


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

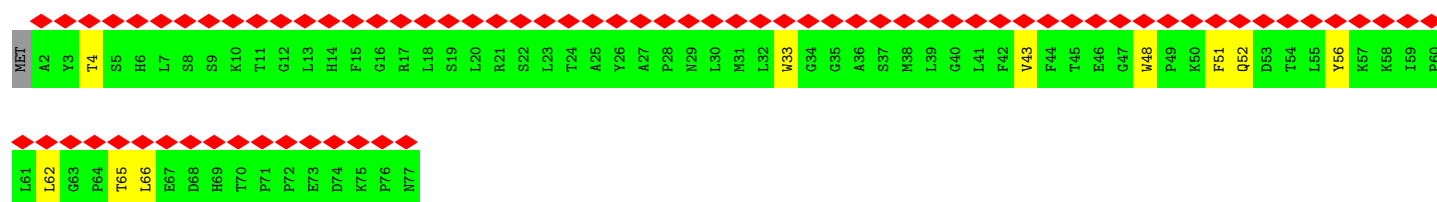
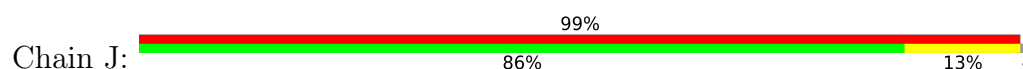


- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9; SYNONYM: COMPLEX III SUBUNIT 9, COMPLEX III SUBUNIT X, CYTOCHROME C1 NON-HEME 7.3 KDA PROTEIN, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KDA PROTEIN

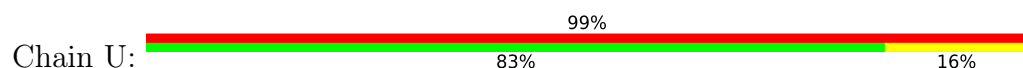




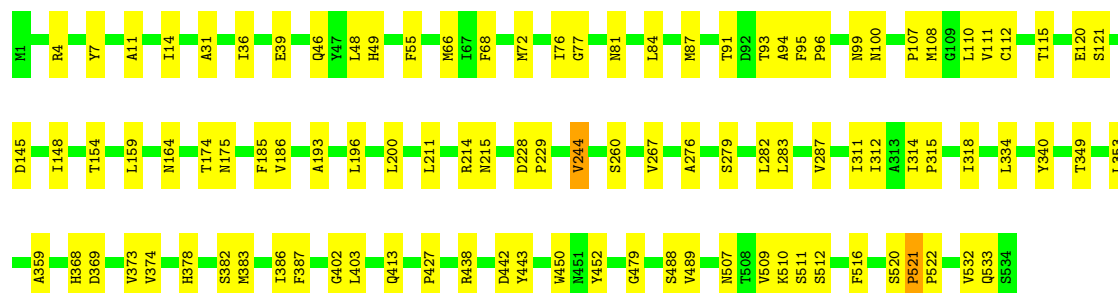
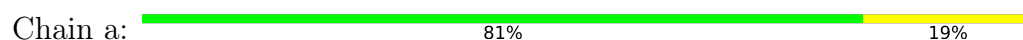
- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN



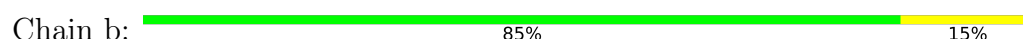
- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 10; SYNONYM: COMPLEX III SUBUNIT 10, COMPLEX III SUBUNIT XI, UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 8.5 KDA PROTEIN

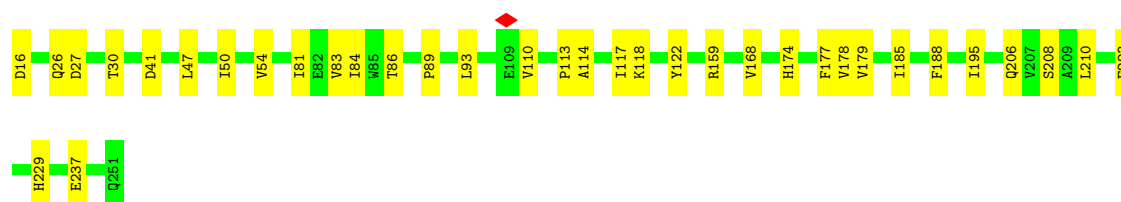


- Molecule 11: CYTOCHROME C OXIDASE SUBUNIT 1; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE I, COX1



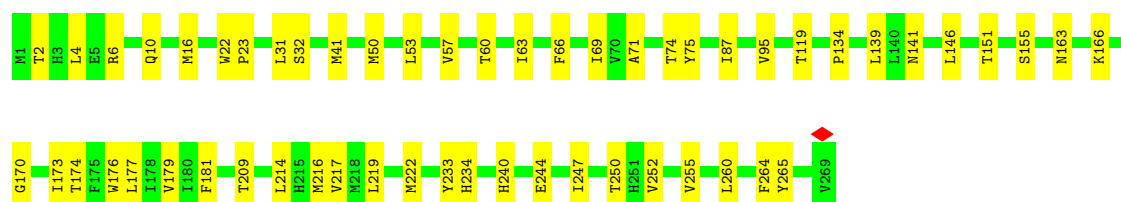
- Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 2; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE II, COX2





- Molecule 13: CYTOCHROME C OXIDASE SUBUNIT 3; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE III, COX3

Chain c: 80% 20%



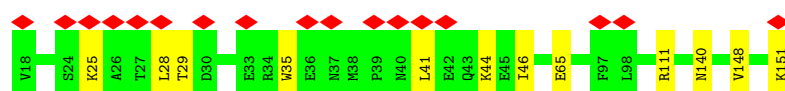
- Molecule 14: CYTOCHROME C OXIDASE SUBUNIT 4, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE IV, COX4

Chain d: 75% 18% 7%



- Molecule 15: CYTOCHROME C OXIDASE POLYPEPTIDE 5B, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VB, COX5B

Chain e: 13% 91% 9%



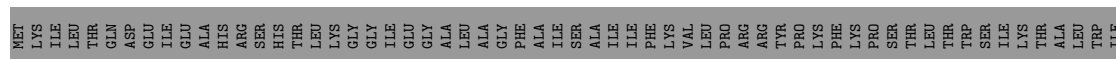
- Molecule 16: CYTOCHROME C OXIDASE SUBUNIT 6, MITOCHONDRIAL; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VI, COX6

Chain f: 86% 10%



- Molecule 17: CYTOCHROME C OXIDASE SUBUNIT 7; SYNONYM: CYTOCHROME C OXIDASE POLYPEPTIDE VII, COX7

Chain g: 93% 7%





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 73042                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 56.4                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.004                                   | Depositor |
| Minimum map value                    | -1.391                                  | Depositor |
| Average map value                    | 0.009                                   | Depositor |
| Map value standard deviation         | 0.081                                   | Depositor |
| Recommended contour level            | 0.424                                   | Depositor |
| Map size (Å)                         | 402.432, 402.432, 402.432               | wwPDB     |
| Map dimensions                       | 384, 384, 384                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.048, 1.048, 1.048                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEF, HEM, CU, FES, CUA, MG, HEC, PCF, HEA, ZN

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     | 0.21         | 0/3406  | 0.49        | 0/4615        |
| 1   | L     | 0.22         | 0/3406  | 0.53        | 0/4615        |
| 2   | B     | 0.22         | 0/2781  | 0.50        | 0/3764        |
| 2   | M     | 0.22         | 0/2781  | 0.51        | 0/3764        |
| 3   | C     | 0.26         | 0/3192  | 0.59        | 1/4354 (0.0%) |
| 3   | N     | 0.26         | 0/3192  | 0.57        | 0/4354        |
| 4   | D     | 0.20         | 0/2012  | 0.44        | 0/2740        |
| 4   | O     | 0.21         | 0/2012  | 0.44        | 0/2740        |
| 5   | E     | 0.28         | 0/1444  | 0.65        | 2/1957 (0.1%) |
| 5   | P     | 0.30         | 0/1444  | 0.67        | 0/1957        |
| 6   | F     | 0.31         | 0/647   | 0.71        | 2/870 (0.2%)  |
| 6   | Q     | 0.28         | 0/647   | 0.67        | 2/870 (0.2%)  |
| 7   | G     | 0.24         | 0/1040  | 0.54        | 0/1408        |
| 7   | R     | 0.22         | 0/1040  | 0.47        | 0/1408        |
| 8   | H     | 0.19         | 0/804   | 0.44        | 0/1088        |
| 8   | S     | 0.22         | 0/804   | 0.48        | 0/1088        |
| 9   | I     | 0.22         | 0/479   | 0.48        | 0/646         |
| 9   | T     | 0.20         | 0/479   | 0.47        | 0/646         |
| 10  | J     | 0.21         | 0/619   | 0.52        | 0/841         |
| 10  | U     | 0.26         | 0/619   | 0.58        | 0/841         |
| 11  | a     | 0.29         | 0/4290  | 0.66        | 1/5857 (0.0%) |
| 12  | b     | 0.26         | 0/1941  | 0.66        | 0/2653        |
| 13  | c     | 0.27         | 0/2218  | 0.62        | 0/3036        |
| 14  | d     | 0.26         | 0/932   | 0.61        | 0/1269        |
| 15  | e     | 0.24         | 0/1111  | 0.59        | 0/1503        |
| 16  | f     | 0.28         | 0/884   | 0.56        | 0/1196        |
| 17  | g     | 0.30         | 0/500   | 0.70        | 1/681 (0.1%)  |
| 18  | h     | 0.25         | 0/424   | 0.68        | 2/569 (0.4%)  |
| 19  | i     | 0.25         | 0/468   | 0.56        | 0/626         |
| 20  | j     | 0.31         | 0/664   | 0.75        | 1/899 (0.1%)  |
| 21  | k     | 0.24         | 0/1002  | 0.55        | 0/1364        |
| 22  | l     | 0.25         | 0/372   | 0.64        | 0/502         |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 23  | m     | 0.29         | 0/813   | 0.64        | 0/1093          |
| All | All   | 0.25         | 0/48467 | 0.57        | 12/65814 (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   | L     | 0                   | 1                   |
| 2   | B     | 0                   | 1                   |
| 3   | N     | 0                   | 1                   |
| 5   | E     | 0                   | 1                   |
| 5   | P     | 0                   | 1                   |
| 11  | a     | 0                   | 4                   |
| 13  | c     | 0                   | 1                   |
| 14  | d     | 0                   | 1                   |
| 21  | k     | 0                   | 1                   |
| All | All   | 0                   | 12                  |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 20  | j     | 46  | ALA  | N-CA-C | 10.14 | 117.34      | 108.22   |
| 11  | a     | 14  | ILE  | N-CA-C | -6.09 | 106.86      | 112.96   |
| 18  | h     | 77  | ALA  | CA-C-N | 5.71  | 131.98      | 121.70   |
| 18  | h     | 77  | ALA  | C-N-CA | 5.71  | 131.98      | 121.70   |
| 6   | F     | 117 | LEU  | CA-C-N | 5.64  | 132.30      | 121.54   |
| 6   | F     | 117 | LEU  | C-N-CA | 5.64  | 132.30      | 121.54   |
| 5   | E     | 123 | PRO  | CA-C-N | 5.47  | 131.99      | 121.54   |
| 5   | E     | 123 | PRO  | C-N-CA | 5.47  | 131.99      | 121.54   |
| 17  | g     | 43  | THR  | N-CA-C | 5.41  | 121.76      | 109.81   |
| 6   | Q     | 117 | LEU  | CA-C-N | 5.39  | 131.84      | 121.54   |
| 6   | Q     | 117 | LEU  | C-N-CA | 5.39  | 131.84      | 121.54   |
| 3   | C     | 222 | HIS  | N-CA-C | 5.27  | 116.88      | 111.03   |

There are no chirality outliers.

All (12) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | B     | 220 | GLU  | Peptide |
| 5   | E     | 167 | ILE  | Peptide |
| 1   | L     | 444 | ASP  | Peptide |
| 3   | N     | 345 | GLU  | Peptide |
| 5   | P     | 125 | GLU  | Peptide |
| 11  | a     | 120 | GLU  | Peptide |
| 11  | a     | 442 | ASP  | Peptide |
| 11  | a     | 520 | SER  | Peptide |
| 11  | a     | 91  | THR  | Peptide |
| 13  | c     | 22  | TRP  | Peptide |
| 14  | d     | 143 | LEU  | Peptide |
| 21  | k     | 95  | ASP  | Peptide |

## 5.2 Too-close contacts [i](#)

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     | 3345  | 0        | 3323     | 29      | 0            |
| 1   | L     | 3345  | 0        | 3323     | 37      | 0            |
| 2   | B     | 2735  | 0        | 2774     | 30      | 0            |
| 2   | M     | 2735  | 0        | 2774     | 35      | 0            |
| 3   | C     | 3090  | 0        | 3127     | 42      | 0            |
| 3   | N     | 3090  | 0        | 3129     | 45      | 0            |
| 4   | D     | 1951  | 0        | 1874     | 22      | 0            |
| 4   | O     | 1951  | 0        | 1874     | 28      | 0            |
| 5   | E     | 1411  | 0        | 1386     | 30      | 0            |
| 5   | P     | 1411  | 0        | 1386     | 29      | 0            |
| 6   | F     | 633   | 0        | 587      | 7       | 0            |
| 6   | Q     | 633   | 0        | 587      | 4       | 0            |
| 7   | G     | 1019  | 0        | 1034     | 11      | 0            |
| 7   | R     | 1019  | 0        | 1034     | 11      | 0            |
| 8   | H     | 773   | 0        | 736      | 14      | 0            |
| 8   | S     | 773   | 0        | 735      | 8       | 0            |
| 9   | I     | 465   | 0        | 459      | 6       | 0            |
| 9   | T     | 465   | 0        | 459      | 7       | 0            |
| 10  | J     | 599   | 0        | 594      | 8       | 0            |
| 10  | U     | 599   | 0        | 594      | 9       | 0            |
| 11  | a     | 4162  | 0        | 4189     | 66      | 0            |
| 12  | b     | 1889  | 0        | 1866     | 26      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | c     | 2146  | 0        | 2137     | 38      | 0            |
| 14  | d     | 913   | 0        | 910      | 20      | 0            |
| 15  | e     | 1083  | 0        | 1081     | 9       | 0            |
| 16  | f     | 866   | 0        | 834      | 6       | 0            |
| 17  | g     | 484   | 0        | 517      | 2       | 0            |
| 18  | h     | 409   | 0        | 408      | 5       | 0            |
| 19  | i     | 456   | 0        | 469      | 4       | 0            |
| 20  | j     | 642   | 0        | 586      | 7       | 0            |
| 21  | k     | 967   | 0        | 933      | 11      | 0            |
| 22  | l     | 361   | 0        | 363      | 4       | 0            |
| 23  | m     | 799   | 0        | 819      | 4       | 0            |
| 24  | A     | 31    | 0        | 35       | 2       | 0            |
| 24  | C     | 83    | 0        | 113      | 3       | 0            |
| 24  | E     | 43    | 0        | 62       | 2       | 0            |
| 24  | H     | 32    | 0        | 37       | 0       | 0            |
| 24  | J     | 29    | 0        | 31       | 0       | 0            |
| 24  | L     | 36    | 0        | 43       | 1       | 0            |
| 24  | N     | 83    | 0        | 118      | 3       | 0            |
| 24  | P     | 42    | 0        | 60       | 1       | 0            |
| 24  | S     | 36    | 0        | 48       | 1       | 0            |
| 24  | U     | 47    | 0        | 73       | 0       | 0            |
| 24  | a     | 33    | 0        | 39       | 1       | 0            |
| 24  | b     | 73    | 0        | 95       | 1       | 0            |
| 24  | c     | 77    | 0        | 100      | 2       | 0            |
| 24  | e     | 42    | 0        | 60       | 1       | 0            |
| 25  | C     | 86    | 0        | 60       | 3       | 0            |
| 25  | N     | 86    | 0        | 60       | 5       | 0            |
| 26  | C     | 55    | 0        | 52       | 0       | 0            |
| 26  | D     | 67    | 0        | 78       | 1       | 0            |
| 26  | H     | 53    | 0        | 50       | 3       | 0            |
| 26  | L     | 58    | 0        | 60       | 2       | 0            |
| 26  | N     | 66    | 0        | 75       | 4       | 0            |
| 26  | O     | 71    | 0        | 89       | 2       | 0            |
| 26  | S     | 53    | 0        | 50       | 2       | 0            |
| 27  | C     | 50    | 0        | 80       | 0       | 0            |
| 27  | I     | 39    | 0        | 52       | 0       | 0            |
| 27  | N     | 39    | 0        | 55       | 3       | 0            |
| 27  | S     | 32    | 0        | 38       | 0       | 0            |
| 27  | T     | 50    | 0        | 80       | 1       | 0            |
| 27  | e     | 36    | 0        | 44       | 3       | 0            |
| 28  | D     | 43    | 0        | 31       | 1       | 0            |
| 28  | O     | 43    | 0        | 31       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | E     | 4     | 0        | 0        | 0       | 0            |
| 29  | P     | 4     | 0        | 0        | 1       | 0            |
| 30  | a     | 1     | 0        | 0        | 0       | 0            |
| 31  | a     | 120   | 0        | 105      | 9       | 0            |
| 32  | a     | 1     | 0        | 0        | 0       | 0            |
| 33  | b     | 2     | 0        | 0        | 0       | 0            |
| 34  | d     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 48966 | 0        | 48905    | 533     | 0            |

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 5.

All (533) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:i:34:TRP:O     | 19:i:38:MET:HB2   | 1.84                     | 0.78              |
| 11:a:66:MET:HG2   | 31:a:602:HEA:HBC1 | 1.65                     | 0.76              |
| 2:M:50:LEU:O      | 2:M:54:PHE:HB2    | 1.84                     | 0.75              |
| 5:E:118:ILE:HA    | 5:E:153:LEU:O     | 1.87                     | 0.72              |
| 2:B:255:VAL:HG12  | 2:B:321:THR:HG21  | 1.74                     | 0.69              |
| 11:a:159:LEU:HB2  | 11:a:200:LEU:HD11 | 1.75                     | 0.68              |
| 13:c:260:LEU:O    | 13:c:264:PHE:HB2  | 1.95                     | 0.67              |
| 5:P:175:GLY:HA3   | 5:P:185:TYR:O     | 1.95                     | 0.67              |
| 9:T:13:ARG:HH21   | 10:U:29:ASN:HD22  | 1.40                     | 0.67              |
| 11:a:383:MET:O    | 11:a:387:PHE:HB2  | 1.94                     | 0.67              |
| 11:a:87:MET:HE1   | 11:a:185:PHE:HB3  | 1.76                     | 0.66              |
| 3:N:297:ALA:O     | 3:N:301:VAL:HB    | 1.95                     | 0.65              |
| 8:H:40:ILE:O      | 8:H:44:ALA:HB2    | 1.97                     | 0.65              |
| 2:B:19:VAL:HG11   | 2:B:201:VAL:HG11  | 1.77                     | 0.64              |
| 3:C:297:ALA:O     | 3:C:301:VAL:HB    | 1.97                     | 0.64              |
| 5:E:116:VAL:HA    | 5:E:156:LEU:HA    | 1.80                     | 0.63              |
| 13:c:216:MET:HG3  | 13:c:219:LEU:HD23 | 1.81                     | 0.63              |
| 5:E:123:PRO:HA    | 5:E:126:ILE:HB    | 1.78                     | 0.63              |
| 2:M:255:VAL:HG22  | 2:M:321:THR:HG21  | 1.80                     | 0.62              |
| 16:f:131:VAL:O    | 16:f:135:LEU:HB2  | 1.99                     | 0.62              |
| 11:a:94:ALA:O     | 11:a:164:ASN:ND2  | 2.32                     | 0.62              |
| 12:b:117:ILE:HB   | 12:b:177:PHE:HB3  | 1.82                     | 0.62              |
| 12:b:110:VAL:HG13 | 12:b:208:SER:HB2  | 1.82                     | 0.61              |
| 4:O:238:ASP:HB2   | 9:T:55:ARG:HH12   | 1.66                     | 0.61              |
| 1:L:441:GLY:HA2   | 8:S:13:TRP:HB3    | 1.83                     | 0.60              |
| 9:I:34:THR:HG21   | 10:J:65:THR:HB    | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:373:VAL:HG13 | 31:a:603:HEA:HHa  | 1.84                     | 0.60              |
| 11:a:7:TYR:O      | 11:a:100:ASN:ND2  | 2.34                     | 0.60              |
| 4:O:268:ARG:HD2   | 9:T:37:THR:HG22   | 1.84                     | 0.60              |
| 5:E:146:ARG:NH1   | 5:E:155:MET:SD    | 2.75                     | 0.60              |
| 3:N:183:HIS:HE1   | 25:N:601:HEM:NB   | 2.00                     | 0.60              |
| 1:L:184:SER:OG    | 5:P:35:ARG:NH1    | 2.35                     | 0.59              |
| 14:d:115:PRO:HD2  | 14:d:118:SER:HB2  | 1.84                     | 0.59              |
| 20:j:41:LYS:NZ    | 20:j:45:PHE:O     | 2.35                     | 0.59              |
| 3:N:59:GLU:HG3    | 3:N:60:LEU:HG     | 1.84                     | 0.59              |
| 13:c:74:THR:HG21  | 13:c:234:HIS:HD2  | 1.66                     | 0.59              |
| 14:d:91:LYS:NZ    | 14:d:137:CYS:O    | 2.35                     | 0.59              |
| 12:b:223:GLU:O    | 12:b:229:HIS:CE1  | 2.56                     | 0.58              |
| 11:a:68:PHE:HB3   | 11:a:154:THR:HG21 | 1.84                     | 0.58              |
| 11:a:279:SER:O    | 11:a:283:LEU:HB2  | 2.04                     | 0.58              |
| 2:M:305:VAL:HG21  | 2:M:368:LEU:HB3   | 1.86                     | 0.58              |
| 11:a:349:THR:HG21 | 12:b:54:VAL:HG11  | 1.86                     | 0.58              |
| 11:a:215:ASN:ND2  | 13:c:41:MET:SD    | 2.77                     | 0.57              |
| 8:H:55:GLN:NE2    | 26:H:601:CDL:OB3  | 2.37                     | 0.57              |
| 3:N:346:VAL:HG11  | 8:S:80:LEU:HD22   | 1.85                     | 0.57              |
| 1:A:270:VAL:HG11  | 1:A:396:ILE:HD13  | 1.86                     | 0.57              |
| 13:c:4:LEU:HA     | 14:d:148:VAL:HG21 | 1.85                     | 0.57              |
| 16:f:117:ASN:HD22 | 22:l:26:GLU:HG2   | 1.70                     | 0.57              |
| 5:E:184:HIS:HB2   | 5:E:193:LYS:HB2   | 1.86                     | 0.57              |
| 13:c:134:PRO:HB3  | 13:c:265:TYR:HB3  | 1.85                     | 0.57              |
| 5:P:159:CYS:HB2   | 29:P:301:FES:S2   | 2.44                     | 0.57              |
| 2:B:30:THR:HG22   | 2:B:190:GLU:HG3   | 1.87                     | 0.56              |
| 1:L:126:GLN:HE21  | 1:L:127:GLN:HE21  | 1.53                     | 0.56              |
| 3:C:270:VAL:HG23  | 3:C:276:LEU:HD21  | 1.87                     | 0.56              |
| 2:B:305:VAL:HG11  | 2:B:368:LEU:HB3   | 1.88                     | 0.56              |
| 1:L:99:ARG:NH2    | 1:L:176:LEU:O     | 2.39                     | 0.56              |
| 11:a:369:ASP:HA   | 11:a:438:ARG:HE   | 1.70                     | 0.56              |
| 11:a:39:GLU:HG3   | 11:a:48:LEU:HG    | 1.88                     | 0.55              |
| 11:a:244:VAL:HG11 | 31:a:603:HEA:HHd  | 1.88                     | 0.55              |
| 9:I:24:GLY:O      | 9:I:28:PHE:HB3    | 2.07                     | 0.55              |
| 14:d:134:CYS:HB3  | 14:d:138:GLY:H    | 1.71                     | 0.55              |
| 8:H:82:SER:OG     | 8:H:83:LYS:N      | 2.40                     | 0.55              |
| 1:L:317:HIS:HE1   | 1:L:351:TRP:HE1   | 1.54                     | 0.55              |
| 11:a:95:PHE:HE1   | 13:c:87:ILE:HG22  | 1.71                     | 0.55              |
| 12:b:83:VAL:HA    | 12:b:86:THR:HG22  | 1.88                     | 0.55              |
| 4:D:181:VAL:HG12  | 4:D:191:ILE:HG13  | 1.88                     | 0.55              |
| 16:f:96:ARG:NH1   | 16:f:99:ASN:OD1   | 2.40                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:456:ARG:HB2   | 10:U:33:TRP:HE1   | 1.72                     | 0.55              |
| 8:H:42:HIS:O      | 8:H:46:PHE:HB2    | 2.06                     | 0.55              |
| 4:O:181:VAL:HG12  | 4:O:191:ILE:HG13  | 1.89                     | 0.55              |
| 2:M:54:PHE:HZ     | 2:M:114:PHE:HA    | 1.72                     | 0.54              |
| 15:e:41:LEU:HA    | 15:e:44:LYS:HE3   | 1.89                     | 0.54              |
| 1:A:317:HIS:HE1   | 1:A:351:TRP:HE1   | 1.53                     | 0.54              |
| 1:L:236:PRO:HB3   | 15:e:41:LEU:HB3   | 1.90                     | 0.54              |
| 2:M:84:ARG:HH12   | 2:M:144:ASP:HB3   | 1.72                     | 0.54              |
| 26:N:603:CDL:H542 | 26:N:603:CDL:HA61 | 1.90                     | 0.54              |
| 3:N:127:THR:HA    | 3:N:130:LEU:HD12  | 1.88                     | 0.54              |
| 2:B:154:GLY:O     | 2:B:157:ASN:ND2   | 2.41                     | 0.54              |
| 3:C:210:LEU:HD21  | 7:G:82:GLU:HG3    | 1.88                     | 0.54              |
| 11:a:46:GLN:OE1   | 15:e:111:ARG:NH2  | 2.41                     | 0.54              |
| 11:a:77:GLY:O     | 11:a:81:ASN:HB2   | 2.08                     | 0.54              |
| 3:N:213:THR:HG22  | 7:R:51:GLU:HG2    | 1.90                     | 0.54              |
| 1:A:145:LEU:HD21  | 1:A:186:GLU:HG2   | 1.89                     | 0.54              |
| 24:A:501:PEF:H12  | 3:C:3:PHE:HB3     | 1.90                     | 0.54              |
| 2:B:272:SER:OG    | 2:B:288:PHE:O     | 2.23                     | 0.54              |
| 11:a:108:MET:HA   | 11:a:111:VAL:HG12 | 1.89                     | 0.54              |
| 15:e:25:LYS:O     | 15:e:29:THR:OG1   | 2.24                     | 0.54              |
| 12:b:41:ASP:OD2   | 19:i:37:HIS:ND1   | 2.40                     | 0.53              |
| 5:P:72:LYS:HG3    | 10:U:44:PHE:HA    | 1.89                     | 0.53              |
| 1:L:375:GLY:HA3   | 2:M:28:ILE:HG13   | 1.88                     | 0.53              |
| 2:M:26:THR:OG1    | 2:M:191:ASN:ND2   | 2.41                     | 0.53              |
| 11:a:174:THR:OG1  | 11:a:175:ASN:N    | 2.41                     | 0.53              |
| 3:N:31:ASN:HB3    | 3:N:232:THR:HG21  | 1.91                     | 0.53              |
| 7:G:47:ASP:OD1    | 7:G:102:TYR:OH    | 2.26                     | 0.53              |
| 2:M:30:THR:OG1    | 2:M:190:GLU:OE1   | 2.27                     | 0.53              |
| 12:b:178:VAL:HG12 | 12:b:206:GLN:HB3  | 1.91                     | 0.53              |
| 6:Q:122:ASP:O     | 8:S:83:LYS:NZ     | 2.35                     | 0.53              |
| 24:c:302:PEF:N    | 21:k:122:ASN:OD1  | 2.42                     | 0.53              |
| 5:E:96:VAL:HG11   | 5:E:118:ILE:HG21  | 1.91                     | 0.53              |
| 5:E:129:ALA:HB1   | 5:E:188:SER:HB2   | 1.91                     | 0.53              |
| 1:A:317:HIS:CE1   | 1:A:351:TRP:HE1   | 2.27                     | 0.52              |
| 5:E:82:MET:O      | 3:N:178:ARG:NH2   | 2.42                     | 0.52              |
| 3:N:82:HIS:CE1    | 25:N:601:HEM:NC   | 2.78                     | 0.52              |
| 12:b:16:ASP:N     | 15:e:140:ASN:OD1  | 2.42                     | 0.52              |
| 3:N:314:ARG:NH1   | 7:R:52:GLU:OE2    | 2.42                     | 0.52              |
| 5:P:51:LYS:HE2    | 26:S:101:CDL:HA32 | 1.90                     | 0.52              |
| 5:P:116:VAL:HG12  | 5:P:156:LEU:HB3   | 1.91                     | 0.52              |
| 15:e:35:TRP:HZ3   | 15:e:46:ILE:HD11  | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:138:LYS:NZ    | 5:E:194:GLY:O     | 2.42                     | 0.52              |
| 1:L:108:SER:OG    | 1:L:109:LEU:N     | 2.42                     | 0.52              |
| 2:M:149:ILE:HG21  | 2:M:229:ASN:HB2   | 1.91                     | 0.52              |
| 5:P:166:PRO:HG3   | 5:P:178:CYS:HB2   | 1.91                     | 0.52              |
| 13:c:119:THR:OG1  | 21:k:97:GLU:OE2   | 2.26                     | 0.52              |
| 1:A:431:ILE:O     | 1:A:445:TYR:OH    | 2.27                     | 0.52              |
| 1:L:297:LEU:HB3   | 2:M:65:LEU:HD12   | 1.92                     | 0.52              |
| 4:O:284:SER:HA    | 4:O:287:VAL:HG12  | 1.92                     | 0.52              |
| 11:a:402:GLY:HA3  | 11:a:521:PRO:HD3  | 1.91                     | 0.52              |
| 2:B:35:VAL:HG12   | 2:B:185:LEU:HB3   | 1.92                     | 0.52              |
| 5:P:57:TYR:HA     | 5:P:60:VAL:HG22   | 1.92                     | 0.52              |
| 1:A:283:GLN:OE1   | 1:A:373:GLN:NE2   | 2.43                     | 0.52              |
| 2:B:149:ILE:HG21  | 2:B:229:ASN:HB2   | 1.91                     | 0.52              |
| 2:B:47:VAL:HG22   | 2:B:167:VAL:HG21  | 1.92                     | 0.52              |
| 13:c:173:ILE:O    | 13:c:177:LEU:HB2  | 2.09                     | 0.52              |
| 22:l:28:TRP:HA    | 22:l:31:THR:HG22  | 1.92                     | 0.52              |
| 20:j:35:HIS:O     | 20:j:39:ASN:ND2   | 2.42                     | 0.51              |
| 1:A:149:GLN:HB3   | 1:A:182:LEU:HD21  | 1.92                     | 0.51              |
| 3:C:54:TYR:OH     | 3:C:134:CYS:O     | 2.29                     | 0.51              |
| 5:E:57:TYR:HA     | 5:E:60:VAL:HG12   | 1.93                     | 0.51              |
| 11:a:353:LEU:HD22 | 12:b:47:LEU:HG    | 1.93                     | 0.51              |
| 13:c:10:GLN:NE2   | 13:c:16:MET:SD    | 2.83                     | 0.51              |
| 10:J:52:GLN:HE21  | 10:J:66:LEU:HD23  | 1.75                     | 0.51              |
| 11:a:112:CYS:HA   | 11:a:115:THR:HG22 | 1.92                     | 0.51              |
| 1:L:317:HIS:CE1   | 1:L:351:TRP:HE1   | 2.29                     | 0.51              |
| 3:N:137:GLY:H     | 3:N:140:SER:HB3   | 1.75                     | 0.51              |
| 12:b:114:ALA:O    | 20:j:11:THR:OG1   | 2.27                     | 0.51              |
| 14:d:59:ASP:OD1   | 14:d:59:ASP:N     | 2.43                     | 0.51              |
| 5:E:102:PRO:HD2   | 5:E:105:LYS:HD3   | 1.91                     | 0.51              |
| 2:M:355:ALA:HB1   | 2:M:362:LEU:HD13  | 1.93                     | 0.51              |
| 6:Q:78:LEU:HD13   | 6:Q:142:LEU:HD22  | 1.93                     | 0.51              |
| 4:D:249:LYS:NZ    | 6:F:147:LYS:O     | 2.44                     | 0.51              |
| 2:B:190:GLU:OE1   | 2:B:191:ASN:ND2   | 2.44                     | 0.51              |
| 2:B:252:GLN:HE21  | 2:B:346:PHE:HD1   | 1.58                     | 0.51              |
| 26:H:601:CDL:HA4  | 26:H:601:CDL:H522 | 1.92                     | 0.51              |
| 5:P:104:GLY:HA2   | 5:P:119:ARG:HE    | 1.76                     | 0.50              |
| 4:O:272:LYS:HG2   | 9:T:36:ILE:HG21   | 1.93                     | 0.50              |
| 9:T:24:GLY:O      | 9:T:28:PHE:HB3    | 2.10                     | 0.50              |
| 5:E:164:CYS:SG    | 5:E:165:VAL:N     | 2.81                     | 0.50              |
| 3:N:65:VAL:HG21   | 3:N:135:VAL:HG23  | 1.93                     | 0.50              |
| 3:C:226:ILE:HG23  | 24:C:604:PEF:H341 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:L:501:CDL:H542 | 26:L:501:CDL:H322 | 1.94                     | 0.50              |
| 7:R:47:ASP:OD1    | 7:R:102:TYR:OH    | 2.30                     | 0.50              |
| 2:B:229:ASN:O     | 2:B:354:VAL:HA    | 2.12                     | 0.50              |
| 3:C:159:ASN:HA    | 3:C:162:VAL:HG12  | 1.93                     | 0.50              |
| 3:C:82:HIS:CE1    | 25:C:601:HEM:NC   | 2.79                     | 0.50              |
| 4:O:84:THR:OG1    | 4:O:85:PHE:N      | 2.44                     | 0.50              |
| 11:a:488:SER:OG   | 11:a:489:VAL:N    | 2.45                     | 0.50              |
| 3:C:117:GLY:C     | 25:C:602:HEM:HBC2 | 2.37                     | 0.50              |
| 5:E:121:ARG:HH11  | 5:E:150:PRO:HA    | 1.77                     | 0.50              |
| 1:A:98:SER:OG     | 1:A:99:ARG:N      | 2.45                     | 0.49              |
| 3:C:345:GLU:OE1   | 4:D:62:MET:N      | 2.44                     | 0.49              |
| 13:c:141:ASN:HB2  | 13:c:181:PHE:HD1  | 1.77                     | 0.49              |
| 23:m:176:HIS:HB3  | 23:m:179:LYS:HE3  | 1.93                     | 0.49              |
| 3:C:14:ASN:HA     | 3:C:18:ILE:HB     | 1.94                     | 0.49              |
| 5:E:110:LYS:HA    | 5:E:115:PRO:HA    | 1.94                     | 0.49              |
| 5:E:117:PHE:O     | 5:E:154:ILE:HA    | 2.12                     | 0.49              |
| 1:L:230:LEU:O     | 1:L:231:GLN:NE2   | 2.44                     | 0.49              |
| 4:O:205:GLY:HA3   | 6:Q:122:ASP:HA    | 1.95                     | 0.49              |
| 12:b:27:ASP:OD1   | 12:b:27:ASP:N     | 2.45                     | 0.49              |
| 1:A:99:ARG:NH1    | 1:A:162:GLU:OE1   | 2.44                     | 0.49              |
| 3:N:117:GLY:C     | 25:N:602:HEM:HBC2 | 2.38                     | 0.49              |
| 4:O:110:VAL:HG21  | 4:O:258:CYS:HB2   | 1.93                     | 0.49              |
| 31:a:603:HEA:H211 | 12:b:50:ILE:HG21  | 1.94                     | 0.49              |
| 21:k:24:PRO:O     | 21:k:27:LYS:NZ    | 2.42                     | 0.49              |
| 4:D:190:TYR:OH    | 28:D:401:HEC:O2A  | 2.29                     | 0.49              |
| 3:N:383:VAL:HG12  | 7:R:101:PRO:HG2   | 1.94                     | 0.49              |
| 11:a:107:PRO:HA   | 11:a:110:LEU:HB3  | 1.94                     | 0.49              |
| 8:H:29:VAL:HB     | 8:H:34:GLN:HE21   | 1.77                     | 0.49              |
| 4:O:181:VAL:HG21  | 4:O:256:ASN:HA    | 1.94                     | 0.49              |
| 4:O:288:LYS:NZ    | 26:O:402:CDL:OA3  | 2.37                     | 0.49              |
| 11:a:507:ASN:ND2  | 14:d:133:ARG:O    | 2.45                     | 0.49              |
| 3:C:25:SER:OG     | 7:G:82:GLU:OE1    | 2.31                     | 0.49              |
| 4:D:72:PRO:HG3    | 6:F:135:ASP:HB3   | 1.94                     | 0.49              |
| 1:L:125:ILE:HG23  | 1:L:230:LEU:HG    | 1.95                     | 0.49              |
| 1:L:352:ASN:ND2   | 1:L:452:MET:O     | 2.46                     | 0.49              |
| 13:c:155:SER:HB2  | 13:c:170:GLY:HA3  | 1.94                     | 0.49              |
| 1:L:376:GLN:HE21  | 2:M:92:THR:HG21   | 1.78                     | 0.49              |
| 3:C:31:ASN:HB3    | 3:C:232:THR:HG21  | 1.95                     | 0.48              |
| 13:c:222:MET:HG3  | 24:c:301:PEF:H331 | 1.95                     | 0.48              |
| 3:C:311:SER:HB3   | 3:C:371:SER:HB2   | 1.95                     | 0.48              |
| 8:S:40:ILE:O      | 8:S:44:ALA:HB2    | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:95:PHE:O     | 11:a:164:ASN:ND2  | 2.46                     | 0.48              |
| 24:A:501:PEF:H42  | 3:C:3:PHE:HB2     | 1.95                     | 0.48              |
| 2:B:228:GLU:HG3   | 2:B:353:TYR:HD2   | 1.78                     | 0.48              |
| 6:F:117:LEU:H     | 6:F:120:LYS:HZ1   | 1.61                     | 0.48              |
| 5:E:114:LYS:HZ3   | 5:E:158:ILE:HD13  | 1.79                     | 0.48              |
| 5:P:85:THR:OG1    | 5:P:87:ASP:OD1    | 2.30                     | 0.48              |
| 1:L:345:HIS:HE1   | 26:L:501:CDL:H1   | 1.79                     | 0.48              |
| 2:M:65:LEU:HD11   | 2:M:69:ARG:HH11   | 1.78                     | 0.48              |
| 3:N:339:ILE:HD11  | 3:N:351:MET:HE2   | 1.96                     | 0.48              |
| 22:l:54:PRO:HA    | 22:l:57:VAL:HG12  | 1.94                     | 0.48              |
| 2:M:265:SER:HB3   | 2:M:267:LEU:H     | 1.76                     | 0.48              |
| 17:g:23:HIS:HB3   | 17:g:26:SER:HB2   | 1.95                     | 0.48              |
| 3:C:7:ASN:HD21    | 24:C:605:PEF:H111 | 1.78                     | 0.48              |
| 10:J:52:GLN:HA    | 10:J:56:TYR:HB2   | 1.94                     | 0.48              |
| 24:N:604:PEF:H132 | 5:P:63:MET:HE3    | 1.96                     | 0.48              |
| 12:b:30:THR:HG23  | 12:b:210:LEU:H    | 1.79                     | 0.48              |
| 14:d:96:ASP:OD1   | 14:d:96:ASP:N     | 2.46                     | 0.48              |
| 3:N:84:ASN:ND2    | 3:N:243:PHE:O     | 2.46                     | 0.48              |
| 3:N:124:THR:HA    | 3:N:127:THR:HG22  | 1.96                     | 0.48              |
| 11:a:452:TYR:OH   | 27:e:202:PCF:O22  | 2.31                     | 0.48              |
| 1:L:431:ILE:O     | 1:L:445:TYR:OH    | 2.31                     | 0.48              |
| 11:a:228:ASP:N    | 11:a:228:ASP:OD1  | 2.46                     | 0.48              |
| 1:L:67:ASN:HD21   | 1:L:176:LEU:HB3   | 1.79                     | 0.47              |
| 3:N:72:VAL:HG23   | 5:P:85:THR:HG22   | 1.96                     | 0.47              |
| 1:A:359:THR:OG1   | 1:A:362:GLU:OE1   | 2.24                     | 0.47              |
| 3:C:362:TYR:HA    | 3:C:366:ILE:HB    | 1.95                     | 0.47              |
| 4:D:272:LYS:HG2   | 9:I:36:ILE:HG21   | 1.96                     | 0.47              |
| 24:C:604:PEF:H142 | 5:E:63:MET:HE3    | 1.96                     | 0.47              |
| 11:a:95:PHE:HB2   | 11:a:164:ASN:HD22 | 1.79                     | 0.47              |
| 15:e:28:LEU:HD21  | 15:e:65:GLU:HA    | 1.96                     | 0.47              |
| 11:a:368:HIS:ND1  | 31:a:603:HEA:O1A  | 2.39                     | 0.47              |
| 12:b:118:LYS:NZ   | 20:j:57:ALA:O     | 2.48                     | 0.47              |
| 14:d:128:VAL:HG23 | 14:d:145:PRO:HG3  | 1.96                     | 0.47              |
| 2:B:271:ILE:HA    | 2:B:289:VAL:HG22  | 1.96                     | 0.47              |
| 11:a:521:PRO:HA   | 11:a:522:PRO:HD3  | 1.80                     | 0.47              |
| 13:c:244:GLU:HA   | 13:c:247:ILE:HG12 | 1.95                     | 0.47              |
| 1:A:114:ASP:N     | 1:A:114:ASP:OD2   | 2.45                     | 0.47              |
| 2:B:69:ARG:NH2    | 7:R:121:ASP:OD1   | 2.47                     | 0.47              |
| 2:B:162:ASP:OD1   | 2:B:162:ASP:N     | 2.44                     | 0.47              |
| 4:D:238:ASP:HB2   | 9:I:55:ARG:HH12   | 1.79                     | 0.47              |
| 1:L:108:SER:OG    | 1:L:112:SER:O     | 2.30                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:108:MET:HB3  | 13:c:31:LEU:HB2   | 1.97                     | 0.47              |
| 11:a:511:SER:OG   | 11:a:512:SER:N    | 2.46                     | 0.47              |
| 14:d:48:GLY:HA3   | 14:d:68:ARG:HH12  | 1.79                     | 0.47              |
| 4:D:284:SER:HA    | 4:D:287:VAL:HG12  | 1.97                     | 0.47              |
| 4:O:83:GLU:HA     | 9:T:44:ASN:HD21   | 1.80                     | 0.47              |
| 11:a:4:ARG:NH1    | 18:h:36:GLU:O     | 2.47                     | 0.47              |
| 13:c:247:ILE:HA   | 13:c:250:THR:HG22 | 1.96                     | 0.47              |
| 21:k:125:ILE:HG23 | 21:k:127:HIS:H    | 1.80                     | 0.47              |
| 4:O:224:ALA:HB3   | 28:O:401:HEC:HBD2 | 1.97                     | 0.47              |
| 5:E:43:LEU:HD21   | 8:H:29:VAL:HG11   | 1.96                     | 0.47              |
| 1:A:297:LEU:HB3   | 2:B:65:LEU:HD12   | 1.97                     | 0.47              |
| 3:C:65:VAL:HG21   | 3:C:135:VAL:HG23  | 1.97                     | 0.47              |
| 2:M:231:VAL:HB    | 2:M:356:VAL:HG22  | 1.96                     | 0.47              |
| 1:A:263:LEU:HD13  | 1:A:431:ILE:HD12  | 1.97                     | 0.46              |
| 1:A:300:ILE:HG22  | 1:A:302:LEU:H     | 1.80                     | 0.46              |
| 6:F:104:ARG:O     | 6:F:108:GLN:HB2   | 2.14                     | 0.46              |
| 5:P:184:HIS:HB2   | 5:P:193:LYS:HB2   | 1.96                     | 0.46              |
| 1:L:189:VAL:HG23  | 1:L:191:ALA:H     | 1.80                     | 0.46              |
| 3:N:330:VAL:HG13  | 27:N:606:PCF:H472 | 1.97                     | 0.46              |
| 2:B:62:ARG:HB2    | 2:B:66:LYS:HD3    | 1.97                     | 0.46              |
| 1:L:57:SER:HB3    | 1:L:205:ASN:HD21  | 1.80                     | 0.46              |
| 13:c:2:THR:HG23   | 21:k:18:LEU:HA    | 1.96                     | 0.46              |
| 13:c:209:THR:HG22 | 13:c:260:LEU:HD21 | 1.96                     | 0.46              |
| 2:B:117:HIS:HB2   | 7:R:62:ARG:HG2    | 1.98                     | 0.46              |
| 3:C:214:GLY:HA2   | 7:G:79:HIS:HE1    | 1.81                     | 0.46              |
| 2:M:35:VAL:HG12   | 2:M:185:LEU:HB3   | 1.97                     | 0.46              |
| 3:N:9:TYR:HB3     | 24:N:605:PEF:H181 | 1.97                     | 0.46              |
| 11:a:49:HIS:NE2   | 18:h:77:ALA:O     | 2.44                     | 0.46              |
| 13:c:50:MET:HE3   | 13:c:53:LEU:HB3   | 1.97                     | 0.46              |
| 13:c:95:VAL:HG11  | 13:c:252:VAL:HG11 | 1.98                     | 0.46              |
| 14:d:78:ILE:HG21  | 21:k:22:PHE:HB3   | 1.96                     | 0.46              |
| 1:L:121:ASN:HB2   | 1:L:228:LEU:HD12  | 1.98                     | 0.46              |
| 3:N:257:TYR:HB2   | 4:O:183:ALA:HB2   | 1.98                     | 0.46              |
| 12:b:177:PHE:HZ   | 12:b:195:ILE:HD13 | 1.81                     | 0.46              |
| 19:i:10:ILE:HD12  | 19:i:10:ILE:HA    | 1.85                     | 0.46              |
| 12:b:122:TYR:OH   | 20:j:62:ASP:OD2   | 2.33                     | 0.46              |
| 14:d:78:ILE:HD11  | 21:k:25:PRO:HB3   | 1.98                     | 0.46              |
| 1:L:354:LEU:HD23  | 1:L:354:LEU:HA    | 1.83                     | 0.46              |
| 3:N:142:TRP:HA    | 3:N:145:THR:HG22  | 1.98                     | 0.46              |
| 12:b:113:PRO:HA   | 12:b:174:HIS:HB2  | 1.96                     | 0.46              |
| 2:M:240:ALA:HA    | 2:M:287:LEU:O     | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:S:80:LEU:HD21   | 8:S:89:LEU:HA     | 1.96                     | 0.46              |
| 11:a:443:TYR:O    | 12:b:159:ARG:NH1  | 2.48                     | 0.46              |
| 11:a:533:GLN:HE21 | 14:d:121:ILE:HG12 | 1.80                     | 0.46              |
| 31:a:603:HEA:H243 | 12:b:89:PRO:HB3   | 1.97                     | 0.46              |
| 13:c:146:LEU:HD11 | 23:m:156:PHE:HB2  | 1.98                     | 0.46              |
| 3:C:245:PHE:O     | 4:D:266:ARG:NH2   | 2.48                     | 0.46              |
| 4:D:65:ALA:HB2    | 6:F:124:VAL:HG21  | 1.97                     | 0.46              |
| 3:C:137:GLY:H     | 3:C:140:SER:HB3   | 1.80                     | 0.46              |
| 8:H:10:MET:HG3    | 8:H:16:MET:HE1    | 1.98                     | 0.46              |
| 11:a:521:PRO:HG2  | 18:h:34:VAL:HA    | 1.97                     | 0.46              |
| 16:f:82:VAL:HG12  | 16:f:114:LYS:HE3  | 1.96                     | 0.46              |
| 4:D:84:THR:OG1    | 4:D:85:PHE:N      | 2.48                     | 0.45              |
| 6:F:76:ASP:OD1    | 6:F:76:ASP:N      | 2.49                     | 0.45              |
| 3:N:184:TYR:CZ    | 25:N:601:HEM:HBC1 | 2.50                     | 0.45              |
| 12:b:81:ILE:HA    | 12:b:84:ILE:HG22  | 1.98                     | 0.45              |
| 5:E:121:ARG:O     | 5:E:151:GLN:NE2   | 2.49                     | 0.45              |
| 2:M:49:HIS:HD2    | 2:M:161:TYR:H     | 1.65                     | 0.45              |
| 13:c:141:ASN:HB2  | 13:c:181:PHE:CD1  | 2.51                     | 0.45              |
| 10:U:26:TYR:HB3   | 10:U:30:LEU:HD23  | 1.98                     | 0.45              |
| 11:a:315:PRO:HA   | 11:a:318:ILE:HG12 | 1.99                     | 0.45              |
| 13:c:2:THR:HG22   | 13:c:4:LEU:H      | 1.81                     | 0.45              |
| 10:J:48:TRP:HD1   | 10:J:51:PHE:H     | 1.64                     | 0.45              |
| 1:A:376:GLN:HE21  | 2:B:92:THR:HG21   | 1.82                     | 0.45              |
| 2:M:33:VAL:HG22   | 2:M:187:VAL:HG22  | 1.99                     | 0.45              |
| 11:a:403:LEU:HB3  | 11:a:479:GLY:HA3  | 1.98                     | 0.45              |
| 4:D:80:GLY:O      | 4:D:267:LYS:NZ    | 2.47                     | 0.45              |
| 3:N:42:ILE:HG12   | 24:P:302:PEF:H422 | 1.98                     | 0.45              |
| 23:m:185:MET:HA   | 23:m:188:TRP:HB3  | 1.98                     | 0.45              |
| 1:A:374:LEU:HD12  | 1:A:410:ILE:HD11  | 1.97                     | 0.45              |
| 24:E:302:PEF:H362 | 24:E:302:PEF:H332 | 1.82                     | 0.45              |
| 13:c:233:TYR:OH   | 14:d:53:GLU:O     | 2.31                     | 0.45              |
| 1:A:265:VAL:HG12  | 1:A:431:ILE:HG22  | 1.99                     | 0.45              |
| 8:H:40:ILE:O      | 8:H:44:ALA:CB     | 2.64                     | 0.45              |
| 3:N:284:SER:OG    | 3:N:285:ILE:N     | 2.50                     | 0.45              |
| 1:A:247:SER:OG    | 1:A:248:GLU:N     | 2.47                     | 0.45              |
| 5:E:175:GLY:HA3   | 5:E:185:TYR:O     | 2.17                     | 0.45              |
| 8:H:80:LEU:HD12   | 8:H:80:LEU:HA     | 1.82                     | 0.45              |
| 3:N:214:GLY:HA2   | 7:R:79:HIS:HE1    | 1.82                     | 0.45              |
| 13:c:252:VAL:HA   | 13:c:255:VAL:HG12 | 1.99                     | 0.45              |
| 14:d:133:ARG:HG2  | 14:d:140:VAL:HG12 | 1.98                     | 0.45              |
| 20:j:46:ALA:HB1   | 20:j:48:CYS:H     | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:80:SER:HA     | 2:M:88:THR:O      | 2.16                     | 0.45              |
| 2:M:115:LYS:HB2   | 2:M:118:GLU:HG3   | 1.99                     | 0.45              |
| 3:N:36:LEU:HD11   | 3:N:93:MET:HA     | 1.98                     | 0.45              |
| 4:O:229:LEU:HD22  | 4:O:247:MET:HE3   | 1.98                     | 0.45              |
| 5:P:95:GLU:HG3    | 5:P:213:ILE:HA    | 1.99                     | 0.45              |
| 5:P:141:GLN:HE21  | 5:P:199:ASN:HD22  | 1.64                     | 0.45              |
| 11:a:145:ASP:OD2  | 11:a:214:ARG:NH1  | 2.49                     | 0.45              |
| 3:C:10:LEU:HA     | 3:C:13:VAL:HG22   | 1.98                     | 0.44              |
| 1:L:74:LYS:HB2    | 1:L:97:ILE:HD11   | 1.97                     | 0.44              |
| 27:e:202:PCF:H231 | 27:e:202:PCF:H262 | 1.77                     | 0.44              |
| 1:A:456:ARG:HB2   | 10:J:33:TRP:HE1   | 1.82                     | 0.44              |
| 2:M:238:VAL:HG22  | 2:M:356:VAL:HB    | 1.99                     | 0.44              |
| 3:N:81:LEU:HD23   | 3:N:244:VAL:HG21  | 1.98                     | 0.44              |
| 4:O:143:ASN:OD1   | 4:O:143:ASN:N     | 2.50                     | 0.44              |
| 5:P:107:VAL:O     | 5:P:117:PHE:HA    | 2.17                     | 0.44              |
| 13:c:71:ALA:O     | 13:c:75:TYR:HB2   | 2.17                     | 0.44              |
| 1:A:74:LYS:HB2    | 1:A:97:ILE:HD11   | 2.00                     | 0.44              |
| 7:G:66:ASP:OD1    | 7:G:66:ASP:N      | 2.49                     | 0.44              |
| 12:b:168:VAL:HA   | 12:b:237:GLU:O    | 2.18                     | 0.44              |
| 3:C:142:TRP:HA    | 3:C:145:THR:HG22  | 2.00                     | 0.44              |
| 1:L:37:VAL:HB     | 1:L:207:VAL:HG22  | 1.99                     | 0.44              |
| 1:L:300:ILE:HG22  | 1:L:302:LEU:H     | 1.82                     | 0.44              |
| 11:a:287:VAL:HG21 | 11:a:312:ILE:HG13 | 1.98                     | 0.44              |
| 11:a:427:PRO:HB3  | 11:a:450:TRP:HB3  | 1.99                     | 0.44              |
| 13:c:60:THR:HA    | 13:c:63:ILE:HG22  | 1.98                     | 0.44              |
| 5:E:205:TYR:HB3   | 5:E:214:VAL:HG22  | 2.00                     | 0.44              |
| 7:G:47:ASP:OD2    | 7:G:74:ARG:NH2    | 2.50                     | 0.44              |
| 1:L:300:ILE:HB    | 1:L:303:LEU:HG    | 2.00                     | 0.44              |
| 3:N:212:ILE:HD12  | 7:R:75:ILE:HG23   | 2.00                     | 0.44              |
| 11:a:11:ALA:HB2   | 11:a:93:THR:HG22  | 2.00                     | 0.44              |
| 12:b:16:ASP:O     | 12:b:26:GLN:NE2   | 2.50                     | 0.44              |
| 3:N:211:GLY:HA2   | 3:N:314:ARG:HD2   | 2.00                     | 0.44              |
| 4:O:272:LYS:HE2   | 4:O:272:LYS:HB3   | 1.77                     | 0.44              |
| 5:P:110:LYS:HA    | 5:P:115:PRO:HA    | 1.99                     | 0.44              |
| 11:a:359:ALA:HB2  | 31:a:603:HEA:HMB1 | 1.99                     | 0.44              |
| 2:B:97:ASP:OD1    | 10:J:4:THR:OG1    | 2.36                     | 0.44              |
| 4:D:243:THR:HB    | 6:F:76:ASP:HA     | 1.99                     | 0.44              |
| 5:E:73:SER:HA     | 5:E:76:GLU:HG2    | 1.99                     | 0.44              |
| 5:E:74:THR:HA     | 5:E:77:THR:HG22   | 2.00                     | 0.44              |
| 24:L:502:PEF:H12  | 3:N:3:PHE:HB3     | 2.00                     | 0.44              |
| 24:N:604:PEF:H151 | 24:N:604:PEF:H182 | 1.80                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:240:ALA:HA    | 2:B:287:LEU:O     | 2.17                     | 0.44              |
| 3:C:110:ARG:HD3   | 3:C:113:LEU:HD23  | 2.00                     | 0.44              |
| 8:H:35:LYS:HG3    | 8:H:38:GLN:HB2    | 1.99                     | 0.44              |
| 1:L:102:GLN:HE22  | 1:L:196:PHE:HE2   | 1.64                     | 0.44              |
| 5:P:142:THR:OG1   | 5:P:143:ASP:N     | 2.48                     | 0.44              |
| 7:R:47:ASP:OD2    | 7:R:74:ARG:NH2    | 2.51                     | 0.44              |
| 13:c:163:ASN:HD22 | 13:c:166:LYS:HG2  | 1.82                     | 0.44              |
| 13:c:176:TRP:HA   | 13:c:179:VAL:HG12 | 1.99                     | 0.44              |
| 3:N:54:TYR:OH     | 3:N:134:CYS:O     | 2.36                     | 0.44              |
| 24:S:102:PEF:H422 | 24:S:102:PEF:H391 | 1.86                     | 0.44              |
| 3:C:178:ARG:HD3   | 5:P:82:MET:HE3    | 1.99                     | 0.43              |
| 7:G:121:ASP:OD1   | 2:M:69:ARG:NH2    | 2.51                     | 0.43              |
| 2:M:40:ARG:NH1    | 2:M:281:ASP:OD2   | 2.51                     | 0.43              |
| 3:N:93:MET:HE2    | 25:N:602:HEM:HAB  | 1.99                     | 0.43              |
| 4:O:64:ALA:HA     | 4:O:67:HIS:HB2    | 1.98                     | 0.43              |
| 13:c:214:LEU:HA   | 13:c:217:VAL:HG22 | 1.99                     | 0.43              |
| 18:h:31:LYS:HD3   | 18:h:31:LYS:HA    | 1.74                     | 0.43              |
| 23:m:109:VAL:O    | 23:m:113:SER:HB3  | 2.18                     | 0.43              |
| 2:B:233:PHE:HB3   | 2:B:357:GLY:HA2   | 2.00                     | 0.43              |
| 9:I:2:SER:O       | 9:I:2:SER:OG      | 2.34                     | 0.43              |
| 4:O:297:THR:OG1   | 8:S:34:GLN:NE2    | 2.44                     | 0.43              |
| 11:a:340:TYR:OH   | 11:a:413:GLN:OE1  | 2.34                     | 0.43              |
| 1:A:49:ALA:HA     | 1:A:212:GLY:HA3   | 1.99                     | 0.43              |
| 3:C:36:LEU:HD11   | 3:C:93:MET:HA     | 2.01                     | 0.43              |
| 4:D:289:LYS:HD3   | 8:H:37:LEU:HD23   | 1.98                     | 0.43              |
| 2:M:55:ASN:OD1    | 2:M:180:TYR:OH    | 2.33                     | 0.43              |
| 2:B:50:LEU:O      | 2:B:54:PHE:HB2    | 2.18                     | 0.43              |
| 3:C:208:ASN:N     | 3:C:208:ASN:OD1   | 2.49                     | 0.43              |
| 5:E:206:GLU:O     | 5:E:212:VAL:HA    | 2.19                     | 0.43              |
| 1:L:349:LYS:HD3   | 1:L:349:LYS:HA    | 1.75                     | 0.43              |
| 1:L:352:ASN:HB2   | 1:L:454:MET:HE2   | 2.01                     | 0.43              |
| 3:N:178:ARG:HE    | 3:N:178:ARG:HB2   | 1.47                     | 0.43              |
| 5:P:55:TYR:OH     | 26:S:101:CDL:OB9  | 2.36                     | 0.43              |
| 5:P:151:GLN:O     | 5:P:151:GLN:NE2   | 2.51                     | 0.43              |
| 2:B:167:VAL:HG23  | 2:B:171:ASP:HB3   | 2.00                     | 0.43              |
| 9:I:26:PHE:HB2    | 10:J:43:VAL:HG12  | 1.99                     | 0.43              |
| 1:L:211:THR:OG1   | 1:L:383:PRO:O     | 2.36                     | 0.43              |
| 1:A:428:ASP:OD1   | 1:A:453:SER:OG    | 2.30                     | 0.43              |
| 3:C:339:ILE:HD11  | 3:C:351:MET:HE2   | 1.99                     | 0.43              |
| 4:O:118:VAL:HG11  | 4:O:257:TRP:CE2   | 2.53                     | 0.43              |
| 5:P:146:ARG:HH11  | 5:P:155:MET:HE2   | 1.83                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:374:VAL:O    | 11:a:378:HIS:HB2  | 2.19                     | 0.43              |
| 21:k:118:ASN:HB3  | 21:k:121:VAL:HG22 | 2.01                     | 0.43              |
| 2:M:169:LEU:HG    | 2:M:173:LYS:HE3   | 1.99                     | 0.43              |
| 4:D:297:THR:HG21  | 5:E:42:VAL:HG11   | 2.01                     | 0.43              |
| 2:M:229:ASN:O     | 2:M:354:VAL:HA    | 2.18                     | 0.43              |
| 3:N:166:TRP:O     | 3:N:175:THR:OG1   | 2.30                     | 0.43              |
| 10:U:59:ILE:HD12  | 10:U:60:PRO:HD2   | 2.00                     | 0.43              |
| 4:D:143:ASN:OD1   | 4:D:143:ASN:N     | 2.50                     | 0.43              |
| 3:N:28:TYR:HB2    | 26:N:603:CDL:HA32 | 2.00                     | 0.43              |
| 4:O:304:PRO:HA    | 4:O:305:PRO:HD3   | 1.87                     | 0.43              |
| 5:P:134:MET:HA    | 5:P:137:LEU:HG    | 2.00                     | 0.43              |
| 11:a:96:PRO:HA    | 11:a:99:ASN:HD21  | 1.84                     | 0.43              |
| 2:B:50:LEU:HD23   | 2:B:50:LEU:HA     | 1.90                     | 0.42              |
| 4:O:190:TYR:OH    | 28:O:401:HEC:O2A  | 2.29                     | 0.42              |
| 5:P:118:ILE:HA    | 5:P:153:LEU:O     | 2.19                     | 0.42              |
| 8:S:10:MET:HG3    | 8:S:16:MET:HE1    | 2.01                     | 0.42              |
| 11:a:509:VAL:HG11 | 11:a:516:PHE:HB3  | 2.01                     | 0.42              |
| 13:c:32:SER:HB2   | 17:g:41:VAL:HG23  | 2.01                     | 0.42              |
| 14:d:132:ALA:O    | 14:d:140:VAL:HA   | 2.19                     | 0.42              |
| 4:D:304:PRO:HA    | 4:D:305:PRO:HD3   | 1.86                     | 0.42              |
| 2:M:324:LYS:HA    | 2:M:324:LYS:HD2   | 1.89                     | 0.42              |
| 3:N:245:PHE:O     | 4:O:266:ARG:NH2   | 2.51                     | 0.42              |
| 9:T:26:PHE:HB2    | 10:U:43:VAL:HG12  | 2.01                     | 0.42              |
| 14:d:77:GLY:HA2   | 21:k:30:ALA:HB3   | 2.00                     | 0.42              |
| 3:C:263:LEU:HD22  | 5:P:115:PRO:HD3   | 2.01                     | 0.42              |
| 3:C:310:ARG:HA    | 7:G:2:PRO:HB2     | 2.01                     | 0.42              |
| 4:D:166:ARG:NH2   | 4:D:171:GLY:O     | 2.52                     | 0.42              |
| 2:M:53:ARG:HA     | 2:M:53:ARG:HD3    | 1.78                     | 0.42              |
| 2:M:304:ILE:HD13  | 2:M:304:ILE:HA    | 1.90                     | 0.42              |
| 13:c:151:THR:HG23 | 13:c:174:THR:HB   | 2.01                     | 0.42              |
| 1:A:72:LEU:HD23   | 1:A:193:LEU:HD11  | 2.01                     | 0.42              |
| 27:T:101:PCF:H481 | 27:T:101:PCF:H412 | 2.01                     | 0.42              |
| 11:a:279:SER:HA   | 11:a:282:LEU:HG   | 2.00                     | 0.42              |
| 3:C:29:TRP:HB3    | 3:C:99:LYS:HG3    | 2.00                     | 0.42              |
| 3:C:212:ILE:HG22  | 7:G:48:LEU:HA     | 2.01                     | 0.42              |
| 5:E:101:ILE:HD13  | 5:E:107:VAL:HG21  | 2.02                     | 0.42              |
| 26:N:603:CDL:H111 | 26:O:402:CDL:H321 | 2.01                     | 0.42              |
| 5:P:143:ASP:HA    | 5:P:146:ARG:HB2   | 2.01                     | 0.42              |
| 1:A:61:ASN:HB3    | 1:A:200:HIS:CE1   | 2.55                     | 0.42              |
| 4:D:177:LEU:HD22  | 4:D:180:ILE:HG21  | 2.01                     | 0.42              |
| 19:i:33:TRP:O     | 19:i:37:HIS:HB3   | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:183:HIS:HE1   | 25:C:601:HEM:NB   | 2.18                     | 0.42              |
| 11:a:510:LYS:HA   | 14:d:122:MET:HE3  | 2.02                     | 0.42              |
| 13:c:57:VAL:HA    | 13:c:60:THR:HG22  | 2.02                     | 0.42              |
| 3:N:290:LEU:HA    | 3:N:293:ILE:HG12  | 2.02                     | 0.42              |
| 5:P:123:PRO:HA    | 5:P:126:ILE:HB    | 2.01                     | 0.42              |
| 7:R:103:LEU:HG    | 7:R:107:ILE:HD11  | 2.02                     | 0.42              |
| 11:a:36:ILE:HG23  | 11:a:55:PHE:HE1   | 1.84                     | 0.42              |
| 11:a:148:ILE:HD11 | 11:a:211:LEU:HD12 | 2.02                     | 0.42              |
| 15:e:151:LYS:HB2  | 22:l:62:LYS:HE2   | 2.02                     | 0.42              |
| 16:f:90:LYS:HA    | 16:f:90:LYS:HD3   | 1.80                     | 0.42              |
| 11:a:382:SER:O    | 11:a:386:ILE:HB   | 2.20                     | 0.42              |
| 31:a:603:HEA:H251 | 12:b:93:LEU:HD21  | 2.01                     | 0.42              |
| 3:N:288:LYS:HD3   | 3:N:288:LYS:HA    | 1.73                     | 0.42              |
| 4:O:138:PRO:HB3   | 4:O:144:PRO:HA    | 2.01                     | 0.42              |
| 11:a:108:MET:HB3  | 13:c:31:LEU:HD13  | 2.02                     | 0.42              |
| 13:c:6:ARG:NH2    | 13:c:6:ARG:O      | 2.53                     | 0.42              |
| 14:d:78:ILE:H     | 14:d:78:ILE:HG13  | 1.68                     | 0.42              |
| 3:C:27:ASN:HD22   | 26:H:601:CDL:H1   | 1.85                     | 0.41              |
| 5:E:137:LEU:HD11  | 5:E:190:ARG:HD3   | 2.02                     | 0.41              |
| 7:R:90:ARG:HD2    | 7:R:90:ARG:HA     | 1.85                     | 0.41              |
| 11:a:229:PRO:HB2  | 12:b:185:ILE:HD11 | 2.02                     | 0.41              |
| 13:c:240:HIS:O    | 13:c:240:HIS:ND1  | 2.53                     | 0.41              |
| 20:j:37:CYS:SG    | 20:j:38:VAL:N     | 2.92                     | 0.41              |
| 5:E:78:PHE:HE2    | 24:E:302:PEF:H421 | 1.86                     | 0.41              |
| 7:G:58:THR:HA     | 7:G:61:ARG:HG2    | 2.02                     | 0.41              |
| 4:O:84:THR:OG1    | 4:O:264:ASP:OD1   | 2.32                     | 0.41              |
| 5:P:130:ASN:ND2   | 5:P:142:THR:OG1   | 2.53                     | 0.41              |
| 10:U:32:LEU:HD23  | 10:U:32:LEU:HA    | 1.91                     | 0.41              |
| 3:C:36:LEU:HG     | 3:C:92:VAL:HG12   | 2.03                     | 0.41              |
| 8:H:57:LEU:HD23   | 8:H:57:LEU:HA     | 1.91                     | 0.41              |
| 2:M:62:ARG:HB2    | 2:M:66:LYS:HD3    | 2.01                     | 0.41              |
| 3:N:58:ILE:HD11   | 3:N:136:TYR:CZ    | 2.55                     | 0.41              |
| 14:d:119:HIS:CE1  | 14:d:137:CYS:HB2  | 2.55                     | 0.41              |
| 1:A:443:LEU:HD13  | 1:A:447:ARG:HE    | 1.85                     | 0.41              |
| 3:C:99:LYS:HG2    | 3:C:103:TYR:HD2   | 1.85                     | 0.41              |
| 1:L:39:ALA:O      | 1:L:209:VAL:HA    | 2.21                     | 0.41              |
| 3:N:346:VAL:HG13  | 8:S:92:VAL:HG11   | 2.03                     | 0.41              |
| 11:a:84:LEU:HD12  | 11:a:186:VAL:HG22 | 2.03                     | 0.41              |
| 11:a:193:ALA:HA   | 11:a:196:LEU:HD12 | 2.03                     | 0.41              |
| 16:f:60:PHE:HE2   | 16:f:87:VAL:HG13  | 1.85                     | 0.41              |
| 3:C:178:ARG:HE    | 3:C:178:ARG:HB2   | 1.46                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:N:99:LYS:HG2    | 3:N:103:TYR:HD2   | 1.85                     | 0.41              |
| 11:a:31:ALA:HB3   | 18:h:64:PRO:HG2   | 2.02                     | 0.41              |
| 11:a:72:MET:HG3   | 11:a:76:ILE:HD13  | 2.03                     | 0.41              |
| 11:a:334:LEU:HD13 | 24:e:201:PEF:H111 | 2.02                     | 0.41              |
| 2:B:255:VAL:HG21  | 2:B:343:VAL:HG21  | 2.03                     | 0.41              |
| 3:C:383:VAL:HG22  | 7:G:101:PRO:HG2   | 2.01                     | 0.41              |
| 2:M:151:PHE:CE1   | 2:M:221:PRO:HG2   | 2.55                     | 0.41              |
| 4:O:177:LEU:HD22  | 4:O:180:ILE:HG21  | 2.02                     | 0.41              |
| 4:O:228:VAL:HG21  | 28:O:401:HEC:HMC2 | 2.02                     | 0.41              |
| 11:a:276:ALA:HB2  | 11:a:318:ILE:HD11 | 2.03                     | 0.41              |
| 11:a:532:VAL:HG13 | 14:d:86:LEU:HD22  | 2.02                     | 0.41              |
| 24:a:605:PEF:H162 | 24:a:605:PEF:H131 | 1.79                     | 0.41              |
| 21:k:19:LYS:HB3   | 21:k:19:LYS:HE2   | 1.94                     | 0.41              |
| 3:C:216:LEU:HD21  | 8:H:19:PRO:HG2    | 2.01                     | 0.41              |
| 3:C:348:TYR:OH    | 8:H:74:ASN:OD1    | 2.37                     | 0.41              |
| 4:D:289:LYS:NZ    | 26:D:402:CDL:OA4  | 2.47                     | 0.41              |
| 1:L:64:PRO:HG3    | 1:L:176:LEU:HD21  | 2.03                     | 0.41              |
| 1:L:408:LYS:HE3   | 1:L:408:LYS:HB2   | 1.86                     | 0.41              |
| 26:N:603:CDL:H512 | 27:N:606:PCF:H331 | 2.02                     | 0.41              |
| 13:c:139:LEU:HD23 | 13:c:139:LEU:HA   | 1.85                     | 0.41              |
| 2:B:43:THR:OG1    | 2:B:44:LYS:N      | 2.54                     | 0.41              |
| 2:B:241:ILE:HG12  | 2:B:287:LEU:HB3   | 2.01                     | 0.41              |
| 3:C:166:TRP:O     | 3:C:175:THR:OG1   | 2.31                     | 0.41              |
| 1:L:219:LEU:O     | 1:L:223:ILE:HG13  | 2.21                     | 0.41              |
| 2:M:233:PHE:HB3   | 2:M:357:GLY:HA2   | 2.03                     | 0.41              |
| 2:M:301:ILE:HD12  | 2:M:301:ILE:HA    | 1.98                     | 0.41              |
| 4:O:92:ARG:NH2    | 4:O:250:ASP:OD2   | 2.54                     | 0.41              |
| 21:k:24:PRO:HA    | 21:k:25:PRO:HD3   | 1.92                     | 0.41              |
| 1:A:52:GLY:HA3    | 1:A:105:ILE:HD13  | 2.04                     | 0.41              |
| 3:C:60:LEU:O      | 3:C:64:SER:HB3    | 2.21                     | 0.41              |
| 3:N:58:ILE:HD12   | 3:N:58:ILE:HA     | 1.88                     | 0.41              |
| 2:B:124:LEU:HD23  | 2:B:124:LEU:HA    | 1.94                     | 0.40              |
| 1:L:52:GLY:HA3    | 1:L:105:ILE:HD13  | 2.03                     | 0.40              |
| 5:P:116:VAL:HA    | 5:P:156:LEU:HA    | 2.02                     | 0.40              |
| 13:c:66:PHE:HA    | 13:c:69:ILE:HG22  | 2.03                     | 0.40              |
| 5:E:93:LYS:HG2    | 5:E:215:GLY:HA3   | 2.04                     | 0.40              |
| 4:O:246:GLN:HE22  | 6:Q:147:LYS:H     | 1.69                     | 0.40              |
| 11:a:228:ASP:HA   | 11:a:229:PRO:HD3  | 1.94                     | 0.40              |
| 31:a:603:HEA:H241 | 12:b:93:LEU:HG    | 2.03                     | 0.40              |
| 1:A:217:GLU:HA    | 1:A:220:VAL:HG12  | 2.03                     | 0.40              |
| 10:U:48:TRP:HD1   | 10:U:49:PRO:HD2   | 1.87                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:b:302:PEF:H142 | 24:b:302:PEF:H112 | 1.83                     | 0.40              |
| 1:A:428:ASP:O     | 1:A:449:ARG:NH1   | 2.55                     | 0.40              |
| 4:D:122:ASN:HD21  | 4:D:126:ARG:HH22  | 1.69                     | 0.40              |
| 5:E:166:PRO:HG3   | 5:E:178:CYS:HB2   | 2.04                     | 0.40              |
| 11:a:311:ILE:HA   | 11:a:314:ILE:HG22 | 2.04                     | 0.40              |
| 15:e:111:ARG:HG3  | 27:e:202:PCF:H112 | 2.04                     | 0.40              |
| 1:A:292:GLU:HA    | 1:A:293:PRO:HD3   | 1.98                     | 0.40              |
| 4:D:118:VAL:HG11  | 4:D:257:TRP:CE2   | 2.57                     | 0.40              |
| 10:J:62:LEU:O     | 10:J:65:THR:OG1   | 2.39                     | 0.40              |
| 1:L:341:ASP:OD1   | 1:L:341:ASP:N     | 2.54                     | 0.40              |
| 2:M:70:GLU:HB2    | 10:U:7:LEU:HD22   | 2.02                     | 0.40              |
| 3:N:60:LEU:O      | 3:N:64:SER:HB2    | 2.22                     | 0.40              |
| 3:N:98:ALA:HB2    | 27:N:606:PCF:H491 | 2.03                     | 0.40              |
| 11:a:260:SER:HB2  | 11:a:267:VAL:HG13 | 2.03                     | 0.40              |
| 12:b:179:VAL:HG21 | 12:b:188:PHE:HB2  | 2.03                     | 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     | 429/431 (100%) | 397 (92%) | 32 (8%) | 0        | 100         | 100 |
| 1   | L     | 429/431 (100%) | 394 (92%) | 35 (8%) | 0        | 100         | 100 |
| 2   | B     | 350/352 (99%)  | 334 (95%) | 16 (5%) | 0        | 100         | 100 |
| 2   | M     | 350/352 (99%)  | 334 (95%) | 16 (5%) | 0        | 100         | 100 |
| 3   | C     | 383/385 (100%) | 363 (95%) | 20 (5%) | 0        | 100         | 100 |
| 3   | N     | 383/385 (100%) | 357 (93%) | 26 (7%) | 0        | 100         | 100 |
| 4   | D     | 245/248 (99%)  | 239 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 4   | O     | 245/248 (99%)  | 241 (98%) | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 5   | E     | 183/185 (99%)   | 163 (89%)  | 20 (11%) | 0        | 100         | 100 |
| 5   | P     | 183/185 (99%)   | 167 (91%)  | 16 (9%)  | 0        | 100         | 100 |
| 6   | F     | 73/147 (50%)    | 68 (93%)   | 5 (7%)   | 0        | 100         | 100 |
| 6   | Q     | 73/147 (50%)    | 70 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 7   | G     | 124/127 (98%)   | 121 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 7   | R     | 124/127 (98%)   | 119 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 8   | H     | 91/94 (97%)     | 83 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 8   | S     | 91/94 (97%)     | 85 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 9   | I     | 55/66 (83%)     | 54 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 9   | T     | 55/66 (83%)     | 55 (100%)  | 0        | 0        | 100         | 100 |
| 10  | J     | 74/77 (96%)     | 70 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 10  | U     | 74/77 (96%)     | 72 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 11  | a     | 532/534 (100%)  | 490 (92%)  | 40 (8%)  | 2 (0%)   | 30          | 60  |
| 12  | b     | 234/236 (99%)   | 214 (92%)  | 20 (8%)  | 0        | 100         | 100 |
| 13  | c     | 267/269 (99%)   | 256 (96%)  | 10 (4%)  | 1 (0%)   | 30          | 60  |
| 14  | d     | 119/130 (92%)   | 101 (85%)  | 18 (15%) | 0        | 100         | 100 |
| 15  | e     | 132/134 (98%)   | 123 (93%)  | 9 (7%)   | 0        | 100         | 100 |
| 16  | f     | 102/108 (94%)   | 96 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 17  | g     | 57/59 (97%)     | 53 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 18  | h     | 49/51 (96%)     | 48 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 19  | i     | 53/55 (96%)     | 51 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 20  | j     | 75/82 (92%)     | 67 (89%)   | 8 (11%)  | 0        | 100         | 100 |
| 21  | k     | 116/131 (88%)   | 103 (89%)  | 13 (11%) | 0        | 100         | 100 |
| 22  | l     | 43/66 (65%)     | 42 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 23  | m     | 97/224 (43%)    | 91 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| All | All   | 5890/6303 (93%) | 5521 (94%) | 366 (6%) | 3 (0%)   | 49          | 75  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | a     | 121 | SER  |
| 11  | a     | 521 | PRO  |
| 13  | c     | 23  | PRO  |

### 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     | 370/370 (100%) | 370 (100%) | 0        | 100         | 100 |
| 1   | L     | 370/370 (100%) | 370 (100%) | 0        | 100         | 100 |
| 2   | B     | 301/301 (100%) | 300 (100%) | 1 (0%)   | 86          | 86  |
| 2   | M     | 301/301 (100%) | 300 (100%) | 1 (0%)   | 86          | 86  |
| 3   | C     | 338/338 (100%) | 338 (100%) | 0        | 100         | 100 |
| 3   | N     | 338/338 (100%) | 337 (100%) | 1 (0%)   | 86          | 86  |
| 4   | D     | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 4   | O     | 205/206 (100%) | 205 (100%) | 0        | 100         | 100 |
| 5   | E     | 151/151 (100%) | 150 (99%)  | 1 (1%)   | 76          | 80  |
| 5   | P     | 151/151 (100%) | 149 (99%)  | 2 (1%)   | 61          | 74  |
| 6   | F     | 68/131 (52%)   | 68 (100%)  | 0        | 100         | 100 |
| 6   | Q     | 68/131 (52%)   | 67 (98%)   | 1 (2%)   | 57          | 72  |
| 7   | G     | 110/111 (99%)  | 110 (100%) | 0        | 100         | 100 |
| 7   | R     | 110/111 (99%)  | 109 (99%)  | 1 (1%)   | 70          | 78  |
| 8   | H     | 77/78 (99%)    | 77 (100%)  | 0        | 100         | 100 |
| 8   | S     | 77/78 (99%)    | 77 (100%)  | 0        | 100         | 100 |
| 9   | I     | 47/54 (87%)    | 47 (100%)  | 0        | 100         | 100 |
| 9   | T     | 47/54 (87%)    | 47 (100%)  | 0        | 100         | 100 |
| 10  | J     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 10  | U     | 65/66 (98%)    | 65 (100%)  | 0        | 100         | 100 |
| 11  | a     | 447/447 (100%) | 446 (100%) | 1 (0%)   | 87          | 88  |
| 12  | b     | 209/209 (100%) | 209 (100%) | 0        | 100         | 100 |
| 13  | c     | 228/228 (100%) | 228 (100%) | 0        | 100         | 100 |
| 14  | d     | 102/111 (92%)  | 101 (99%)  | 1 (1%)   | 68          | 76  |
| 15  | e     | 115/115 (100%) | 114 (99%)  | 1 (1%)   | 70          | 78  |
| 16  | f     | 92/96 (96%)    | 91 (99%)   | 1 (1%)   | 65          | 76  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 17  | g     | 50/50 (100%)    | 50 (100%)   | 0        | 100         | 100 |
| 18  | h     | 41/41 (100%)    | 41 (100%)   | 0        | 100         | 100 |
| 19  | i     | 46/46 (100%)    | 46 (100%)   | 0        | 100         | 100 |
| 20  | j     | 69/73 (94%)     | 69 (100%)   | 0        | 100         | 100 |
| 21  | k     | 104/113 (92%)   | 104 (100%)  | 0        | 100         | 100 |
| 22  | l     | 36/53 (68%)     | 35 (97%)    | 1 (3%)   | 38          | 62  |
| 23  | m     | 84/191 (44%)    | 84 (100%)   | 0        | 100         | 100 |
| All | All   | 5087/5385 (94%) | 5074 (100%) | 13 (0%)  | 84          | 86  |

All (13) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 30  | THR  |
| 5   | E     | 124 | HIS  |
| 2   | M     | 18  | THR  |
| 3   | N     | 213 | THR  |
| 5   | P     | 118 | ILE  |
| 5   | P     | 212 | VAL  |
| 6   | Q     | 101 | CYS  |
| 7   | R     | 125 | VAL  |
| 11  | a     | 244 | VAL  |
| 14  | d     | 78  | ILE  |
| 15  | e     | 148 | VAL  |
| 16  | f     | 111 | LEU  |
| 22  | l     | 29  | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 47  | HIS  |
| 1   | A     | 61  | ASN  |
| 1   | A     | 75  | ASN  |
| 1   | A     | 121 | ASN  |
| 1   | A     | 126 | GLN  |
| 1   | A     | 156 | HIS  |
| 1   | A     | 200 | HIS  |
| 1   | A     | 271 | ASN  |
| 1   | A     | 298 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 317 | HIS  |
| 1   | A     | 345 | HIS  |
| 1   | A     | 350 | GLN  |
| 1   | A     | 352 | ASN  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 376 | GLN  |
| 1   | A     | 385 | ASN  |
| 1   | A     | 388 | ASN  |
| 2   | B     | 49  | HIS  |
| 2   | B     | 103 | ASN  |
| 2   | B     | 157 | ASN  |
| 2   | B     | 252 | GLN  |
| 2   | B     | 258 | ASN  |
| 2   | B     | 292 | GLN  |
| 2   | B     | 325 | ASN  |
| 3   | C     | 7   | ASN  |
| 3   | C     | 138 | GLN  |
| 3   | C     | 173 | ASN  |
| 3   | C     | 204 | HIS  |
| 3   | C     | 215 | ASN  |
| 3   | C     | 384 | ASN  |
| 4   | D     | 122 | ASN  |
| 4   | D     | 127 | ASN  |
| 4   | D     | 246 | GLN  |
| 5   | E     | 97  | ASN  |
| 5   | E     | 106 | ASN  |
| 5   | E     | 112 | GLN  |
| 5   | E     | 130 | ASN  |
| 7   | G     | 30  | ASN  |
| 7   | G     | 79  | HIS  |
| 7   | G     | 86  | HIS  |
| 8   | H     | 34  | GLN  |
| 8   | H     | 43  | ASN  |
| 8   | H     | 77  | ASN  |
| 9   | I     | 42  | ASN  |
| 10  | J     | 29  | ASN  |
| 10  | J     | 52  | GLN  |
| 1   | L     | 75  | ASN  |
| 1   | L     | 102 | GLN  |
| 1   | L     | 121 | ASN  |
| 1   | L     | 126 | GLN  |
| 1   | L     | 154 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 205 | ASN  |
| 1   | L     | 274 | ASN  |
| 1   | L     | 307 | GLN  |
| 1   | L     | 316 | ASN  |
| 1   | L     | 317 | HIS  |
| 1   | L     | 345 | HIS  |
| 1   | L     | 352 | ASN  |
| 1   | L     | 373 | GLN  |
| 1   | L     | 376 | GLN  |
| 1   | L     | 385 | ASN  |
| 2   | M     | 52  | ASN  |
| 2   | M     | 58  | ASN  |
| 2   | M     | 103 | ASN  |
| 2   | M     | 191 | ASN  |
| 2   | M     | 258 | ASN  |
| 2   | M     | 325 | ASN  |
| 3   | N     | 138 | GLN  |
| 3   | N     | 173 | ASN  |
| 3   | N     | 375 | ASN  |
| 3   | N     | 384 | ASN  |
| 4   | O     | 122 | ASN  |
| 4   | O     | 127 | ASN  |
| 4   | O     | 246 | GLN  |
| 5   | P     | 130 | ASN  |
| 5   | P     | 141 | GLN  |
| 6   | Q     | 131 | GLN  |
| 7   | R     | 3   | GLN  |
| 7   | R     | 30  | ASN  |
| 7   | R     | 86  | HIS  |
| 8   | S     | 34  | GLN  |
| 8   | S     | 43  | ASN  |
| 8   | S     | 72  | ASN  |
| 9   | T     | 44  | ASN  |
| 10  | U     | 14  | HIS  |
| 10  | U     | 29  | ASN  |
| 10  | U     | 52  | GLN  |
| 10  | U     | 69  | HIS  |
| 11  | a     | 53  | GLN  |
| 11  | a     | 99  | ASN  |
| 11  | a     | 100 | ASN  |
| 11  | a     | 164 | ASN  |
| 11  | a     | 171 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | a     | 175 | ASN  |
| 11  | a     | 257 | HIS  |
| 11  | a     | 399 | GLN  |
| 11  | a     | 475 | GLN  |
| 11  | a     | 478 | ASN  |
| 11  | a     | 481 | ASN  |
| 11  | a     | 482 | ASN  |
| 11  | a     | 505 | ASN  |
| 11  | a     | 533 | GLN  |
| 12  | b     | 26  | GLN  |
| 12  | b     | 33  | GLN  |
| 12  | b     | 40  | HIS  |
| 12  | b     | 42  | ASN  |
| 12  | b     | 68  | ASN  |
| 12  | b     | 77  | HIS  |
| 12  | b     | 249 | ASN  |
| 13  | c     | 12  | HIS  |
| 13  | c     | 47  | ASN  |
| 13  | c     | 163 | ASN  |
| 13  | c     | 185 | GLN  |
| 15  | e     | 43  | GLN  |
| 15  | e     | 49  | ASN  |
| 15  | e     | 115 | ASN  |
| 15  | e     | 123 | ASN  |
| 15  | e     | 127 | GLN  |
| 15  | e     | 140 | ASN  |
| 16  | f     | 44  | HIS  |
| 16  | f     | 74  | ASN  |
| 17  | g     | 13  | GLN  |
| 18  | h     | 53  | HIS  |
| 19  | i     | 42  | ASN  |
| 20  | j     | 29  | GLN  |
| 20  | j     | 81  | ASN  |
| 21  | k     | 43  | HIS  |
| 23  | m     | 173 | ASN  |

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 3 are monoatomic - leaving 42 for Mogul analysis.

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 | $\# Z  > 2$ |
| 24  | PEF  | C     | 605 | -    | 42,42,46     | 1.01 | 2 (4%)      | 45,47,51    | 1.16 | 3 (6%)      |
| 27  | PCF  | e     | 202 | -    | 35,35,49     | 1.14 | 2 (5%)      | 41,43,57    | 1.08 | 3 (7%)      |
| 24  | PEF  | L     | 502 | -    | 35,35,46     | 1.08 | 2 (5%)      | 38,40,51    | 1.15 | 4 (10%)     |
| 28  | HEC  | O     | 401 | 4    | 46,50,50     | 2.67 | 27 (58%)    | 58,82,82    | 2.15 | 20 (34%)    |
| 24  | PEF  | c     | 302 | -    | 40,40,46     | 1.02 | 2 (5%)      | 43,45,51    | 1.05 | 2 (4%)      |
| 29  | FES  | E     | 301 | 5    | 0,4,4        | -    | -           | -           | -    | -           |
| 27  | PCF  | S     | 103 | -    | 31,31,49     | 1.20 | 2 (6%)      | 37,39,57    | 1.11 | 4 (10%)     |
| 25  | HEM  | N     | 601 | 3    | 50,50,50     | 1.61 | 10 (20%)    | 67,82,82    | 1.67 | 13 (19%)    |
| 26  | CDL  | D     | 402 | -    | 66,66,99     | 1.12 | 4 (6%)      | 72,78,111   | 1.21 | 6 (8%)      |
| 24  | PEF  | c     | 301 | -    | 35,35,46     | 1.09 | 2 (5%)      | 38,40,51    | 1.16 | 3 (7%)      |
| 24  | PEF  | N     | 604 | -    | 43,43,46     | 0.98 | 2 (4%)      | 46,48,51    | 1.06 | 3 (6%)      |
| 24  | PEF  | a     | 605 | -    | 32,32,46     | 1.16 | 2 (6%)      | 35,37,51    | 1.20 | 3 (8%)      |
| 24  | PEF  | C     | 604 | 27   | 39,39,46     | 1.04 | 2 (5%)      | 42,44,51    | 1.11 | 3 (7%)      |
| 31  | HEA  | a     | 603 | 11   | 67,67,67     | 2.40 | 24 (35%)    | 81,103,103  | 2.64 | 34 (41%)    |
| 24  | PEF  | U     | 101 | -    | 46,46,46     | 0.96 | 2 (4%)      | 49,51,51    | 1.04 | 2 (4%)      |
| 27  | PCF  | I     | 101 | 24   | 38,38,49     | 1.08 | 2 (5%)      | 44,46,57    | 1.10 | 4 (9%)      |
| 26  | CDL  | C     | 603 | -    | 54,54,99     | 1.16 | 4 (7%)      | 60,66,111   | 1.25 | 6 (10%)     |
| 28  | HEC  | D     | 401 | 4    | 46,50,50     | 2.66 | 27 (58%)    | 58,82,82    | 2.10 | 19 (32%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 31  | HEA  | a     | 602 | 11   | 67,67,67     | 2.38 | 25 (37%) | 81,103,103  | 2.53 | 35 (43%) |
| 24  | PEF  | e     | 201 | -    | 41,41,46     | 1.04 | 2 (4%)   | 44,46,51    | 0.98 | 2 (4%)   |
| 25  | HEM  | C     | 602 | 3    | 50,50,50     | 1.63 | 9 (18%)  | 67,82,82    | 1.63 | 13 (19%) |
| 24  | PEF  | b     | 302 | -    | 39,39,46     | 1.05 | 2 (5%)   | 42,44,51    | 1.06 | 2 (4%)   |
| 24  | PEF  | S     | 102 | -    | 35,35,46     | 1.09 | 2 (5%)   | 38,40,51    | 1.12 | 3 (7%)   |
| 26  | CDL  | N     | 603 | 26   | 65,65,99     | 1.13 | 4 (6%)   | 71,77,111   | 1.18 | 7 (9%)   |
| 26  | CDL  | O     | 402 | 26   | 70,70,99     | 1.09 | 4 (5%)   | 76,82,111   | 1.22 | 7 (9%)   |
| 26  | CDL  | H     | 601 | -    | 52,52,99     | 1.27 | 4 (7%)   | 58,64,111   | 1.28 | 6 (10%)  |
| 24  | PEF  | N     | 605 | -    | 38,38,46     | 1.08 | 2 (5%)   | 41,43,51    | 1.00 | 2 (4%)   |
| 25  | HEM  | N     | 602 | 3    | 50,50,50     | 1.61 | 9 (18%)  | 67,82,82    | 1.62 | 14 (20%) |
| 26  | CDL  | S     | 101 | -    | 52,52,99     | 1.26 | 4 (7%)   | 58,64,111   | 1.27 | 7 (12%)  |
| 27  | PCF  | N     | 606 | -    | 38,38,49     | 1.11 | 2 (5%)   | 44,46,57    | 1.06 | 3 (6%)   |
| 24  | PEF  | E     | 302 | -    | 42,42,46     | 1.01 | 2 (4%)   | 45,47,51    | 1.12 | 3 (6%)   |
| 27  | PCF  | C     | 606 | -    | 49,49,49     | 0.97 | 2 (4%)   | 55,57,57    | 1.02 | 4 (7%)   |
| 33  | CUA  | b     | 301 | 12   | 0,1,1        | -    | -        | -           | -    | -        |
| 29  | FES  | P     | 301 | 5    | 0,4,4        | -    | -        | -           | -    | -        |
| 24  | PEF  | A     | 501 | -    | 30,30,46     | 1.18 | 2 (6%)   | 33,35,51    | 1.14 | 3 (9%)   |
| 24  | PEF  | H     | 602 | -    | 31,31,46     | 1.16 | 2 (6%)   | 34,36,51    | 1.25 | 4 (11%)  |
| 27  | PCF  | T     | 101 | -    | 49,49,49     | 0.97 | 2 (4%)   | 55,57,57    | 1.03 | 3 (5%)   |
| 24  | PEF  | J     | 101 | -    | 28,28,46     | 1.22 | 2 (7%)   | 31,33,51    | 1.20 | 3 (9%)   |
| 24  | PEF  | P     | 302 | -    | 41,41,46     | 1.01 | 2 (4%)   | 44,46,51    | 1.06 | 3 (6%)   |
| 25  | HEM  | C     | 601 | 3    | 50,50,50     | 1.61 | 10 (20%) | 67,82,82    | 1.69 | 14 (20%) |
| 26  | CDL  | L     | 501 | -    | 57,57,99     | 1.21 | 4 (7%)   | 63,69,111   | 1.22 | 6 (9%)   |
| 24  | PEF  | b     | 303 | -    | 32,32,46     | 1.13 | 2 (6%)   | 35,37,51    | 1.24 | 4 (11%)  |

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 |
|-----|------|-------|-----|------|---------|-------------|-------|
| 24  | PEF  | C     | 605 | -    | -       | 13/46/46/50 | -     |
| 27  | PCF  | e     | 202 | -    | -       | 8/39/39/53  | -     |
| 24  | PEF  | L     | 502 | -    | -       | 14/39/39/50 | -     |
| 28  | HEC  | O     | 401 | 4    | -       | 3/14/54/54  | -     |
| 24  | PEF  | c     | 302 | -    | -       | 11/44/44/50 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 29  | FES  | E     | 301 | 5    | -       | -            | 0/1/1/1 |
| 27  | PCF  | S     | 103 | -    | -       | 8/35/35/53   | -       |
| 25  | HEM  | N     | 601 | 3    | -       | 10/14/54/54  | -       |
| 26  | CDL  | D     | 402 | -    | -       | 28/77/77/110 | -       |
| 24  | PEF  | c     | 301 | -    | -       | 10/39/39/50  | -       |
| 24  | PEF  | N     | 604 | -    | -       | 9/47/47/50   | -       |
| 24  | PEF  | a     | 605 | -    | -       | 4/36/36/50   | -       |
| 24  | PEF  | C     | 604 | 27   | -       | 8/43/43/50   | -       |
| 31  | HEA  | a     | 603 | 11   | -       | 6/36/76/76   | -       |
| 24  | PEF  | U     | 101 | -    | -       | 12/50/50/50  | -       |
| 27  | PCF  | I     | 101 | 24   | -       | 6/42/42/53   | -       |
| 26  | CDL  | C     | 603 | -    | -       | 22/64/64/110 | -       |
| 28  | HEC  | D     | 401 | 4    | -       | 0/14/54/54   | -       |
| 31  | HEA  | a     | 602 | 11   | -       | 14/36/76/76  | -       |
| 24  | PEF  | e     | 201 | -    | -       | 13/45/45/50  | -       |
| 25  | HEM  | C     | 602 | 3    | -       | 6/14/54/54   | -       |
| 24  | PEF  | b     | 302 | -    | -       | 19/43/43/50  | -       |
| 24  | PEF  | S     | 102 | -    | -       | 8/39/39/50   | -       |
| 26  | CDL  | N     | 603 | 26   | -       | 10/76/76/110 | -       |
| 26  | CDL  | O     | 402 | 26   | -       | 17/81/81/110 | -       |
| 26  | CDL  | H     | 601 | -    | -       | 18/63/63/110 | -       |
| 24  | PEF  | N     | 605 | -    | -       | 10/42/42/50  | -       |
| 25  | HEM  | N     | 602 | 3    | -       | 6/14/54/54   | -       |
| 26  | CDL  | S     | 101 | -    | -       | 20/63/63/110 | -       |
| 27  | PCF  | N     | 606 | -    | -       | 11/42/42/53  | -       |
| 24  | PEF  | E     | 302 | -    | -       | 13/46/46/50  | -       |
| 27  | PCF  | C     | 606 | -    | -       | 16/53/53/53  | -       |
| 29  | FES  | P     | 301 | 5    | -       | -            | 0/1/1/1 |
| 24  | PEF  | A     | 501 | -    | -       | 7/34/34/50   | -       |
| 24  | PEF  | H     | 602 | -    | -       | 4/35/35/50   | -       |
| 27  | PCF  | T     | 101 | -    | -       | 7/53/53/53   | -       |
| 24  | PEF  | J     | 101 | -    | -       | 14/32/32/50  | -       |
| 24  | PEF  | P     | 302 | -    | -       | 13/45/45/50  | -       |
| 25  | HEM  | C     | 601 | 3    | -       | 10/14/54/54  | -       |
| 26  | CDL  | L     | 501 | -    | -       | 17/68/68/110 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings |
|-----|------|-------|-----|------|---------|-------------|-------|
| 24  | PEF  | b     | 303 | -    | -       | 14/36/36/50 | -     |

All (217) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 31  | a     | 602 | HEA  | FE-NB   | 5.53 | 2.11        | 1.94     |
| 31  | a     | 603 | HEA  | FE-NB   | 5.48 | 2.11        | 1.94     |
| 31  | a     | 603 | HEA  | FE-ND   | 5.41 | 2.11        | 1.94     |
| 31  | a     | 602 | HEA  | C3B-C2B | 5.35 | 1.46        | 1.34     |
| 28  | O     | 401 | HEC  | CHC-C4B | 5.34 | 1.48        | 1.38     |
| 31  | a     | 602 | HEA  | FE-ND   | 5.32 | 2.11        | 1.94     |
| 31  | a     | 603 | HEA  | C3B-C2B | 5.29 | 1.46        | 1.34     |
| 25  | C     | 601 | HEM  | FE-NB   | 5.24 | 2.11        | 1.94     |
| 25  | N     | 601 | HEM  | FE-NB   | 5.24 | 2.11        | 1.94     |
| 25  | C     | 602 | HEM  | FE-NB   | 5.22 | 2.11        | 1.94     |
| 25  | N     | 602 | HEM  | FE-NB   | 5.19 | 2.10        | 1.94     |
| 28  | D     | 401 | HEC  | CHC-C4B | 5.19 | 1.48        | 1.38     |
| 28  | O     | 401 | HEC  | CHD-C4C | 4.95 | 1.48        | 1.38     |
| 28  | D     | 401 | HEC  | CHD-C4C | 4.94 | 1.48        | 1.38     |
| 28  | D     | 401 | HEC  | CAC-C3C | 4.82 | 1.50        | 1.35     |
| 31  | a     | 603 | HEA  | C3D-C2D | 4.81 | 1.47        | 1.36     |
| 28  | O     | 401 | HEC  | CAC-C3C | 4.79 | 1.50        | 1.35     |
| 28  | O     | 401 | HEC  | C2A-C3A | 4.79 | 1.47        | 1.36     |
| 28  | D     | 401 | HEC  | C2A-C3A | 4.76 | 1.47        | 1.36     |
| 31  | a     | 603 | HEA  | CHB-C4A | 4.75 | 1.47        | 1.38     |
| 28  | O     | 401 | HEC  | CHB-C4A | 4.64 | 1.47        | 1.38     |
| 31  | a     | 602 | HEA  | C3D-C2D | 4.63 | 1.46        | 1.36     |
| 28  | D     | 401 | HEC  | CHB-C4A | 4.61 | 1.47        | 1.38     |
| 28  | D     | 401 | HEC  | CHA-C1A | 4.61 | 1.47        | 1.38     |
| 28  | D     | 401 | HEC  | CAB-C3B | 4.60 | 1.49        | 1.35     |
| 28  | O     | 401 | HEC  | CHA-C1A | 4.55 | 1.47        | 1.38     |
| 28  | O     | 401 | HEC  | CAB-C3B | 4.55 | 1.49        | 1.35     |
| 31  | a     | 603 | HEA  | FE-NC   | 4.54 | 2.10        | 1.95     |
| 24  | N     | 605 | PEF  | O2-C10  | 4.53 | 1.47        | 1.34     |
| 31  | a     | 602 | HEA  | C3A-C2A | 4.45 | 1.47        | 1.37     |
| 31  | a     | 603 | HEA  | C3A-C2A | 4.44 | 1.47        | 1.37     |
| 31  | a     | 602 | HEA  | CHC-C4B | 4.43 | 1.47        | 1.38     |
| 24  | e     | 201 | PEF  | O2-C10  | 4.37 | 1.46        | 1.34     |
| 31  | a     | 602 | HEA  | FE-NC   | 4.35 | 2.09        | 1.95     |
| 24  | C     | 605 | PEF  | O2-C10  | 4.34 | 1.46        | 1.34     |
| 26  | O     | 402 | CDL  | OB8-CB7 | 4.34 | 1.46        | 1.33     |
| 26  | C     | 603 | CDL  | OB6-CB5 | 4.30 | 1.46        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 26  | D     | 402 | CDL  | OB8-CB7 | 4.30 | 1.45        | 1.33     |
| 24  | a     | 605 | PEF  | O2-C10  | 4.29 | 1.46        | 1.34     |
| 31  | a     | 602 | HEA  | CHA-C1A | 4.29 | 1.46        | 1.38     |
| 24  | e     | 201 | PEF  | O3-C30  | 4.29 | 1.45        | 1.33     |
| 24  | A     | 501 | PEF  | O3-C30  | 4.28 | 1.45        | 1.33     |
| 26  | L     | 501 | CDL  | OB8-CB7 | 4.27 | 1.45        | 1.33     |
| 24  | U     | 101 | PEF  | O3-C30  | 4.27 | 1.45        | 1.33     |
| 24  | J     | 101 | PEF  | O3-C30  | 4.27 | 1.45        | 1.33     |
| 26  | S     | 101 | CDL  | OB8-CB7 | 4.25 | 1.45        | 1.33     |
| 26  | S     | 101 | CDL  | OA8-CA7 | 4.25 | 1.45        | 1.33     |
| 24  | E     | 302 | PEF  | O3-C30  | 4.25 | 1.45        | 1.33     |
| 27  | C     | 606 | PCF  | O31-C31 | 4.24 | 1.45        | 1.33     |
| 24  | C     | 604 | PEF  | O3-C30  | 4.24 | 1.45        | 1.33     |
| 26  | H     | 601 | CDL  | OB8-CB7 | 4.24 | 1.45        | 1.33     |
| 27  | e     | 202 | PCF  | O31-C31 | 4.24 | 1.45        | 1.33     |
| 24  | H     | 602 | PEF  | O3-C30  | 4.23 | 1.45        | 1.33     |
| 24  | c     | 301 | PEF  | O3-C30  | 4.23 | 1.45        | 1.33     |
| 24  | b     | 302 | PEF  | O3-C30  | 4.22 | 1.45        | 1.33     |
| 27  | N     | 606 | PCF  | O31-C31 | 4.22 | 1.45        | 1.33     |
| 26  | D     | 402 | CDL  | OA8-CA7 | 4.22 | 1.45        | 1.33     |
| 27  | N     | 606 | PCF  | O21-C21 | 4.22 | 1.46        | 1.34     |
| 26  | L     | 501 | CDL  | OA8-CA7 | 4.22 | 1.45        | 1.33     |
| 26  | N     | 603 | CDL  | OA8-CA7 | 4.21 | 1.45        | 1.33     |
| 24  | S     | 102 | PEF  | O2-C10  | 4.21 | 1.46        | 1.34     |
| 24  | a     | 605 | PEF  | O3-C30  | 4.21 | 1.45        | 1.33     |
| 26  | O     | 402 | CDL  | OA8-CA7 | 4.21 | 1.45        | 1.33     |
| 31  | a     | 602 | HEA  | CHB-C4A | 4.21 | 1.46        | 1.38     |
| 24  | b     | 303 | PEF  | O3-C30  | 4.21 | 1.45        | 1.33     |
| 26  | H     | 601 | CDL  | OA8-CA7 | 4.21 | 1.45        | 1.33     |
| 26  | H     | 601 | CDL  | OA6-CA5 | 4.20 | 1.46        | 1.34     |
| 27  | S     | 103 | PCF  | O21-C21 | 4.20 | 1.46        | 1.34     |
| 26  | L     | 501 | CDL  | OB6-CB5 | 4.19 | 1.46        | 1.34     |
| 27  | T     | 101 | PCF  | O31-C31 | 4.18 | 1.45        | 1.33     |
| 27  | T     | 101 | PCF  | O21-C21 | 4.18 | 1.46        | 1.34     |
| 24  | E     | 302 | PEF  | O2-C10  | 4.18 | 1.46        | 1.34     |
| 24  | N     | 604 | PEF  | O3-C30  | 4.18 | 1.45        | 1.33     |
| 27  | S     | 103 | PCF  | O31-C31 | 4.17 | 1.45        | 1.33     |
| 26  | N     | 603 | CDL  | OB6-CB5 | 4.17 | 1.46        | 1.34     |
| 25  | C     | 601 | HEM  | FE-NC   | 4.17 | 2.08        | 1.95     |
| 24  | N     | 605 | PEF  | O3-C30  | 4.17 | 1.45        | 1.33     |
| 24  | b     | 302 | PEF  | O2-C10  | 4.17 | 1.46        | 1.34     |
| 25  | N     | 602 | HEM  | FE-NC   | 4.17 | 2.08        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 26  | C     | 603 | CDL  | OB8-CB7 | 4.17 | 1.45        | 1.33     |
| 26  | N     | 603 | CDL  | OB8-CB7 | 4.16 | 1.45        | 1.33     |
| 31  | a     | 602 | HEA  | CHD-C1D | 4.16 | 1.46        | 1.38     |
| 24  | c     | 302 | PEF  | O3-C30  | 4.16 | 1.45        | 1.33     |
| 24  | H     | 602 | PEF  | O2-C10  | 4.16 | 1.46        | 1.34     |
| 24  | J     | 101 | PEF  | O2-C10  | 4.16 | 1.46        | 1.34     |
| 24  | C     | 605 | PEF  | O3-C30  | 4.15 | 1.45        | 1.33     |
| 24  | c     | 302 | PEF  | O2-C10  | 4.14 | 1.46        | 1.34     |
| 26  | S     | 101 | CDL  | OB6-CB5 | 4.13 | 1.46        | 1.34     |
| 24  | P     | 302 | PEF  | O2-C10  | 4.13 | 1.45        | 1.34     |
| 27  | I     | 101 | PCF  | O31-C31 | 4.12 | 1.45        | 1.33     |
| 26  | L     | 501 | CDL  | OA6-CA5 | 4.12 | 1.45        | 1.34     |
| 25  | C     | 602 | HEM  | FE-NC   | 4.11 | 2.08        | 1.95     |
| 31  | a     | 603 | HEA  | CHA-C1A | 4.10 | 1.46        | 1.38     |
| 24  | L     | 502 | PEF  | O2-C10  | 4.10 | 1.45        | 1.34     |
| 24  | P     | 302 | PEF  | O3-C30  | 4.10 | 1.45        | 1.33     |
| 24  | L     | 502 | PEF  | O3-C30  | 4.10 | 1.45        | 1.33     |
| 25  | N     | 601 | HEM  | FE-NC   | 4.09 | 2.08        | 1.95     |
| 26  | D     | 402 | CDL  | OA6-CA5 | 4.09 | 1.45        | 1.34     |
| 27  | C     | 606 | PCF  | O21-C21 | 4.08 | 1.45        | 1.34     |
| 26  | N     | 603 | CDL  | OA6-CA5 | 4.08 | 1.45        | 1.34     |
| 24  | C     | 604 | PEF  | O2-C10  | 4.08 | 1.45        | 1.34     |
| 26  | H     | 601 | CDL  | OB6-CB5 | 4.08 | 1.45        | 1.34     |
| 26  | O     | 402 | CDL  | OA6-CA5 | 4.08 | 1.45        | 1.34     |
| 26  | C     | 603 | CDL  | OA6-CA5 | 4.07 | 1.45        | 1.34     |
| 24  | U     | 101 | PEF  | O2-C10  | 4.07 | 1.45        | 1.34     |
| 26  | S     | 101 | CDL  | OA6-CA5 | 4.07 | 1.45        | 1.34     |
| 24  | S     | 102 | PEF  | O3-C30  | 4.07 | 1.45        | 1.33     |
| 24  | A     | 501 | PEF  | O2-C10  | 4.07 | 1.45        | 1.34     |
| 31  | a     | 603 | HEA  | C4A-NA  | 4.06 | 1.47        | 1.39     |
| 27  | e     | 202 | PCF  | O21-C21 | 4.05 | 1.45        | 1.34     |
| 31  | a     | 603 | HEA  | C1A-NA  | 4.05 | 1.47        | 1.39     |
| 24  | c     | 301 | PEF  | O2-C10  | 4.04 | 1.45        | 1.34     |
| 26  | O     | 402 | CDL  | OB6-CB5 | 4.03 | 1.45        | 1.34     |
| 24  | N     | 604 | PEF  | O2-C10  | 4.03 | 1.45        | 1.34     |
| 26  | D     | 402 | CDL  | OB6-CB5 | 4.02 | 1.45        | 1.34     |
| 27  | I     | 101 | PCF  | O21-C21 | 4.01 | 1.45        | 1.34     |
| 24  | b     | 303 | PEF  | O2-C10  | 3.95 | 1.45        | 1.34     |
| 31  | a     | 603 | HEA  | CHC-C4B | 3.82 | 1.46        | 1.38     |
| 31  | a     | 602 | HEA  | C1A-NA  | 3.74 | 1.46        | 1.39     |
| 28  | O     | 401 | HEC  | CHD-C1D | 3.72 | 1.47        | 1.39     |
| 28  | D     | 401 | HEC  | CHD-C1D | 3.67 | 1.47        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | D     | 401 | HEC  | CHB-C1B | 3.66  | 1.47        | 1.39     |
| 28  | O     | 401 | HEC  | CHB-C1B | 3.66  | 1.47        | 1.39     |
| 28  | D     | 401 | HEC  | CHA-C4D | 3.64  | 1.47        | 1.39     |
| 31  | a     | 602 | HEA  | C4A-NA  | 3.64  | 1.46        | 1.39     |
| 31  | a     | 602 | HEA  | CHC-C1C | 3.62  | 1.47        | 1.39     |
| 28  | O     | 401 | HEC  | CHC-C1C | 3.62  | 1.47        | 1.39     |
| 28  | D     | 401 | HEC  | CHC-C1C | 3.60  | 1.47        | 1.39     |
| 28  | O     | 401 | HEC  | CHA-C4D | 3.60  | 1.47        | 1.39     |
| 31  | a     | 603 | HEA  | CHD-C1D | 3.59  | 1.45        | 1.38     |
| 25  | C     | 602 | HEM  | C1B-NB  | -3.57 | 1.34        | 1.40     |
| 31  | a     | 603 | HEA  | CHD-C4C | 3.54  | 1.47        | 1.39     |
| 31  | a     | 603 | HEA  | C1D-ND  | -3.52 | 1.34        | 1.40     |
| 25  | N     | 602 | HEM  | C1B-NB  | -3.49 | 1.34        | 1.40     |
| 31  | a     | 602 | HEA  | CHD-C4C | 3.38  | 1.47        | 1.39     |
| 31  | a     | 603 | HEA  | CHB-C1B | 3.37  | 1.46        | 1.39     |
| 25  | C     | 601 | HEM  | C1B-NB  | -3.35 | 1.34        | 1.40     |
| 25  | C     | 602 | HEM  | C4D-ND  | -3.33 | 1.34        | 1.40     |
| 25  | N     | 601 | HEM  | C1B-NB  | -3.32 | 1.34        | 1.40     |
| 25  | N     | 602 | HEM  | C4D-ND  | -3.30 | 1.34        | 1.40     |
| 31  | a     | 602 | HEA  | CHA-C4D | 3.26  | 1.46        | 1.39     |
| 28  | O     | 401 | HEC  | C3D-C2D | 3.22  | 1.47        | 1.38     |
| 28  | D     | 401 | HEC  | C3D-C2D | 3.20  | 1.47        | 1.38     |
| 31  | a     | 603 | HEA  | CHA-C4D | 3.13  | 1.46        | 1.39     |
| 31  | a     | 603 | HEA  | CHC-C1C | 3.12  | 1.46        | 1.39     |
| 31  | a     | 602 | HEA  | CHB-C1B | 3.10  | 1.46        | 1.39     |
| 25  | N     | 601 | HEM  | C4D-ND  | -2.98 | 1.35        | 1.40     |
| 31  | a     | 602 | HEA  | C1D-ND  | -2.96 | 1.35        | 1.40     |
| 25  | C     | 601 | HEM  | C4D-ND  | -2.95 | 1.35        | 1.40     |
| 31  | a     | 603 | HEA  | C4B-NB  | -2.89 | 1.35        | 1.40     |
| 31  | a     | 602 | HEA  | C4B-NB  | -2.86 | 1.35        | 1.40     |
| 31  | a     | 602 | HEA  | C4B-C3B | 2.73  | 1.49        | 1.44     |
| 25  | N     | 602 | HEM  | C1C-C2C | -2.66 | 1.40        | 1.45     |
| 25  | C     | 602 | HEM  | C1C-C2C | -2.66 | 1.40        | 1.45     |
| 28  | D     | 401 | HEC  | C4A-NA  | -2.65 | 1.34        | 1.39     |
| 28  | D     | 401 | HEC  | C1D-ND  | -2.63 | 1.34        | 1.39     |
| 26  | C     | 603 | CDL  | OA8-CA7 | 2.60  | 1.45        | 1.33     |
| 28  | O     | 401 | HEC  | C1D-ND  | -2.59 | 1.34        | 1.39     |
| 28  | O     | 401 | HEC  | C4A-NA  | -2.59 | 1.34        | 1.39     |
| 25  | N     | 601 | HEM  | C1C-C2C | -2.58 | 1.40        | 1.45     |
| 28  | O     | 401 | HEC  | C1A-NA  | -2.57 | 1.34        | 1.39     |
| 25  | N     | 602 | HEM  | FE-ND   | -2.56 | 1.87        | 1.94     |
| 25  | C     | 602 | HEM  | FE-ND   | -2.56 | 1.87        | 1.94     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | O     | 401 | HEC  | C1C-NC  | -2.55 | 1.34        | 1.39     |
| 25  | C     | 601 | HEM  | C1C-C2C | -2.55 | 1.40        | 1.45     |
| 31  | a     | 603 | HEA  | C4C-NC  | -2.52 | 1.34        | 1.39     |
| 31  | a     | 603 | HEA  | C4D-C3D | 2.52  | 1.49        | 1.45     |
| 28  | O     | 401 | HEC  | C1C-C2C | 2.51  | 1.49        | 1.43     |
| 28  | D     | 401 | HEC  | C1C-NC  | -2.49 | 1.34        | 1.39     |
| 31  | a     | 602 | HEA  | C4C-NC  | -2.47 | 1.35        | 1.39     |
| 28  | O     | 401 | HEC  | C4C-NC  | -2.47 | 1.35        | 1.39     |
| 28  | D     | 401 | HEC  | C4C-NC  | -2.46 | 1.35        | 1.39     |
| 28  | D     | 401 | HEC  | C1C-C2C | 2.43  | 1.48        | 1.43     |
| 28  | D     | 401 | HEC  | C4B-NB  | -2.40 | 1.35        | 1.39     |
| 31  | a     | 603 | HEA  | C1C-NC  | -2.39 | 1.35        | 1.39     |
| 28  | D     | 401 | HEC  | C1D-C2D | 2.39  | 1.48        | 1.43     |
| 28  | D     | 401 | HEC  | C1A-NA  | -2.37 | 1.35        | 1.39     |
| 28  | D     | 401 | HEC  | C1B-NB  | -2.37 | 1.35        | 1.39     |
| 28  | O     | 401 | HEC  | C1D-C2D | 2.37  | 1.48        | 1.43     |
| 28  | D     | 401 | HEC  | C4D-ND  | -2.36 | 1.35        | 1.39     |
| 28  | O     | 401 | HEC  | C4D-ND  | -2.34 | 1.35        | 1.39     |
| 31  | a     | 602 | HEA  | C1C-C2C | 2.34  | 1.48        | 1.43     |
| 25  | C     | 601 | HEM  | FE-ND   | -2.33 | 1.87        | 1.94     |
| 31  | a     | 602 | HEA  | C1C-NC  | -2.33 | 1.35        | 1.39     |
| 25  | C     | 602 | HEM  | C3C-C4C | -2.32 | 1.42        | 1.46     |
| 31  | a     | 602 | HEA  | C11-C3B | -2.32 | 1.48        | 1.51     |
| 28  | O     | 401 | HEC  | C4B-NB  | -2.32 | 1.35        | 1.39     |
| 25  | N     | 601 | HEM  | FE-ND   | -2.31 | 1.87        | 1.94     |
| 25  | C     | 601 | HEM  | C1D-ND  | -2.30 | 1.34        | 1.38     |
| 25  | N     | 601 | HEM  | C1D-ND  | -2.29 | 1.34        | 1.38     |
| 28  | O     | 401 | HEC  | C1B-NB  | -2.29 | 1.35        | 1.39     |
| 28  | D     | 401 | HEC  | C1B-C2B | 2.29  | 1.48        | 1.43     |
| 31  | a     | 603 | HEA  | C1C-C2C | 2.28  | 1.48        | 1.43     |
| 25  | N     | 601 | HEM  | C3C-C4C | -2.26 | 1.42        | 1.46     |
| 25  | C     | 602 | HEM  | C1D-ND  | -2.26 | 1.34        | 1.38     |
| 31  | a     | 603 | HEA  | C1B-C2B | 2.25  | 1.49        | 1.44     |
| 28  | O     | 401 | HEC  | C3B-C2B | 2.24  | 1.48        | 1.41     |
| 28  | D     | 401 | HEC  | C3B-C2B | 2.23  | 1.48        | 1.41     |
| 31  | a     | 603 | HEA  | C4B-C3B | 2.23  | 1.48        | 1.44     |
| 25  | N     | 602 | HEM  | C1D-ND  | -2.20 | 1.34        | 1.38     |
| 28  | D     | 401 | HEC  | C3C-C2C | 2.20  | 1.48        | 1.41     |
| 28  | O     | 401 | HEC  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 31  | a     | 602 | HEA  | C4D-C3D | 2.19  | 1.48        | 1.45     |
| 25  | N     | 602 | HEM  | C3C-C4C | -2.17 | 1.42        | 1.46     |
| 28  | O     | 401 | HEC  | C3B-C4B | 2.17  | 1.49        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 25  | C     | 601 | HEM  | C4B-NB  | -2.16 | 1.34        | 1.38     |
| 28  | O     | 401 | HEC  | C3C-C2C | 2.15  | 1.48        | 1.41     |
| 28  | O     | 401 | HEC  | C4D-C3D | 2.15  | 1.48        | 1.44     |
| 25  | N     | 602 | HEM  | C4B-NB  | -2.12 | 1.34        | 1.38     |
| 25  | C     | 602 | HEM  | C4B-NB  | -2.12 | 1.34        | 1.38     |
| 25  | C     | 601 | HEM  | C1A-C2A | -2.11 | 1.40        | 1.44     |
| 25  | C     | 601 | HEM  | C3C-C4C | -2.10 | 1.42        | 1.46     |
| 28  | D     | 401 | HEC  | C3B-C4B | 2.09  | 1.49        | 1.46     |
| 25  | N     | 601 | HEM  | C4B-NB  | -2.07 | 1.34        | 1.38     |
| 28  | D     | 401 | HEC  | C4D-C3D | 2.05  | 1.48        | 1.44     |
| 31  | a     | 602 | HEA  | C4D-ND  | -2.03 | 1.34        | 1.38     |
| 25  | N     | 601 | HEM  | C1A-C2A | -2.01 | 1.40        | 1.44     |

All (280) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 603 | HEA  | C3D-C4D-ND  | 6.67  | 116.80      | 110.35   |
| 31  | a     | 603 | HEA  | C2D-C1D-ND  | 6.56  | 117.38      | 109.84   |
| 31  | a     | 602 | HEA  | C2B-C1B-NB  | 6.22  | 117.09      | 109.90   |
| 31  | a     | 603 | HEA  | C3B-C4B-NB  | 6.15  | 116.91      | 109.84   |
| 31  | a     | 602 | HEA  | C3D-C4D-ND  | 6.09  | 116.24      | 110.35   |
| 31  | a     | 602 | HEA  | C2D-C1D-ND  | 5.76  | 116.46      | 109.84   |
| 28  | O     | 401 | HEC  | C2A-C1A-NA  | 5.75  | 115.88      | 110.32   |
| 31  | a     | 603 | HEA  | CHA-C4D-ND  | -5.65 | 118.34      | 124.42   |
| 28  | D     | 401 | HEC  | C2A-C1A-NA  | 5.54  | 115.67      | 110.32   |
| 31  | a     | 603 | HEA  | C3C-C2C-C1C | -5.43 | 100.77      | 107.17   |
| 31  | a     | 603 | HEA  | C2A-C1A-NA  | 5.41  | 115.54      | 110.32   |
| 31  | a     | 602 | HEA  | C3B-C4B-NB  | 5.23  | 115.85      | 109.84   |
| 25  | C     | 601 | HEM  | CHC-C4B-NB  | 5.21  | 130.03      | 124.42   |
| 31  | a     | 602 | HEA  | C3C-C4C-NC  | 5.13  | 114.12      | 109.80   |
| 24  | C     | 605 | PEF  | O2-C10-C11  | 5.02  | 122.35      | 111.48   |
| 31  | a     | 603 | HEA  | C3C-C4C-NC  | 5.00  | 114.01      | 109.80   |
| 31  | a     | 603 | HEA  | C1A-CHA-C4D | -4.99 | 115.42      | 126.02   |
| 28  | O     | 401 | HEC  | C3D-C4D-ND  | 4.94  | 115.64      | 110.15   |
| 25  | N     | 602 | HEM  | CHC-C4B-NB  | 4.91  | 129.71      | 124.42   |
| 28  | D     | 401 | HEC  | C3D-C4D-ND  | 4.91  | 115.60      | 110.15   |
| 25  | N     | 601 | HEM  | CHC-C4B-NB  | 4.82  | 129.61      | 124.42   |
| 31  | a     | 603 | HEA  | C2B-C1B-NB  | 4.77  | 115.42      | 109.90   |
| 31  | a     | 602 | HEA  | C3C-C2C-C1C | -4.77 | 101.54      | 107.17   |
| 26  | O     | 402 | CDL  | OB6-CB5-C51 | 4.74  | 121.73      | 111.48   |
| 25  | C     | 602 | HEM  | CHC-C4B-NB  | 4.71  | 129.50      | 124.42   |
| 26  | D     | 402 | CDL  | OB6-CB5-C51 | 4.65  | 121.55      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 602 | HEA  | C2A-C1A-NA  | 4.59  | 114.75      | 110.32   |
| 25  | C     | 601 | HEM  | CHD-C1D-ND  | 4.56  | 129.33      | 124.42   |
| 25  | N     | 602 | HEM  | CHD-C1D-ND  | 4.52  | 129.29      | 124.42   |
| 31  | a     | 602 | HEA  | C1D-C2D-C3D | -4.48 | 102.27      | 106.98   |
| 25  | C     | 601 | HEM  | CAD-C3D-C4D | 4.45  | 132.45      | 124.70   |
| 25  | N     | 601 | HEM  | CHD-C1D-ND  | 4.38  | 129.14      | 124.42   |
| 24  | J     | 101 | PEF  | O2-C10-C11  | 4.37  | 120.94      | 111.48   |
| 31  | a     | 603 | HEA  | C1D-C2D-C3D | -4.36 | 102.39      | 106.98   |
| 25  | N     | 601 | HEM  | CAD-C3D-C4D | 4.35  | 132.28      | 124.70   |
| 25  | C     | 602 | HEM  | CHD-C1D-ND  | 4.25  | 129.00      | 124.42   |
| 27  | T     | 101 | PCF  | O21-C21-C22 | 4.25  | 120.67      | 111.48   |
| 31  | a     | 602 | HEA  | CHB-C1B-NB  | -4.20 | 119.90      | 124.42   |
| 31  | a     | 602 | HEA  | C1B-C2B-C3B | -4.18 | 101.95      | 106.80   |
| 28  | O     | 401 | HEC  | C2B-C1B-NB  | 4.14  | 116.78      | 110.14   |
| 28  | D     | 401 | HEC  | C2B-C1B-NB  | 4.10  | 116.71      | 110.14   |
| 26  | C     | 603 | CDL  | OA6-CA5-C11 | 4.09  | 120.32      | 111.48   |
| 31  | a     | 603 | HEA  | C2C-C1C-NC  | 4.06  | 116.65      | 110.14   |
| 24  | b     | 303 | PEF  | O2-C10-C11  | 4.05  | 120.24      | 111.48   |
| 26  | S     | 101 | CDL  | OA6-CA5-C11 | 4.03  | 120.21      | 111.48   |
| 26  | C     | 603 | CDL  | OB6-CB5-C51 | 4.03  | 120.19      | 111.48   |
| 24  | C     | 604 | PEF  | O2-C10-C11  | 3.98  | 120.09      | 111.48   |
| 24  | H     | 602 | PEF  | O2-C10-C11  | 3.98  | 120.09      | 111.48   |
| 26  | L     | 501 | CDL  | OA6-CA5-C11 | 3.97  | 120.07      | 111.48   |
| 24  | a     | 605 | PEF  | O2-C10-C11  | 3.97  | 120.07      | 111.48   |
| 27  | N     | 606 | PCF  | O21-C21-C22 | 3.97  | 120.06      | 111.48   |
| 24  | c     | 301 | PEF  | O2-C10-C11  | 3.94  | 120.01      | 111.48   |
| 24  | P     | 302 | PEF  | O2-C10-C11  | 3.94  | 120.01      | 111.48   |
| 24  | c     | 302 | PEF  | O2-C10-C11  | 3.94  | 120.01      | 111.48   |
| 28  | D     | 401 | HEC  | C2C-C1C-NC  | 3.93  | 116.44      | 110.14   |
| 24  | S     | 102 | PEF  | O2-C10-C11  | 3.93  | 119.98      | 111.48   |
| 24  | b     | 302 | PEF  | O2-C10-C11  | 3.92  | 119.96      | 111.48   |
| 24  | E     | 302 | PEF  | O2-C10-C11  | 3.88  | 119.87      | 111.48   |
| 24  | A     | 501 | PEF  | O2-C10-C11  | 3.88  | 119.87      | 111.48   |
| 26  | H     | 601 | CDL  | OA6-CA5-C11 | 3.86  | 119.84      | 111.48   |
| 24  | L     | 502 | PEF  | O2-C10-C11  | 3.86  | 119.82      | 111.48   |
| 27  | e     | 202 | PCF  | O21-C21-C22 | 3.85  | 119.81      | 111.48   |
| 31  | a     | 603 | HEA  | C3A-C2A-C1A | -3.85 | 103.41      | 107.05   |
| 28  | D     | 401 | HEC  | C1A-C2A-C3A | -3.84 | 102.05      | 107.11   |
| 28  | O     | 401 | HEC  | C2C-C1C-NC  | 3.81  | 116.24      | 110.14   |
| 26  | S     | 101 | CDL  | OB6-CB5-C51 | 3.80  | 119.71      | 111.48   |
| 26  | N     | 603 | CDL  | OB6-CB5-C51 | 3.75  | 119.58      | 111.48   |
| 24  | N     | 604 | PEF  | O2-C10-C11  | 3.74  | 119.58      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | O     | 401 | HEC  | CMB-C2B-C3B | 3.69  | 135.22      | 126.55   |
| 28  | O     | 401 | HEC  | C1A-C2A-C3A | -3.66 | 102.28      | 107.11   |
| 31  | a     | 602 | HEA  | C26-C15-C16 | 3.66  | 121.58      | 115.23   |
| 27  | C     | 606 | PCF  | O21-C21-C22 | 3.66  | 119.39      | 111.48   |
| 24  | U     | 101 | PEF  | O2-C10-C11  | 3.65  | 119.37      | 111.48   |
| 31  | a     | 602 | HEA  | C13-C12-C11 | -3.64 | 108.58      | 114.39   |
| 31  | a     | 603 | HEA  | C4D-C3D-C2D | -3.63 | 101.61      | 106.89   |
| 26  | H     | 601 | CDL  | OB6-CB5-C51 | 3.62  | 119.31      | 111.48   |
| 27  | I     | 101 | PCF  | O21-C21-C22 | 3.60  | 119.26      | 111.48   |
| 25  | N     | 601 | HEM  | CHB-C1B-NB  | 3.59  | 128.81      | 124.37   |
| 26  | L     | 501 | CDL  | OB6-CB5-C51 | 3.58  | 119.23      | 111.48   |
| 26  | O     | 402 | CDL  | OA6-CA5-C11 | 3.58  | 119.22      | 111.48   |
| 31  | a     | 603 | HEA  | CMB-C2B-C1B | 3.56  | 130.60      | 125.03   |
| 31  | a     | 603 | HEA  | C4B-C3B-C2B | -3.54 | 101.49      | 107.44   |
| 25  | C     | 602 | HEM  | CHB-C1B-NB  | 3.53  | 128.74      | 124.37   |
| 28  | D     | 401 | HEC  | CMB-C2B-C3B | 3.49  | 134.76      | 126.55   |
| 26  | D     | 402 | CDL  | CB4-OB6-CB5 | -3.47 | 109.50      | 117.80   |
| 25  | N     | 602 | HEM  | CHB-C1B-NB  | 3.44  | 128.62      | 124.37   |
| 31  | a     | 603 | HEA  | CHB-C1B-NB  | -3.44 | 120.72      | 124.42   |
| 25  | C     | 601 | HEM  | CHB-C1B-NB  | 3.41  | 128.59      | 124.37   |
| 26  | N     | 603 | CDL  | OA6-CA5-C11 | 3.39  | 118.82      | 111.48   |
| 25  | N     | 602 | HEM  | CHA-C4D-ND  | 3.35  | 128.52      | 124.37   |
| 25  | C     | 602 | HEM  | CHA-C4D-ND  | 3.34  | 128.50      | 124.37   |
| 26  | D     | 402 | CDL  | OA6-CA5-C11 | 3.34  | 118.70      | 111.48   |
| 31  | a     | 602 | HEA  | CMB-C2B-C1B | 3.32  | 130.22      | 125.03   |
| 31  | a     | 602 | HEA  | CHA-C4D-ND  | -3.31 | 120.86      | 124.42   |
| 31  | a     | 602 | HEA  | C2C-C1C-NC  | 3.29  | 115.41      | 110.14   |
| 28  | O     | 401 | HEC  | C1D-C2D-C3D | -3.23 | 103.12      | 106.82   |
| 31  | a     | 602 | HEA  | C3A-C2A-C1A | -3.23 | 103.99      | 107.05   |
| 24  | H     | 602 | PEF  | O3-C30-C31  | 3.22  | 121.65      | 111.83   |
| 27  | C     | 606 | PCF  | O31-C31-C32 | 3.20  | 121.58      | 111.83   |
| 24  | U     | 101 | PEF  | O3-C30-C31  | 3.19  | 121.55      | 111.83   |
| 28  | O     | 401 | HEC  | C2D-C1D-ND  | 3.18  | 115.25      | 110.14   |
| 28  | D     | 401 | HEC  | C1D-C2D-C3D | -3.18 | 103.17      | 106.82   |
| 27  | S     | 103 | PCF  | O21-C21-C22 | 3.17  | 118.34      | 111.48   |
| 31  | a     | 602 | HEA  | CBA-CAA-C2A | -3.14 | 103.85      | 112.53   |
| 24  | N     | 605 | PEF  | O2-C10-C11  | 3.13  | 118.26      | 111.48   |
| 26  | N     | 603 | CDL  | OB8-CB7-C71 | 3.11  | 121.32      | 111.83   |
| 24  | b     | 303 | PEF  | C2-O2-C10   | -3.08 | 110.42      | 117.80   |
| 25  | N     | 601 | HEM  | CBD-CAD-C3D | 3.08  | 121.05      | 112.53   |
| 25  | C     | 601 | HEM  | CBD-CAD-C3D | 3.07  | 121.03      | 112.53   |
| 28  | D     | 401 | HEC  | C2D-C1D-ND  | 3.07  | 115.06      | 110.14   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 28  | O     | 401 | HEC  | C4D-C3D-C2D | -3.04 | 102.17      | 106.87   |
| 31  | a     | 602 | HEA  | C27-C19-C20 | 3.02  | 120.47      | 115.23   |
| 28  | O     | 401 | HEC  | C3A-C4A-NA  | 3.02  | 115.23      | 109.64   |
| 26  | H     | 601 | CDL  | OA8-CA7-C31 | 3.02  | 121.05      | 111.83   |
| 28  | D     | 401 | HEC  | C4D-C3D-C2D | -3.02 | 102.19      | 106.87   |
| 31  | a     | 602 | HEA  | C4D-C3D-C2D | -3.01 | 102.50      | 106.89   |
| 26  | O     | 402 | CDL  | OB8-CB7-C71 | 3.01  | 120.29      | 111.15   |
| 25  | C     | 601 | HEM  | C1B-NB-C4B  | 2.99  | 108.75      | 105.21   |
| 25  | N     | 601 | HEM  | C1B-NB-C4B  | 2.99  | 108.75      | 105.21   |
| 31  | a     | 602 | HEA  | CHB-C4A-NA  | -2.98 | 121.20      | 124.45   |
| 28  | D     | 401 | HEC  | CMC-C2C-C3C | 2.97  | 133.53      | 126.55   |
| 26  | L     | 501 | CDL  | OB8-CB7-C71 | 2.95  | 120.83      | 111.83   |
| 26  | O     | 402 | CDL  | OA8-CA7-C31 | 2.95  | 120.82      | 111.83   |
| 27  | I     | 101 | PCF  | O31-C31-C32 | 2.94  | 120.80      | 111.83   |
| 24  | e     | 201 | PEF  | O2-C10-C11  | 2.94  | 117.83      | 111.48   |
| 25  | N     | 602 | HEM  | C1B-NB-C4B  | 2.93  | 108.68      | 105.21   |
| 25  | C     | 602 | HEM  | CHD-C4C-NC  | 2.93  | 127.65      | 124.45   |
| 24  | E     | 302 | PEF  | C2-O2-C10   | -2.93 | 110.78      | 117.80   |
| 31  | a     | 603 | HEA  | C4A-NA-C1A  | -2.93 | 101.05      | 105.82   |
| 24  | E     | 302 | PEF  | O3-C30-C31  | 2.92  | 120.74      | 111.83   |
| 28  | D     | 401 | HEC  | C3A-C4A-NA  | 2.92  | 115.04      | 109.64   |
| 24  | b     | 302 | PEF  | O3-C30-C31  | 2.92  | 120.73      | 111.83   |
| 26  | S     | 101 | CDL  | OA8-CA7-C31 | 2.91  | 120.71      | 111.83   |
| 26  | S     | 101 | CDL  | OB8-CB7-C71 | 2.91  | 120.70      | 111.83   |
| 26  | O     | 402 | CDL  | CB4-OB6-CB5 | -2.91 | 110.84      | 117.80   |
| 31  | a     | 603 | HEA  | C1B-C2B-C3B | -2.90 | 103.44      | 106.80   |
| 27  | S     | 103 | PCF  | C3-C2-C1    | -2.90 | 105.02      | 111.78   |
| 31  | a     | 603 | HEA  | C13-C12-C11 | -2.87 | 109.80      | 114.39   |
| 31  | a     | 602 | HEA  | C4A-CHB-C1B | -2.87 | 119.92      | 126.02   |
| 26  | H     | 601 | CDL  | OB8-CB7-C71 | 2.86  | 120.55      | 111.83   |
| 25  | N     | 601 | HEM  | CAD-C3D-C2D | -2.86 | 122.52      | 127.87   |
| 31  | a     | 603 | HEA  | C1D-ND-C4D  | -2.85 | 101.83      | 105.21   |
| 25  | C     | 601 | HEM  | CAD-C3D-C2D | -2.85 | 122.54      | 127.87   |
| 25  | C     | 602 | HEM  | C1B-NB-C4B  | 2.84  | 108.57      | 105.21   |
| 24  | b     | 303 | PEF  | O3-C30-C31  | 2.83  | 120.46      | 111.83   |
| 31  | a     | 603 | HEA  | CAD-C3D-C4D | 2.83  | 129.63      | 124.70   |
| 27  | S     | 103 | PCF  | O31-C31-C32 | 2.81  | 120.41      | 111.83   |
| 28  | O     | 401 | HEC  | CMC-C2C-C3C | 2.81  | 133.15      | 126.55   |
| 24  | P     | 302 | PEF  | O3-C30-C31  | 2.81  | 120.39      | 111.83   |
| 27  | N     | 606 | PCF  | O31-C31-C32 | 2.80  | 120.36      | 111.83   |
| 31  | a     | 602 | HEA  | C4B-C3B-C2B | -2.79 | 102.74      | 107.44   |
| 31  | a     | 602 | HEA  | C4A-NA-C1A  | -2.78 | 101.29      | 105.82   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 603 | HEA  | C27-C19-C20 | 2.77  | 120.04      | 115.23   |
| 25  | C     | 601 | HEM  | CHD-C1D-C2D | -2.77 | 120.65      | 125.03   |
| 28  | D     | 401 | HEC  | CHC-C4B-NB  | -2.77 | 121.43      | 124.45   |
| 28  | O     | 401 | HEC  | CHC-C4B-NB  | -2.75 | 121.46      | 124.45   |
| 25  | N     | 601 | HEM  | CHD-C1D-C2D | -2.75 | 120.69      | 125.03   |
| 24  | C     | 604 | PEF  | O3-C30-C31  | 2.74  | 120.19      | 111.83   |
| 26  | C     | 603 | CDL  | OB8-CB7-C71 | 2.74  | 120.18      | 111.83   |
| 31  | a     | 602 | HEA  | CAD-C3D-C4D | 2.73  | 129.46      | 124.70   |
| 24  | L     | 502 | PEF  | O3-C30-C31  | 2.73  | 120.16      | 111.83   |
| 28  | O     | 401 | HEC  | C4A-C3A-C2A | -2.73 | 102.92      | 106.97   |
| 31  | a     | 602 | HEA  | CMD-C2D-C1D | 2.72  | 129.29      | 125.03   |
| 26  | D     | 402 | CDL  | OB8-CB7-C71 | 2.72  | 120.12      | 111.83   |
| 24  | N     | 604 | PEF  | C2-O2-C10   | -2.66 | 111.44      | 117.80   |
| 27  | e     | 202 | PCF  | O31-C31-C32 | 2.65  | 119.90      | 111.83   |
| 24  | a     | 605 | PEF  | O3-C30-C31  | 2.63  | 119.86      | 111.83   |
| 26  | S     | 101 | CDL  | CA4-OA6-CA5 | -2.63 | 111.50      | 117.80   |
| 24  | e     | 201 | PEF  | O3-C30-C31  | 2.63  | 119.84      | 111.83   |
| 24  | N     | 604 | PEF  | O3-C30-C31  | 2.62  | 119.82      | 111.83   |
| 28  | O     | 401 | HEC  | CAA-CBA-CGA | -2.60 | 106.77      | 113.67   |
| 24  | S     | 102 | PEF  | O3-C30-C31  | 2.59  | 119.73      | 111.83   |
| 26  | L     | 501 | CDL  | OA8-CA7-C31 | 2.57  | 119.68      | 111.83   |
| 28  | O     | 401 | HEC  | CHB-C1B-C2B | -2.57 | 119.96      | 127.43   |
| 25  | N     | 602 | HEM  | CHD-C1D-C2D | -2.56 | 120.98      | 125.03   |
| 26  | D     | 402 | CDL  | OA8-CA7-C31 | 2.56  | 119.64      | 111.83   |
| 24  | c     | 301 | PEF  | C2-O2-C10   | -2.56 | 111.68      | 117.80   |
| 31  | a     | 602 | HEA  | CHC-C4B-NB  | -2.55 | 121.21      | 124.37   |
| 24  | C     | 604 | PEF  | C2-O2-C10   | -2.54 | 111.71      | 117.80   |
| 25  | N     | 602 | HEM  | CHD-C4C-NC  | 2.54  | 127.22      | 124.45   |
| 28  | O     | 401 | HEC  | CAD-C3D-C4D | 2.53  | 129.88      | 124.94   |
| 24  | C     | 605 | PEF  | O3-C30-C31  | 2.52  | 119.53      | 111.83   |
| 31  | a     | 603 | HEA  | CHC-C4B-NB  | -2.51 | 121.26      | 124.37   |
| 31  | a     | 603 | HEA  | C13-C14-C15 | -2.49 | 121.94      | 127.62   |
| 26  | N     | 603 | CDL  | OA8-CA7-C31 | 2.48  | 119.39      | 111.83   |
| 26  | N     | 603 | CDL  | CB2-C1-CA2  | -2.48 | 105.52      | 112.65   |
| 25  | C     | 602 | HEM  | CHD-C1D-C2D | -2.47 | 121.12      | 125.03   |
| 24  | J     | 101 | PEF  | O3-C30-C31  | 2.47  | 119.37      | 111.83   |
| 24  | A     | 501 | PEF  | O3-C30-C31  | 2.46  | 119.34      | 111.83   |
| 31  | a     | 603 | HEA  | CHD-C1D-C2D | -2.46 | 119.97      | 126.95   |
| 24  | N     | 605 | PEF  | O3-C30-C31  | 2.44  | 119.28      | 111.83   |
| 28  | D     | 401 | HEC  | CHB-C1B-C2B | -2.43 | 120.36      | 127.43   |
| 31  | a     | 602 | HEA  | C4B-NB-C1B  | -2.43 | 102.33      | 105.21   |
| 28  | D     | 401 | HEC  | C4A-C3A-C2A | -2.42 | 103.38      | 106.97   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 31  | a     | 602 | HEA  | C17-C18-C19 | -2.41 | 122.11      | 127.62   |
| 24  | L     | 502 | PEF  | C2-O2-C10   | -2.41 | 112.04      | 117.80   |
| 26  | C     | 603 | CDL  | CA4-OA6-CA5 | -2.41 | 112.04      | 117.80   |
| 28  | D     | 401 | HEC  | CAA-CBA-CGA | -2.39 | 107.34      | 113.67   |
| 25  | N     | 601 | HEM  | CHD-C4C-NC  | 2.38  | 127.04      | 124.45   |
| 27  | T     | 101 | PCF  | C2-O21-C21  | -2.37 | 112.12      | 117.80   |
| 25  | C     | 602 | HEM  | CHB-C1B-C2B | -2.36 | 120.25      | 126.95   |
| 31  | a     | 603 | HEA  | CAA-CBA-CGA | -2.34 | 107.45      | 113.67   |
| 28  | O     | 401 | HEC  | CAD-CBD-CGD | -2.34 | 107.45      | 113.67   |
| 27  | C     | 606 | PCF  | O31-C31-O32 | -2.34 | 117.78      | 123.63   |
| 31  | a     | 602 | HEA  | C25-C23-C24 | 2.33  | 119.95      | 114.59   |
| 26  | O     | 402 | CDL  | OB6-CB5-OB7 | -2.32 | 118.27      | 123.70   |
| 27  | T     | 101 | PCF  | O31-C31-C32 | 2.30  | 118.86      | 111.83   |
| 28  | O     | 401 | HEC  | CHA-C1A-C2A | -2.30 | 121.22      | 124.86   |
| 24  | c     | 301 | PEF  | O3-C30-C31  | 2.29  | 118.83      | 111.83   |
| 27  | I     | 101 | PCF  | C2-O21-C21  | -2.29 | 112.32      | 117.80   |
| 25  | N     | 602 | HEM  | CAD-CBD-CGD | -2.29 | 107.60      | 113.67   |
| 24  | S     | 102 | PEF  | C2-O2-C10   | -2.28 | 112.33      | 117.80   |
| 25  | C     | 602 | HEM  | C4C-CHD-C1D | -2.28 | 121.17      | 126.02   |
| 28  | D     | 401 | HEC  | CAD-C3D-C4D | 2.27  | 129.38      | 124.94   |
| 31  | a     | 603 | HEA  | C25-C23-C24 | 2.27  | 119.81      | 114.59   |
| 31  | a     | 602 | HEA  | C1D-ND-C4D  | -2.27 | 102.52      | 105.21   |
| 31  | a     | 602 | HEA  | OMA-CMA-C3A | -2.26 | 120.52      | 125.62   |
| 25  | N     | 602 | HEM  | CHB-C1B-C2B | -2.25 | 120.54      | 126.95   |
| 25  | N     | 601 | HEM  | C3B-C4B-NB  | -2.24 | 107.86      | 109.47   |
| 25  | C     | 602 | HEM  | C4A-CHB-C1B | -2.24 | 120.98      | 126.25   |
| 27  | C     | 606 | PCF  | C2-O21-C21  | -2.24 | 112.44      | 117.80   |
| 25  | N     | 602 | HEM  | C4C-CHD-C1D | -2.24 | 121.27      | 126.02   |
| 31  | a     | 603 | HEA  | CHA-C1A-NA  | -2.24 | 122.02      | 124.45   |
| 31  | a     | 602 | HEA  | CAD-CBD-CGD | -2.23 | 107.74      | 113.67   |
| 31  | a     | 603 | HEA  | CMB-C2B-C3B | -2.23 | 125.97      | 130.28   |
| 24  | a     | 605 | PEF  | O2-C2-C1    | 2.22  | 116.31      | 108.34   |
| 28  | D     | 401 | HEC  | CHD-C4C-NC  | -2.22 | 122.03      | 124.45   |
| 25  | N     | 602 | HEM  | C4A-CHB-C1B | -2.21 | 121.04      | 126.25   |
| 27  | e     | 202 | PCF  | C2-O21-C21  | -2.21 | 112.51      | 117.80   |
| 25  | N     | 601 | HEM  | CAA-CBA-CGA | -2.21 | 107.81      | 113.67   |
| 24  | H     | 602 | PEF  | C2-O2-C10   | -2.20 | 112.53      | 117.80   |
| 27  | N     | 606 | PCF  | C2-O21-C21  | -2.20 | 112.53      | 117.80   |
| 26  | H     | 601 | CDL  | CB4-OB6-CB5 | -2.20 | 112.54      | 117.80   |
| 31  | a     | 603 | HEA  | CHC-C1C-C2C | -2.19 | 121.06      | 127.43   |
| 31  | a     | 603 | HEA  | C26-C15-C16 | 2.19  | 119.03      | 115.23   |
| 25  | C     | 602 | HEM  | CAD-CBD-CGD | -2.19 | 107.85      | 113.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 24  | H     | 602 | PEF  | O3-C30-O5   | -2.19 | 118.16      | 123.63   |
| 24  | A     | 501 | PEF  | C2-O2-C10   | -2.18 | 112.57      | 117.80   |
| 25  | C     | 601 | HEM  | CAA-CBA-CGA | -2.18 | 107.89      | 113.67   |
| 24  | C     | 605 | PEF  | O2-C10-O4   | -2.18 | 118.62      | 123.70   |
| 27  | I     | 101 | PCF  | O31-C31-O32 | -2.17 | 118.19      | 123.63   |
| 31  | a     | 603 | HEA  | CMC-C2C-C3C | 2.17  | 131.66      | 126.55   |
| 25  | C     | 601 | HEM  | C3B-C4B-NB  | -2.17 | 107.91      | 109.47   |
| 25  | N     | 602 | HEM  | C4D-ND-C1D  | 2.17  | 107.77      | 105.21   |
| 26  | D     | 402 | CDL  | OB6-CB5-OB7 | -2.16 | 118.66      | 123.70   |
| 25  | N     | 601 | HEM  | CHB-C1B-C2B | -2.15 | 120.83      | 126.95   |
| 26  | S     | 101 | CDL  | CB4-OB6-CB5 | -2.15 | 112.66      | 117.80   |
| 25  | N     | 601 | HEM  | C4C-CHD-C1D | -2.14 | 121.47      | 126.02   |
| 25  | C     | 601 | HEM  | CHD-C4C-NC  | 2.13  | 126.77      | 124.45   |
| 31  | a     | 602 | HEA  | C13-C14-C15 | -2.12 | 122.76      | 127.62   |
| 31  | a     | 602 | HEA  | C4C-C3C-C2C | -2.11 | 104.68      | 107.30   |
| 31  | a     | 603 | HEA  | CHB-C4A-NA  | -2.11 | 122.16      | 124.45   |
| 25  | C     | 601 | HEM  | C4C-CHD-C1D | -2.11 | 121.55      | 126.02   |
| 31  | a     | 603 | HEA  | C4B-NB-C1B  | -2.10 | 102.72      | 105.21   |
| 26  | N     | 603 | CDL  | CA4-OA6-CA5 | -2.09 | 112.79      | 117.80   |
| 26  | C     | 603 | CDL  | OB8-CB7-OB9 | -2.09 | 118.40      | 123.63   |
| 31  | a     | 602 | HEA  | CMC-C2C-C1C | 2.08  | 128.59      | 125.42   |
| 24  | b     | 303 | PEF  | O2-C10-O4   | -2.08 | 118.85      | 123.70   |
| 27  | S     | 103 | PCF  | O31-C31-O32 | -2.07 | 118.44      | 123.63   |
| 24  | L     | 502 | PEF  | O3-C30-O5   | -2.07 | 118.45      | 123.63   |
| 28  | D     | 401 | HEC  | CMD-C2D-C1D | 2.07  | 128.57      | 125.42   |
| 25  | N     | 602 | HEM  | O2A-CGA-CBA | 2.07  | 120.53      | 114.00   |
| 25  | C     | 602 | HEM  | C1A-CHA-C4D | -2.06 | 121.40      | 126.25   |
| 25  | C     | 601 | HEM  | CHB-C1B-C2B | -2.05 | 121.13      | 126.95   |
| 24  | P     | 302 | PEF  | O3-C30-O5   | -2.04 | 118.52      | 123.63   |
| 24  | J     | 101 | PEF  | O2-C10-O4   | -2.04 | 118.94      | 123.70   |
| 26  | S     | 101 | CDL  | OB8-CB7-OB9 | -2.04 | 118.53      | 123.63   |
| 25  | N     | 602 | HEM  | C1A-CHA-C4D | -2.04 | 121.46      | 126.25   |
| 28  | O     | 401 | HEC  | CMD-C2D-C1D | 2.03  | 128.51      | 125.42   |
| 28  | D     | 401 | HEC  | CHC-C1C-C2C | -2.03 | 121.54      | 127.43   |
| 26  | L     | 501 | CDL  | CA4-OA6-CA5 | -2.03 | 112.94      | 117.80   |
| 26  | O     | 402 | CDL  | CA6-CA4-CA3 | -2.02 | 107.07      | 111.78   |
| 28  | O     | 401 | HEC  | CHD-C4C-NC  | -2.02 | 122.25      | 124.45   |
| 25  | C     | 601 | HEM  | CHA-C1A-NA  | 2.02  | 127.53      | 123.86   |
| 26  | L     | 501 | CDL  | OB8-CB7-OB9 | -2.01 | 118.59      | 123.63   |
| 26  | C     | 603 | CDL  | CB4-OB6-CB5 | -2.01 | 112.99      | 117.80   |
| 26  | N     | 603 | CDL  | OB8-CB7-OB9 | -2.01 | 118.61      | 123.63   |
| 25  | C     | 602 | HEM  | C3B-C4B-NB  | -2.01 | 108.03      | 109.47   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 26  | H     | 601 | CDL  | CA4-OA6-CA5 | -2.00 | 113.00      | 117.80   |
| 24  | c     | 302 | PEF  | O3-C30-C31  | 2.00  | 117.94      | 111.83   |

There are no chirality outliers.

All (439) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 24  | A     | 501 | PEF  | C1-O3P-P-O1P  |
| 24  | A     | 501 | PEF  | C1-O3P-P-O2P  |
| 24  | A     | 501 | PEF  | C1-O3P-P-O4P  |
| 24  | C     | 604 | PEF  | C4-O4P-P-O3P  |
| 24  | C     | 605 | PEF  | C11-C10-O2-C2 |
| 24  | C     | 605 | PEF  | O4-C10-O2-C2  |
| 24  | C     | 605 | PEF  | C4-O4P-P-O2P  |
| 24  | E     | 302 | PEF  | C11-C10-O2-C2 |
| 24  | E     | 302 | PEF  | C1-O3P-P-O4P  |
| 24  | E     | 302 | PEF  | C4-O4P-P-O2P  |
| 24  | J     | 101 | PEF  | O2-C2-C3-O3   |
| 24  | J     | 101 | PEF  | C11-C10-O2-C2 |
| 24  | L     | 502 | PEF  | C1-O3P-P-O2P  |
| 24  | L     | 502 | PEF  | C1-O3P-P-O4P  |
| 24  | L     | 502 | PEF  | C4-O4P-P-O2P  |
| 24  | L     | 502 | PEF  | C4-O4P-P-O3P  |
| 24  | N     | 604 | PEF  | C1-O3P-P-O2P  |
| 24  | N     | 604 | PEF  | C1-O3P-P-O4P  |
| 24  | N     | 605 | PEF  | C1-O3P-P-O4P  |
| 24  | P     | 302 | PEF  | C1-O3P-P-O4P  |
| 24  | S     | 102 | PEF  | C4-O4P-P-O1P  |
| 24  | b     | 302 | PEF  | C1-O3P-P-O1P  |
| 24  | b     | 302 | PEF  | C1-O3P-P-O2P  |
| 24  | b     | 302 | PEF  | C1-O3P-P-O4P  |
| 24  | b     | 302 | PEF  | C4-O4P-P-O3P  |
| 24  | b     | 303 | PEF  | O4P-C4-C5-N   |
| 24  | b     | 303 | PEF  | C1-O3P-P-O2P  |
| 24  | b     | 303 | PEF  | C1-O3P-P-O4P  |
| 24  | b     | 303 | PEF  | C4-O4P-P-O2P  |
| 24  | b     | 303 | PEF  | C4-O4P-P-O3P  |
| 24  | c     | 301 | PEF  | C1-O3P-P-O2P  |
| 24  | c     | 301 | PEF  | C1-O3P-P-O4P  |
| 24  | c     | 301 | PEF  | C4-O4P-P-O2P  |
| 24  | c     | 301 | PEF  | C4-O4P-P-O3P  |
| 24  | c     | 302 | PEF  | C1-O3P-P-O4P  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | c     | 302 | PEF  | C4-O4P-P-O3P    |
| 24  | e     | 201 | PEF  | C1-O3P-P-O1P    |
| 24  | e     | 201 | PEF  | C1-O3P-P-O2P    |
| 24  | e     | 201 | PEF  | C1-O3P-P-O4P    |
| 24  | e     | 201 | PEF  | C4-O4P-P-O3P    |
| 25  | C     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 25  | C     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 25  | C     | 602 | HEM  | C2C-C3C-CAC-CBC |
| 25  | N     | 601 | HEM  | C2B-C3B-CAB-CBB |
| 25  | N     | 601 | HEM  | C4B-C3B-CAB-CBB |
| 26  | C     | 603 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | C     | 603 | CDL  | CA2-OA2-PA1-OA4 |
| 26  | C     | 603 | CDL  | CA2-OA2-PA1-OA5 |
| 26  | C     | 603 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | C     | 603 | CDL  | CA3-OA5-PA1-OA3 |
| 26  | C     | 603 | CDL  | CA3-OA5-PA1-OA4 |
| 26  | C     | 603 | CDL  | CB3-OB5-PB2-OB2 |
| 26  | C     | 603 | CDL  | CB3-OB5-PB2-OB3 |
| 26  | C     | 603 | CDL  | CB3-OB5-PB2-OB4 |
| 26  | C     | 603 | CDL  | C51-CB5-OB6-CB4 |
| 26  | D     | 402 | CDL  | CA2-OA2-PA1-OA4 |
| 26  | D     | 402 | CDL  | CA2-OA2-PA1-OA5 |
| 26  | D     | 402 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | D     | 402 | CDL  | CA3-OA5-PA1-OA3 |
| 26  | D     | 402 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | D     | 402 | CDL  | CB2-OB2-PB2-OB4 |
| 26  | D     | 402 | CDL  | CB2-OB2-PB2-OB5 |
| 26  | H     | 601 | CDL  | O1-C1-CB2-OB2   |
| 26  | H     | 601 | CDL  | CA2-OA2-PA1-OA5 |
| 26  | H     | 601 | CDL  | CB2-OB2-PB2-OB5 |
| 26  | L     | 501 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | L     | 501 | CDL  | CA3-OA5-PA1-OA3 |
| 26  | L     | 501 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | L     | 501 | CDL  | CB2-OB2-PB2-OB4 |
| 26  | L     | 501 | CDL  | CB2-OB2-PB2-OB5 |
| 26  | N     | 603 | CDL  | CA3-OA5-PA1-OA3 |
| 26  | O     | 402 | CDL  | O1-C1-CB2-OB2   |
| 26  | O     | 402 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | O     | 402 | CDL  | CA2-OA2-PA1-OA5 |
| 26  | O     | 402 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | O     | 402 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | O     | 402 | CDL  | CB3-OB5-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | S     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | S     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | S     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 26  | S     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 26  | S     | 101 | CDL  | CB3-OB5-PB2-OB2 |
| 26  | S     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 26  | S     | 101 | CDL  | CB3-OB5-PB2-OB4 |
| 27  | C     | 606 | PCF  | C1-O11-P-O12    |
| 27  | N     | 606 | PCF  | C11-O13-P-O11   |
| 27  | N     | 606 | PCF  | C11-O13-P-O12   |
| 27  | N     | 606 | PCF  | C11-O13-P-O14   |
| 27  | N     | 606 | PCF  | O13-C11-C12-N   |
| 27  | S     | 103 | PCF  | O13-C11-C12-N   |
| 27  | S     | 103 | PCF  | O11-C1-C2-O21   |
| 31  | a     | 602 | HEA  | C2A-C3A-CMA-OMA |
| 31  | a     | 602 | HEA  | C4A-C3A-CMA-OMA |
| 31  | a     | 602 | HEA  | C11-C12-C13-C14 |
| 27  | S     | 103 | PCF  | O32-C31-O31-C3  |
| 24  | E     | 302 | PEF  | O4-C10-O2-C2    |
| 24  | J     | 101 | PEF  | O4-C10-O2-C2    |
| 26  | C     | 603 | CDL  | OB7-CB5-OB6-CB4 |
| 27  | S     | 103 | PCF  | C32-C31-O31-C3  |
| 31  | a     | 602 | HEA  | C26-C15-C16-C17 |
| 31  | a     | 602 | HEA  | C14-C15-C16-C17 |
| 24  | U     | 101 | PEF  | C31-C30-O3-C3   |
| 26  | D     | 402 | CDL  | O1-C1-CB2-OB2   |
| 26  | S     | 101 | CDL  | O1-C1-CB2-OB2   |
| 31  | a     | 602 | HEA  | C18-C19-C20-C21 |
| 24  | U     | 101 | PEF  | O5-C30-O3-C3    |
| 26  | H     | 601 | CDL  | CA2-C1-CB2-OB2  |
| 26  | O     | 402 | CDL  | CA2-C1-CB2-OB2  |
| 26  | S     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 31  | a     | 602 | HEA  | C27-C19-C20-C21 |
| 24  | A     | 501 | PEF  | C30-C31-C32-C33 |
| 24  | a     | 605 | PEF  | O4-C10-O2-C2    |
| 26  | D     | 402 | CDL  | OB5-CB3-CB4-OB6 |
| 24  | a     | 605 | PEF  | C11-C10-O2-C2   |
| 24  | L     | 502 | PEF  | C10-C11-C12-C13 |
| 24  | J     | 101 | PEF  | C12-C13-C14-C15 |
| 24  | A     | 501 | PEF  | C10-C11-C12-C13 |
| 24  | U     | 101 | PEF  | C30-C31-C32-C33 |
| 24  | c     | 302 | PEF  | C11-C10-O2-C2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | N     | 603 | CDL  | CB5-C51-C52-C53 |
| 24  | c     | 302 | PEF  | O4-C10-O2-C2    |
| 26  | D     | 402 | CDL  | CA2-C1-CB2-OB2  |
| 27  | N     | 606 | PCF  | C21-C22-C23-C24 |
| 26  | D     | 402 | CDL  | CA7-C31-C32-C33 |
| 25  | C     | 601 | HEM  | C2D-C3D-CAD-CBD |
| 25  | N     | 601 | HEM  | C2D-C3D-CAD-CBD |
| 25  | C     | 601 | HEM  | C4D-C3D-CAD-CBD |
| 26  | D     | 402 | CDL  | C11-CA5-OA6-CA4 |
| 26  | N     | 603 | CDL  | C11-CA5-OA6-CA4 |
| 26  | O     | 402 | CDL  | C51-CB5-OB6-CB4 |
| 24  | b     | 303 | PEF  | C31-C30-O3-C3   |
| 24  | C     | 605 | PEF  | C16-C17-C18-C19 |
| 24  | E     | 302 | PEF  | C11-C12-C13-C14 |
| 24  | P     | 302 | PEF  | C33-C34-C35-C36 |
| 26  | H     | 601 | CDL  | C31-C32-C33-C34 |
| 27  | e     | 202 | PCF  | C26-C27-C28-C29 |
| 24  | E     | 302 | PEF  | C37-C38-C39-C40 |
| 24  | U     | 101 | PEF  | C19-C20-C21-C22 |
| 31  | a     | 603 | HEA  | C4C-C3C-CAC-CBC |
| 24  | a     | 605 | PEF  | C30-C31-C32-C33 |
| 24  | c     | 301 | PEF  | C31-C32-C33-C34 |
| 24  | P     | 302 | PEF  | C12-C13-C14-C15 |
| 24  | C     | 605 | PEF  | C31-C32-C33-C34 |
| 24  | C     | 604 | PEF  | C1-C2-C3-O3     |
| 24  | c     | 302 | PEF  | C38-C39-C40-C41 |
| 27  | I     | 101 | PCF  | C27-C28-C29-C30 |
| 27  | e     | 202 | PCF  | C24-C25-C26-C27 |
| 24  | C     | 604 | PEF  | C11-C10-O2-C2   |
| 26  | L     | 501 | CDL  | C71-CB7-OB8-CB6 |
| 27  | C     | 606 | PCF  | C32-C31-O31-C3  |
| 24  | b     | 303 | PEF  | O5-C30-O3-C3    |
| 26  | D     | 402 | CDL  | OA7-CA5-OA6-CA4 |
| 26  | N     | 603 | CDL  | OA7-CA5-OA6-CA4 |
| 26  | L     | 501 | CDL  | C12-C13-C14-C15 |
| 24  | C     | 605 | PEF  | C19-C20-C21-C22 |
| 24  | b     | 302 | PEF  | C17-C18-C19-C20 |
| 24  | e     | 201 | PEF  | C20-C21-C22-C23 |
| 24  | N     | 605 | PEF  | C14-C15-C16-C17 |
| 24  | N     | 604 | PEF  | C11-C10-O2-C2   |
| 24  | N     | 605 | PEF  | C11-C10-O2-C2   |
| 24  | e     | 201 | PEF  | C11-C10-O2-C2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | D     | 402 | CDL  | C51-CB5-OB6-CB4 |
| 26  | H     | 601 | CDL  | C11-CA5-OA6-CA4 |
| 26  | H     | 601 | CDL  | C51-CB5-OB6-CB4 |
| 26  | S     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 24  | b     | 302 | PEF  | C10-C11-C12-C13 |
| 25  | N     | 601 | HEM  | C4D-C3D-CAD-CBD |
| 24  | N     | 604 | PEF  | O4-C10-O2-C2    |
| 24  | e     | 201 | PEF  | O4-C10-O2-C2    |
| 26  | H     | 601 | CDL  | OB7-CB5-OB6-CB4 |
| 26  | O     | 402 | CDL  | OB7-CB5-OB6-CB4 |
| 24  | U     | 101 | PEF  | C38-C39-C40-C41 |
| 24  | N     | 604 | PEF  | C34-C35-C36-C37 |
| 24  | U     | 101 | PEF  | C11-C12-C13-C14 |
| 25  | N     | 602 | HEM  | C2C-C3C-CAC-CBC |
| 24  | b     | 302 | PEF  | C13-C14-C15-C16 |
| 26  | S     | 101 | CDL  | C71-C72-C73-C74 |
| 27  | C     | 606 | PCF  | O32-C31-O31-C3  |
| 24  | c     | 301 | PEF  | C11-C10-O2-C2   |
| 25  | C     | 602 | HEM  | C4C-C3C-CAC-CBC |
| 26  | D     | 402 | CDL  | C73-C74-C75-C76 |
| 24  | C     | 604 | PEF  | C31-C32-C33-C34 |
| 26  | L     | 501 | CDL  | OB6-CB4-CB6-OB8 |
| 24  | N     | 605 | PEF  | C32-C33-C34-C35 |
| 26  | D     | 402 | CDL  | C58-C59-C60-C61 |
| 26  | N     | 603 | CDL  | C35-C36-C37-C38 |
| 27  | C     | 606 | PCF  | C35-C36-C37-C38 |
| 24  | C     | 604 | PEF  | O4-C10-O2-C2    |
| 24  | N     | 605 | PEF  | C21-C22-C23-C24 |
| 24  | b     | 302 | PEF  | C11-C10-O2-C2   |
| 26  | L     | 501 | CDL  | OB9-CB7-OB8-CB6 |
| 24  | b     | 302 | PEF  | O3P-C1-C2-C3    |
| 26  | D     | 402 | CDL  | OB5-CB3-CB4-CB6 |
| 27  | S     | 103 | PCF  | O11-C1-C2-C3    |
| 24  | N     | 605 | PEF  | O4-C10-O2-C2    |
| 26  | H     | 601 | CDL  | OA7-CA5-OA6-CA4 |
| 26  | S     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 27  | N     | 606 | PCF  | C25-C26-C27-C28 |
| 26  | C     | 603 | CDL  | CB7-C71-C72-C73 |
| 26  | S     | 101 | CDL  | CB5-C51-C52-C53 |
| 24  | b     | 302 | PEF  | C19-C20-C21-C22 |
| 24  | C     | 605 | PEF  | C1-C2-C3-O3     |
| 26  | D     | 402 | CDL  | CA3-CA4-CA6-OA8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | N     | 606 | PCF  | C1-C2-C3-O31    |
| 27  | T     | 101 | PCF  | C24-C25-C26-C27 |
| 27  | I     | 101 | PCF  | C35-C36-C37-C38 |
| 26  | L     | 501 | CDL  | CA5-C11-C12-C13 |
| 24  | a     | 605 | PEF  | C1-C2-O2-C10    |
| 27  | N     | 606 | PCF  | C22-C23-C24-C25 |
| 26  | D     | 402 | CDL  | OA6-CA4-CA6-OA8 |
| 27  | N     | 606 | PCF  | O21-C2-C3-O31   |
| 24  | N     | 605 | PEF  | C13-C14-C15-C16 |
| 24  | E     | 302 | PEF  | C14-C15-C16-C17 |
| 27  | T     | 101 | PCF  | C47-C48-C49-C50 |
| 24  | L     | 502 | PEF  | C31-C30-O3-C3   |
| 26  | O     | 402 | CDL  | CA7-C31-C32-C33 |
| 26  | L     | 501 | CDL  | C52-C53-C54-C55 |
| 27  | C     | 606 | PCF  | C47-C48-C49-C50 |
| 26  | D     | 402 | CDL  | OB7-CB5-OB6-CB4 |
| 31  | a     | 602 | HEA  | C4C-C3C-CAC-CBC |
| 27  | e     | 202 | PCF  | O11-C1-C2-C3    |
| 24  | L     | 502 | PEF  | C20-C21-C22-C23 |
| 24  | C     | 605 | PEF  | C13-C14-C15-C16 |
| 24  | C     | 605 | PEF  | C20-C21-C22-C23 |
| 24  | J     | 101 | PEF  | C1-C2-C3-O3     |
| 24  | U     | 101 | PEF  | C1-C2-C3-O3     |
| 26  | C     | 603 | CDL  | CB3-CB4-CB6-OB8 |
| 26  | L     | 501 | CDL  | CB3-CB4-CB6-OB8 |
| 24  | E     | 302 | PEF  | C35-C36-C37-C38 |
| 24  | b     | 302 | PEF  | O2-C10-C11-C12  |
| 24  | b     | 302 | PEF  | O4-C10-O2-C2    |
| 24  | b     | 303 | PEF  | O3P-C1-C2-O2    |
| 27  | e     | 202 | PCF  | O11-C1-C2-O21   |
| 26  | L     | 501 | CDL  | C53-C54-C55-C56 |
| 24  | S     | 102 | PEF  | O2-C2-C3-O3     |
| 24  | e     | 201 | PEF  | O2-C2-C3-O3     |
| 26  | C     | 603 | CDL  | OB6-CB4-CB6-OB8 |
| 24  | c     | 301 | PEF  | O4-C10-O2-C2    |
| 27  | e     | 202 | PCF  | C21-C22-C23-C24 |
| 26  | N     | 603 | CDL  | C15-C16-C17-C18 |
| 24  | c     | 302 | PEF  | C34-C35-C36-C37 |
| 24  | U     | 101 | PEF  | C14-C15-C16-C17 |
| 24  | J     | 101 | PEF  | C10-C11-C12-C13 |
| 24  | N     | 604 | PEF  | C10-C11-C12-C13 |
| 26  | D     | 402 | CDL  | CB5-C51-C52-C53 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | T     | 101 | PCF  | C23-C24-C25-C26 |
| 24  | L     | 502 | PEF  | C11-C12-C13-C14 |
| 31  | a     | 602 | HEA  | C19-C20-C21-C22 |
| 27  | C     | 606 | PCF  | C41-C42-C43-C44 |
| 24  | P     | 302 | PEF  | C11-C10-O2-C2   |
| 27  | S     | 103 | PCF  | C22-C21-O21-C2  |
| 26  | D     | 402 | CDL  | C61-C62-C63-C64 |
| 24  | J     | 101 | PEF  | C13-C14-C15-C16 |
| 24  | S     | 102 | PEF  | C40-C41-C42-C43 |
| 24  | c     | 302 | PEF  | C31-C32-C33-C34 |
| 24  | A     | 501 | PEF  | O3P-C1-C2-C3    |
| 24  | e     | 201 | PEF  | O3P-C1-C2-C3    |
| 26  | L     | 501 | CDL  | OA5-CA3-CA4-CA6 |
| 27  | C     | 606 | PCF  | O11-C1-C2-C3    |
| 26  | C     | 603 | CDL  | CB5-C51-C52-C53 |
| 26  | N     | 603 | CDL  | CA5-C11-C12-C13 |
| 25  | C     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 25  | N     | 601 | HEM  | C2C-C3C-CAC-CBC |
| 24  | C     | 605 | PEF  | C3-C2-O2-C10    |
| 24  | e     | 201 | PEF  | C1-C2-O2-C10    |
| 27  | T     | 101 | PCF  | C21-C22-C23-C24 |
| 24  | L     | 502 | PEF  | O5-C30-O3-C3    |
| 26  | D     | 402 | CDL  | O1-C1-CA2-OA2   |
| 24  | c     | 301 | PEF  | O3P-C1-C2-O2    |
| 26  | O     | 402 | CDL  | OA5-CA3-CA4-OA6 |
| 26  | S     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 27  | C     | 606 | PCF  | O11-C1-C2-O21   |
| 25  | N     | 602 | HEM  | C4C-C3C-CAC-CBC |
| 27  | N     | 606 | PCF  | C24-C25-C26-C27 |
| 24  | N     | 605 | PEF  | C17-C18-C19-C20 |
| 24  | U     | 101 | PEF  | O2-C2-C3-O3     |
| 27  | I     | 101 | PCF  | O13-C11-C12-N   |
| 27  | T     | 101 | PCF  | O13-C11-C12-N   |
| 27  | e     | 202 | PCF  | O13-C11-C12-N   |
| 24  | P     | 302 | PEF  | O4-C10-O2-C2    |
| 24  | b     | 303 | PEF  | C11-C10-O2-C2   |
| 27  | C     | 606 | PCF  | C22-C21-O21-C2  |
| 24  | N     | 604 | PEF  | O3P-C1-C2-C3    |
| 26  | C     | 603 | CDL  | OA5-CA3-CA4-CA6 |
| 24  | b     | 303 | PEF  | O4-C10-O2-C2    |
| 27  | S     | 103 | PCF  | O22-C21-O21-C2  |
| 24  | P     | 302 | PEF  | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | A     | 501 | PEF  | O3P-C1-C2-O2    |
| 24  | b     | 302 | PEF  | O3P-C1-C2-O2    |
| 26  | C     | 603 | CDL  | OA5-CA3-CA4-OA6 |
| 26  | L     | 501 | CDL  | OA5-CA3-CA4-OA6 |
| 24  | C     | 604 | PEF  | O2-C2-C3-O3     |
| 24  | C     | 605 | PEF  | O2-C2-C3-O3     |
| 24  | S     | 102 | PEF  | C1-C2-C3-O3     |
| 26  | S     | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 24  | E     | 302 | PEF  | C30-C31-C32-C33 |
| 27  | T     | 101 | PCF  | C25-C26-C27-C28 |
| 24  | C     | 604 | PEF  | C4-O4P-P-O1P    |
| 24  | C     | 605 | PEF  | C4-O4P-P-O1P    |
| 24  | C     | 605 | PEF  | C4-O4P-P-O3P    |
| 24  | E     | 302 | PEF  | C1-O3P-P-O1P    |
| 24  | E     | 302 | PEF  | C4-O4P-P-O1P    |
| 24  | E     | 302 | PEF  | C4-O4P-P-O3P    |
| 24  | H     | 602 | PEF  | C1-O3P-P-O1P    |
| 24  | H     | 602 | PEF  | C4-O4P-P-O1P    |
| 24  | J     | 101 | PEF  | C1-O3P-P-O1P    |
| 24  | J     | 101 | PEF  | C1-O3P-P-O2P    |
| 24  | J     | 101 | PEF  | C1-O3P-P-O4P    |
| 24  | N     | 605 | PEF  | C1-O3P-P-O1P    |
| 24  | P     | 302 | PEF  | C1-O3P-P-O1P    |
| 24  | U     | 101 | PEF  | C1-O3P-P-O1P    |
| 24  | b     | 302 | PEF  | C4-O4P-P-O1P    |
| 24  | c     | 302 | PEF  | C1-O3P-P-O1P    |
| 24  | c     | 302 | PEF  | C4-O4P-P-O1P    |
| 24  | e     | 201 | PEF  | C4-O4P-P-O1P    |
| 26  | D     | 402 | CDL  | CA3-OA5-PA1-OA4 |
| 26  | H     | 601 | CDL  | CA2-OA2-PA1-OA3 |
| 26  | H     | 601 | CDL  | CB2-OB2-PB2-OB3 |
| 26  | H     | 601 | CDL  | CB3-OB5-PB2-OB3 |
| 26  | L     | 501 | CDL  | CA3-OA5-PA1-OA4 |
| 26  | L     | 501 | CDL  | CB3-OB5-PB2-OB3 |
| 26  | N     | 603 | CDL  | CA3-OA5-PA1-OA2 |
| 26  | O     | 402 | CDL  | CA2-OA2-PA1-OA4 |
| 26  | O     | 402 | CDL  | CA3-OA5-PA1-OA3 |
| 24  | U     | 101 | PEF  | C39-C40-C41-C42 |
| 31  | a     | 603 | HEA  | C2C-C3C-CAC-CBC |
| 24  | L     | 502 | PEF  | C17-C18-C19-C20 |
| 24  | L     | 502 | PEF  | O2-C10-C11-C12  |
| 26  | C     | 603 | CDL  | C1-CB2-OB2-PB2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 303 | PEF  | C31-C32-C33-C34 |
| 26  | H     | 601 | CDL  | O1-C1-CA2-OA2   |
| 24  | N     | 605 | PEF  | C3-C2-O2-C10    |
| 24  | c     | 301 | PEF  | O3P-C1-C2-C3    |
| 26  | O     | 402 | CDL  | OA5-CA3-CA4-CA6 |
| 26  | S     | 101 | CDL  | OB5-CB3-CB4-CB6 |
| 24  | N     | 604 | PEF  | O3P-C1-C2-O2    |
| 26  | O     | 402 | CDL  | C32-C33-C34-C35 |
| 27  | C     | 606 | PCF  | O22-C21-O21-C2  |
| 24  | J     | 101 | PEF  | C31-C30-O3-C3   |
| 24  | C     | 604 | PEF  | O3P-C1-C2-O2    |
| 24  | P     | 302 | PEF  | O3P-C1-C2-O2    |
| 27  | C     | 606 | PCF  | C40-C41-C42-C43 |
| 24  | J     | 101 | PEF  | O5-C30-O3-C3    |
| 25  | N     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 26  | O     | 402 | CDL  | C31-C32-C33-C34 |
| 25  | N     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 24  | b     | 302 | PEF  | C32-C33-C34-C35 |
| 28  | O     | 401 | HEC  | C3D-CAD-CBD-CGD |
| 31  | a     | 602 | HEA  | C2A-CAA-CBA-CGA |
| 24  | b     | 302 | PEF  | C11-C12-C13-C14 |
| 26  | D     | 402 | CDL  | CA6-CA4-OA6-CA5 |
| 25  | N     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 31  | a     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 31  | a     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 25  | C     | 601 | HEM  | CAA-CBA-CGA-O2A |
| 31  | a     | 602 | HEA  | C2C-C3C-CAC-CBC |
| 26  | C     | 603 | CDL  | C11-CA5-OA6-CA4 |
| 25  | C     | 601 | HEM  | CAA-CBA-CGA-O1A |
| 24  | P     | 302 | PEF  | C34-C35-C36-C37 |
| 26  | S     | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 26  | C     | 603 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | N     | 601 | HEM  | CAA-CBA-CGA-O1A |
| 25  | C     | 601 | HEM  | CAD-CBD-CGD-O2D |
| 25  | N     | 601 | HEM  | CAA-CBA-CGA-O2A |
| 26  | N     | 603 | CDL  | C31-C32-C33-C34 |
| 24  | b     | 302 | PEF  | O4-C10-C11-C12  |
| 24  | S     | 102 | PEF  | O3P-C1-C2-O2    |
| 25  | C     | 602 | HEM  | CAD-CBD-CGD-O1D |
| 27  | T     | 101 | PCF  | C34-C35-C36-C37 |
| 25  | C     | 601 | HEM  | CAD-CBD-CGD-O1D |
| 24  | P     | 302 | PEF  | O3P-C1-C2-C3    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 24  | b     | 303 | PEF  | O3P-C1-C2-C3    |
| 26  | H     | 601 | CDL  | OB5-CB3-CB4-CB6 |
| 24  | c     | 302 | PEF  | C35-C36-C37-C38 |
| 26  | S     | 101 | CDL  | C1-CB2-OB2-PB2  |
| 24  | U     | 101 | PEF  | C33-C34-C35-C36 |
| 28  | O     | 401 | HEC  | CAD-CBD-CGD-O2D |
| 27  | S     | 103 | PCF  | C33-C34-C35-C36 |
| 24  | c     | 302 | PEF  | C15-C16-C17-C18 |
| 25  | N     | 602 | HEM  | CAA-CBA-CGA-O2A |
| 24  | H     | 602 | PEF  | C11-C12-C13-C14 |
| 24  | L     | 502 | PEF  | C12-C13-C14-C15 |
| 31  | a     | 603 | HEA  | CAD-CBD-CGD-O1D |
| 24  | E     | 302 | PEF  | C32-C33-C34-C35 |
| 26  | N     | 603 | CDL  | C32-C33-C34-C35 |
| 26  | H     | 601 | CDL  | CB4-CB3-OB5-PB2 |
| 27  | N     | 606 | PCF  | C2-C1-O11-P     |
| 31  | a     | 603 | HEA  | CAD-CBD-CGD-O2D |
| 25  | C     | 601 | HEM  | C4C-C3C-CAC-CBC |
| 28  | O     | 401 | HEC  | CAD-CBD-CGD-O1D |
| 25  | N     | 602 | HEM  | CAD-CBD-CGD-O1D |
| 31  | a     | 603 | HEA  | CAA-CBA-CGA-O1A |
| 24  | J     | 101 | PEF  | C14-C15-C16-C17 |
| 24  | N     | 604 | PEF  | C32-C33-C34-C35 |
| 25  | N     | 602 | HEM  | CAA-CBA-CGA-O1A |
| 27  | I     | 101 | PCF  | C24-C25-C26-C27 |
| 27  | I     | 101 | PCF  | O31-C31-C32-C33 |
| 24  | H     | 602 | PEF  | C33-C34-C35-C36 |
| 24  | e     | 201 | PEF  | O2-C10-C11-C12  |
| 27  | C     | 606 | PCF  | O31-C31-C32-C33 |
| 24  | S     | 102 | PEF  | O3P-C1-C2-C3    |
| 26  | H     | 601 | CDL  | C72-C71-CB7-OB8 |
| 25  | C     | 602 | HEM  | CAD-CBD-CGD-O2D |
| 24  | b     | 302 | PEF  | O3-C30-C31-C32  |
| 27  | C     | 606 | PCF  | C11-C12-N-C14   |
| 26  | C     | 603 | CDL  | C11-C12-C13-C14 |
| 24  | b     | 303 | PEF  | O3-C30-C31-C32  |
| 31  | a     | 602 | HEA  | C15-C16-C17-C18 |
| 25  | C     | 602 | HEM  | CAA-CBA-CGA-O2A |
| 26  | D     | 402 | CDL  | C71-CB7-OB8-CB6 |
| 24  | L     | 502 | PEF  | O3-C30-C31-C32  |
| 24  | P     | 302 | PEF  | O3-C30-C31-C32  |
| 24  | L     | 502 | PEF  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 26  | S     | 101 | CDL  | C72-C71-CB7-OB8 |
| 25  | N     | 602 | HEM  | CAD-CBD-CGD-O2D |
| 26  | D     | 402 | CDL  | C52-C53-C54-C55 |
| 31  | a     | 603 | HEA  | CAA-CBA-CGA-O2A |
| 24  | P     | 302 | PEF  | C38-C39-C40-C41 |
| 26  | O     | 402 | CDL  | C72-C71-CB7-OB8 |
| 24  | J     | 101 | PEF  | C11-C12-C13-C14 |
| 24  | e     | 201 | PEF  | O4-C10-C11-C12  |
| 26  | H     | 601 | CDL  | C72-C71-CB7-OB9 |
| 26  | H     | 601 | CDL  | CA7-C31-C32-C33 |
| 24  | S     | 102 | PEF  | C35-C36-C37-C38 |
| 27  | C     | 606 | PCF  | O32-C31-C32-C33 |
| 24  | S     | 102 | PEF  | O2-C10-C11-C12  |
| 24  | P     | 302 | PEF  | O5-C30-C31-C32  |
| 27  | I     | 101 | PCF  | O32-C31-C32-C33 |
| 24  | b     | 302 | PEF  | O5-C30-C31-C32  |
| 26  | S     | 101 | CDL  | C72-C71-CB7-OB9 |
| 24  | b     | 303 | PEF  | O5-C30-C31-C32  |
| 24  | c     | 301 | PEF  | O2-C10-C11-C12  |
| 27  | C     | 606 | PCF  | C11-C12-N-C13   |
| 27  | C     | 606 | PCF  | C11-C12-N-C15   |
| 27  | e     | 202 | PCF  | C23-C24-C25-C26 |
| 26  | D     | 402 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | C     | 602 | HEM  | CAA-CBA-CGA-O1A |
| 27  | e     | 202 | PCF  | C22-C21-O21-C2  |
| 26  | C     | 603 | CDL  | C52-C51-CB5-OB6 |

There are no ring outliers.

32 monomers are involved in 59 short contacts:

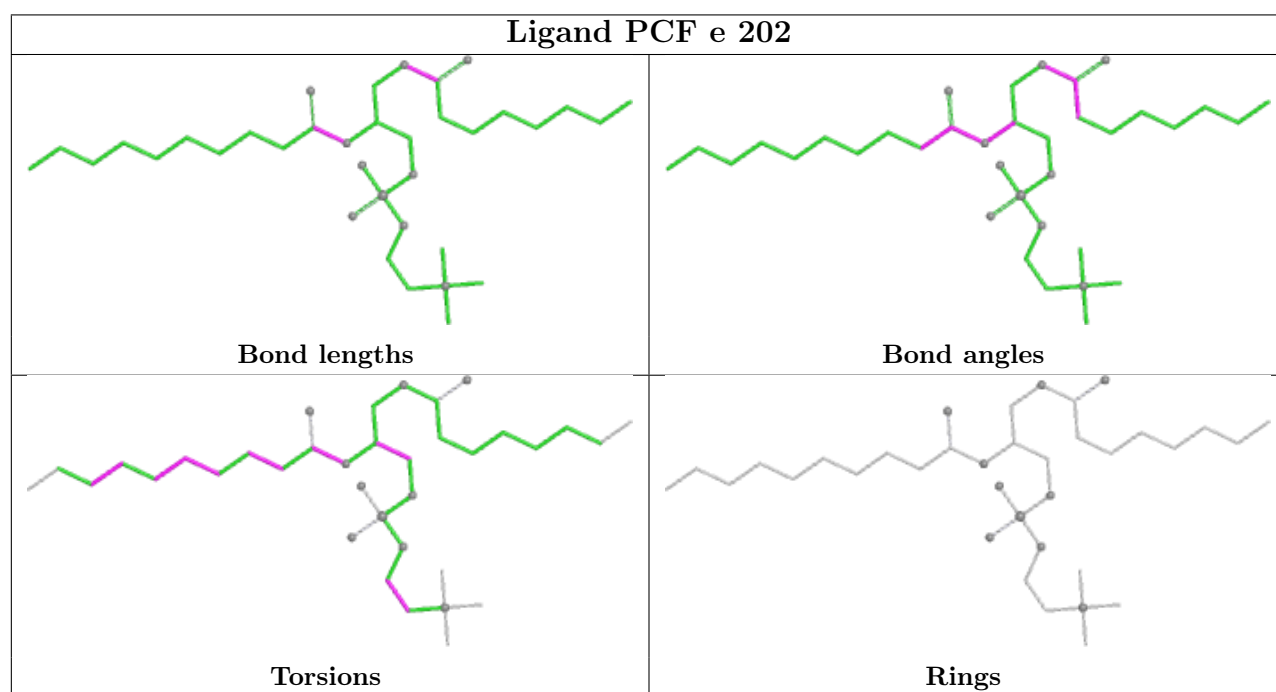
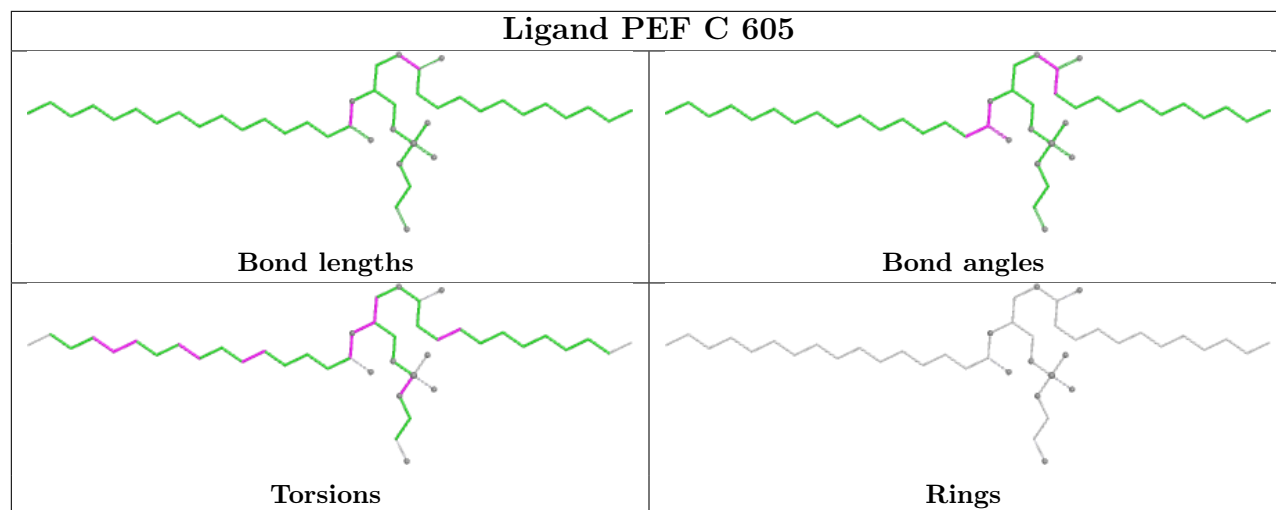
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 24  | C     | 605 | PEF  | 1       | 0            |
| 27  | e     | 202 | PCF  | 3       | 0            |
| 24  | L     | 502 | PEF  | 1       | 0            |
| 28  | O     | 401 | HEC  | 3       | 0            |
| 24  | c     | 302 | PEF  | 1       | 0            |
| 25  | N     | 601 | HEM  | 3       | 0            |
| 26  | D     | 402 | CDL  | 1       | 0            |
| 24  | c     | 301 | PEF  | 1       | 0            |
| 24  | N     | 604 | PEF  | 2       | 0            |
| 24  | a     | 605 | PEF  | 1       | 0            |
| 24  | C     | 604 | PEF  | 2       | 0            |

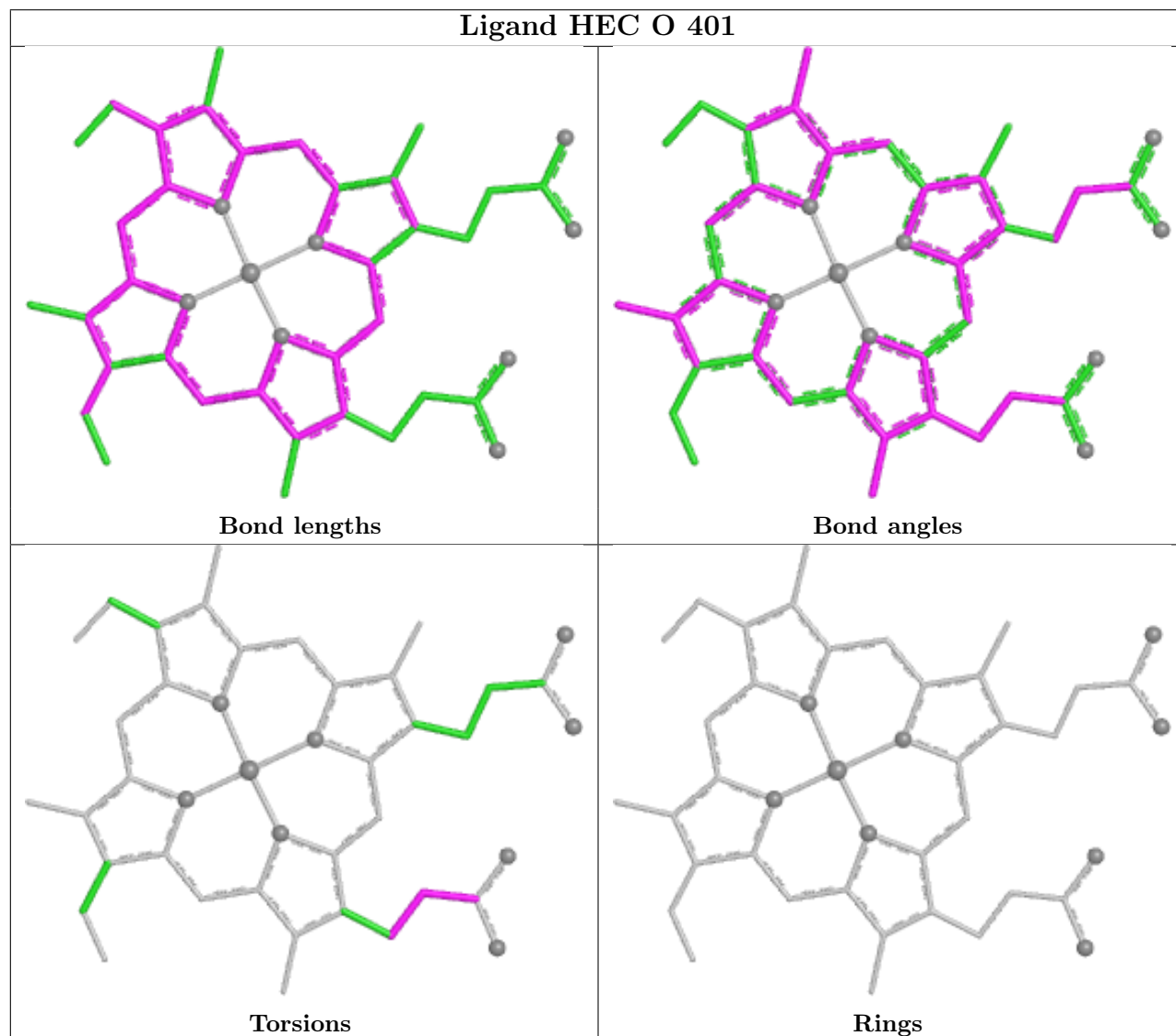
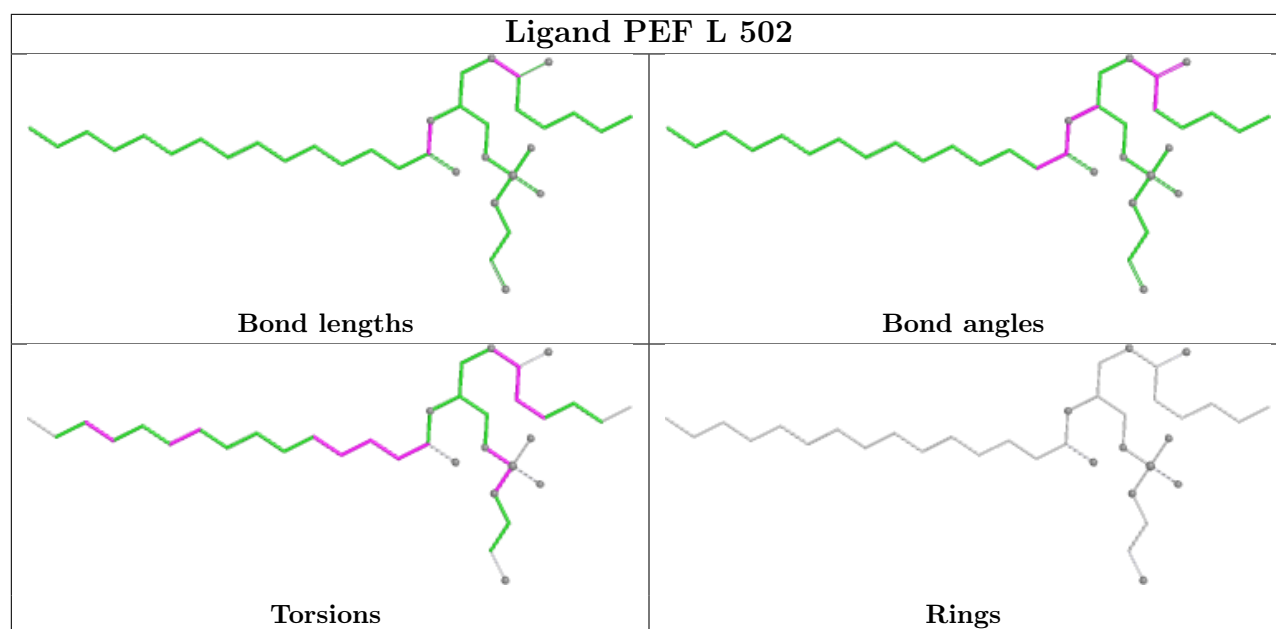
*Continued on next page...*

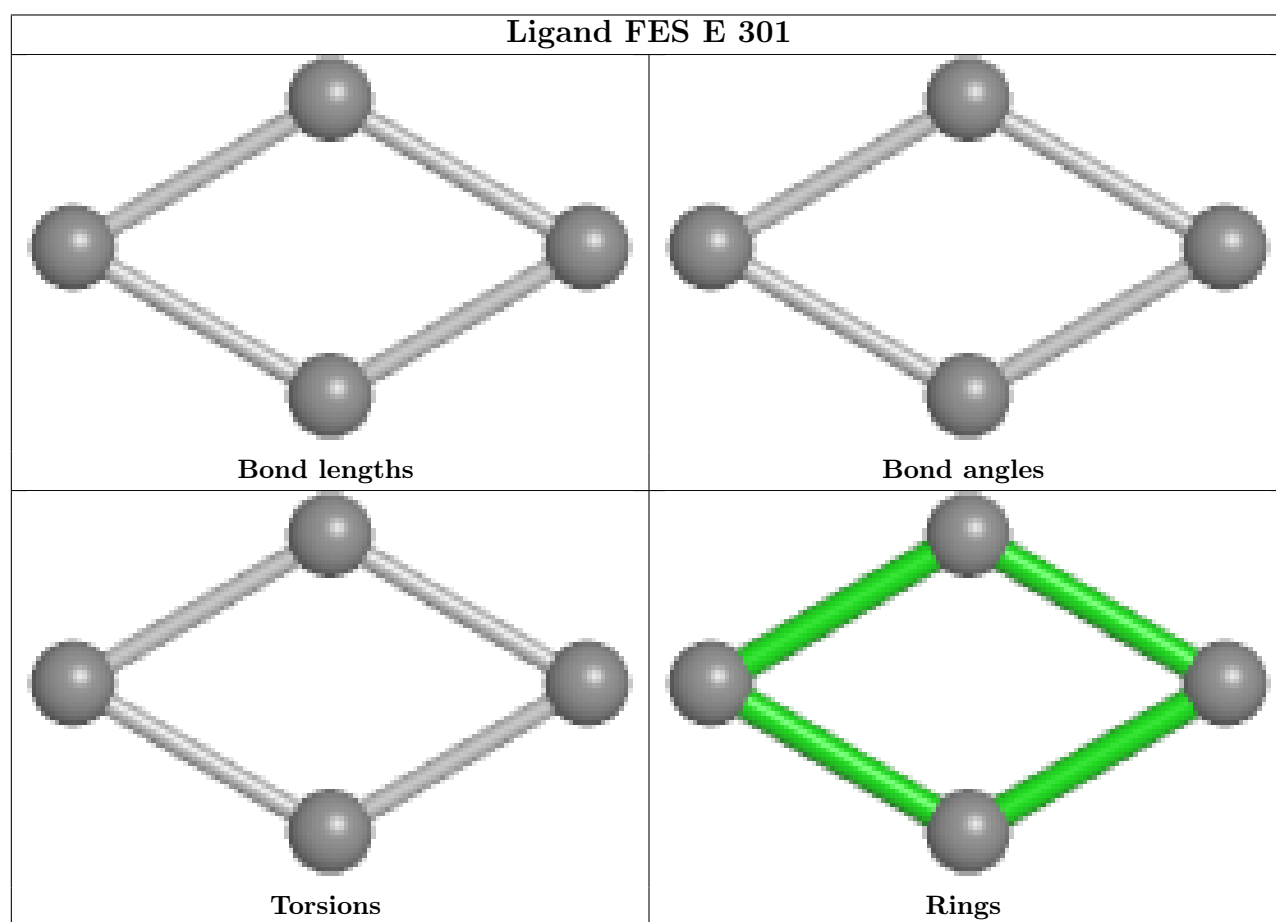
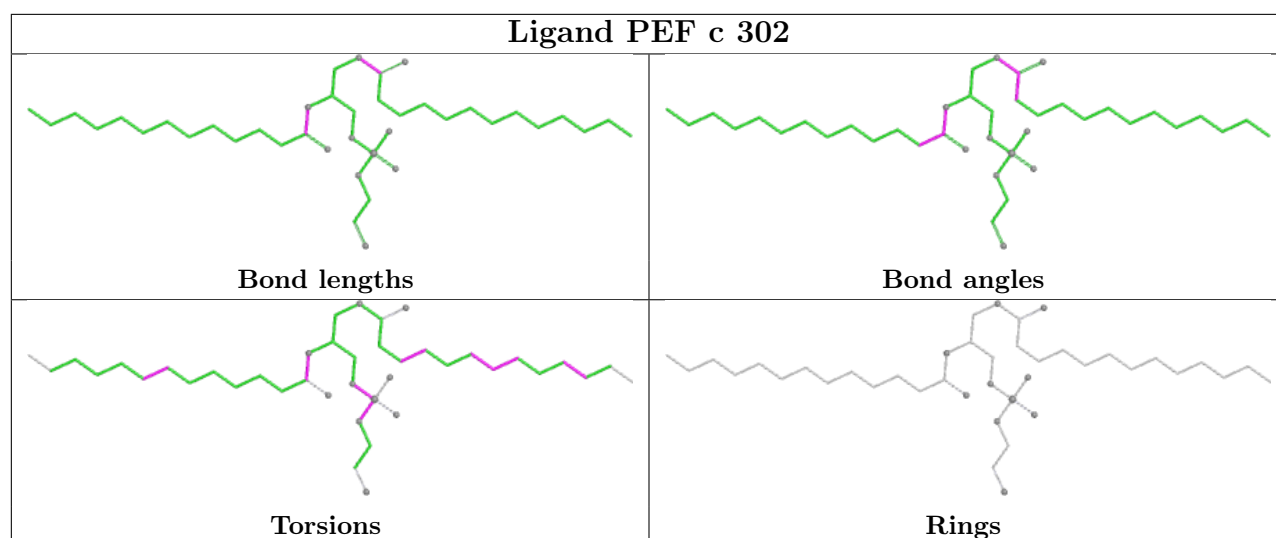
*Continued from previous page...*

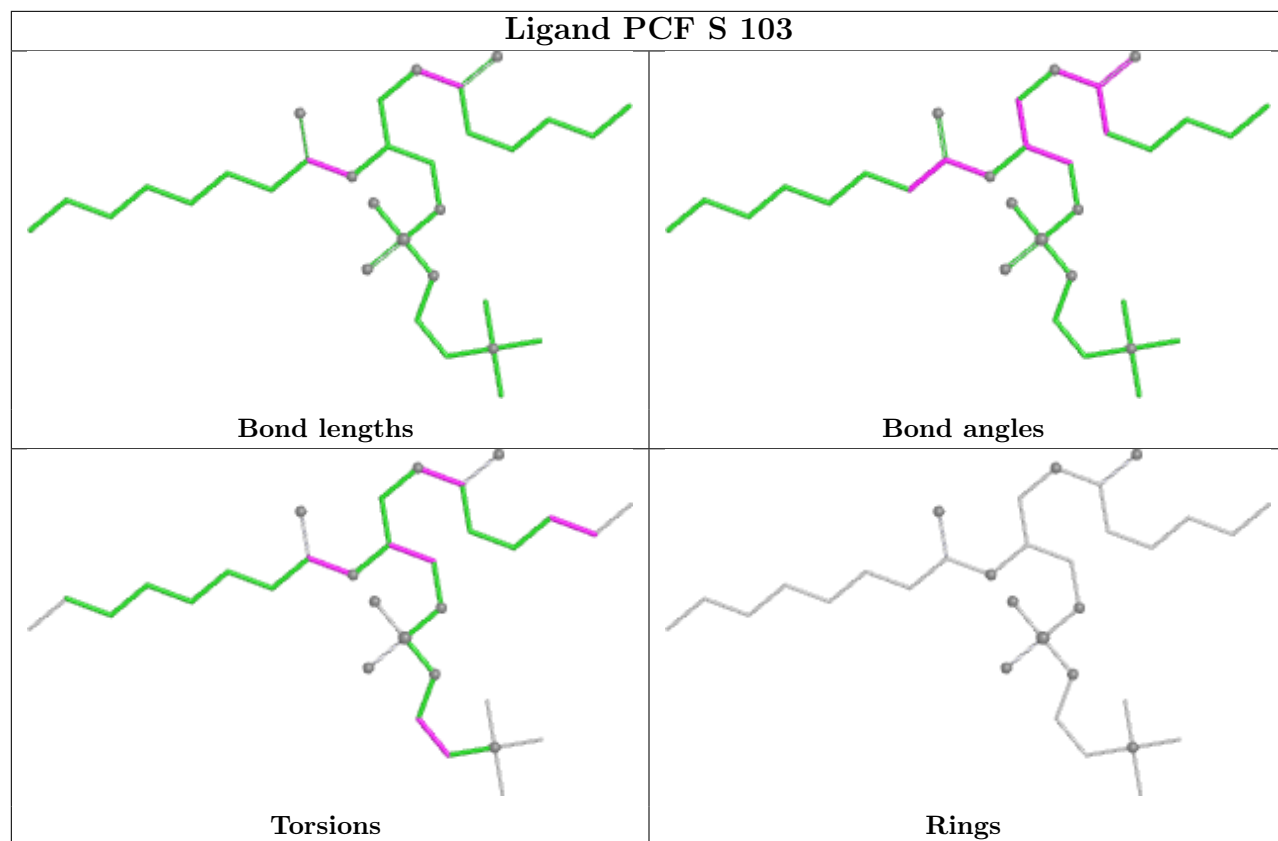
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | a     | 603 | HEA  | 8       | 0            |
| 28  | D     | 401 | HEC  | 1       | 0            |
| 31  | a     | 602 | HEA  | 1       | 0            |
| 24  | e     | 201 | PEF  | 1       | 0            |
| 25  | C     | 602 | HEM  | 1       | 0            |
| 24  | b     | 302 | PEF  | 1       | 0            |
| 24  | S     | 102 | PEF  | 1       | 0            |
| 26  | N     | 603 | CDL  | 4       | 0            |
| 26  | O     | 402 | CDL  | 2       | 0            |
| 26  | H     | 601 | CDL  | 3       | 0            |
| 24  | N     | 605 | PEF  | 1       | 0            |
| 25  | N     | 602 | HEM  | 2       | 0            |
| 26  | S     | 101 | CDL  | 2       | 0            |
| 27  | N     | 606 | PCF  | 3       | 0            |
| 24  | E     | 302 | PEF  | 2       | 0            |
| 29  | P     | 301 | FES  | 1       | 0            |
| 24  | A     | 501 | PEF  | 2       | 0            |
| 27  | T     | 101 | PCF  | 1       | 0            |
| 24  | P     | 302 | PEF  | 1       | 0            |
| 25  | C     | 601 | HEM  | 2       | 0            |
| 26  | L     | 501 | CDL  | 2       | 0            |

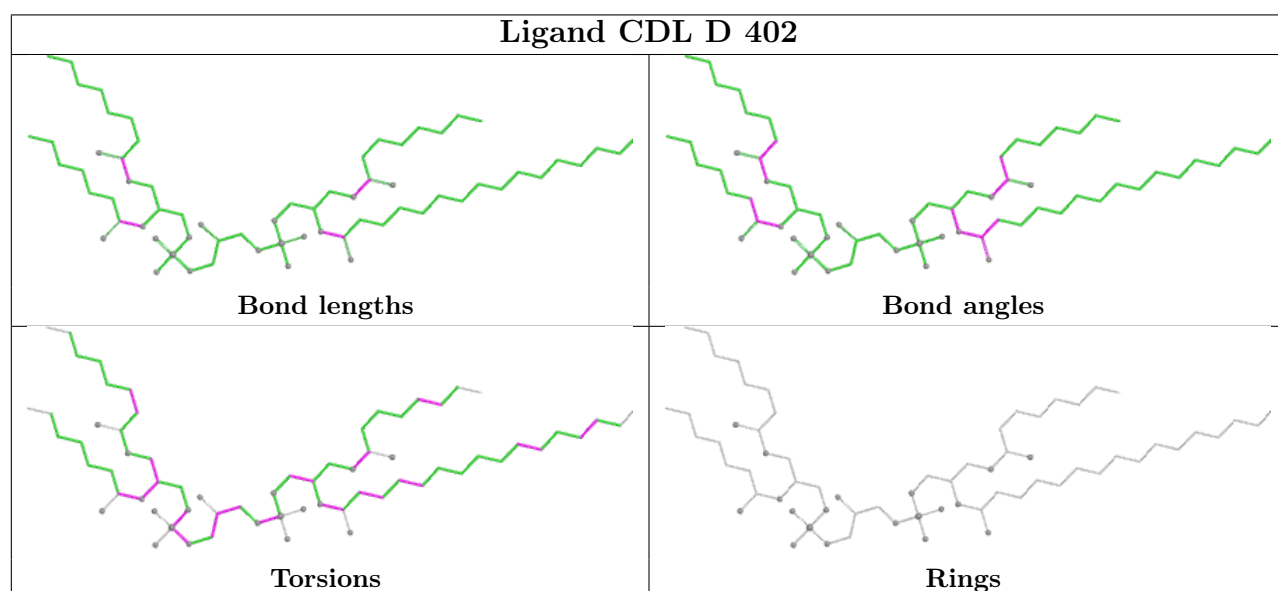
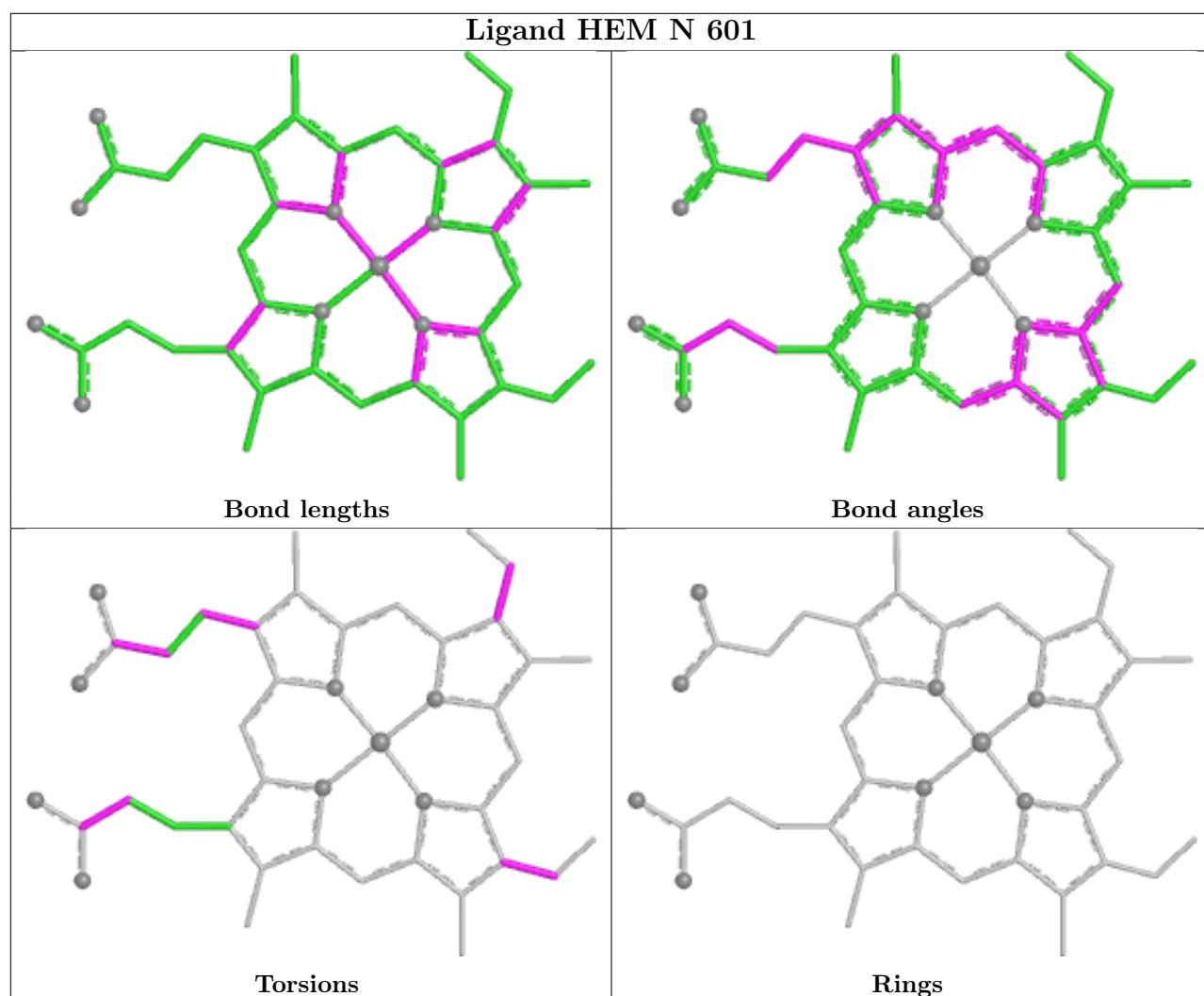
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

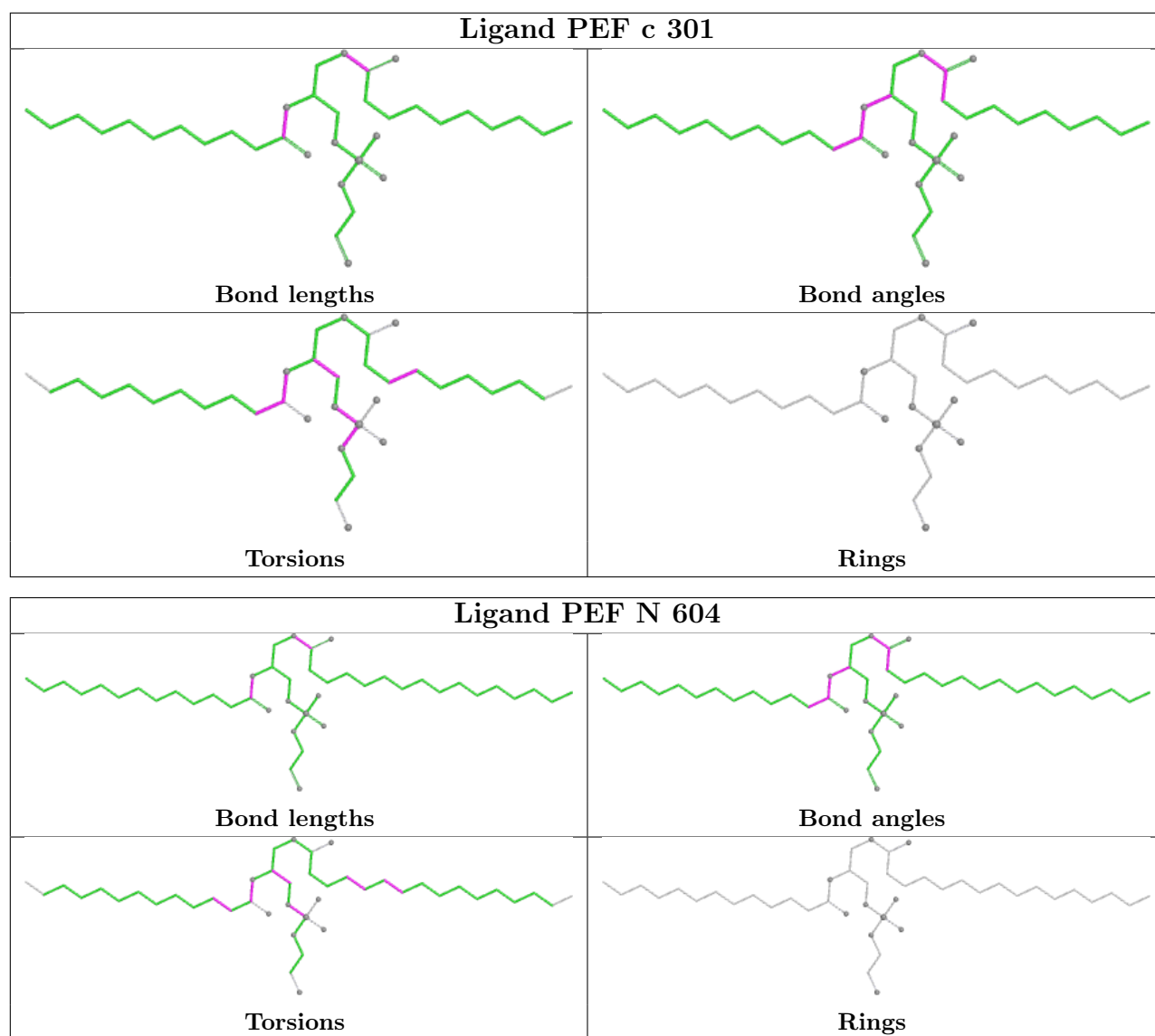


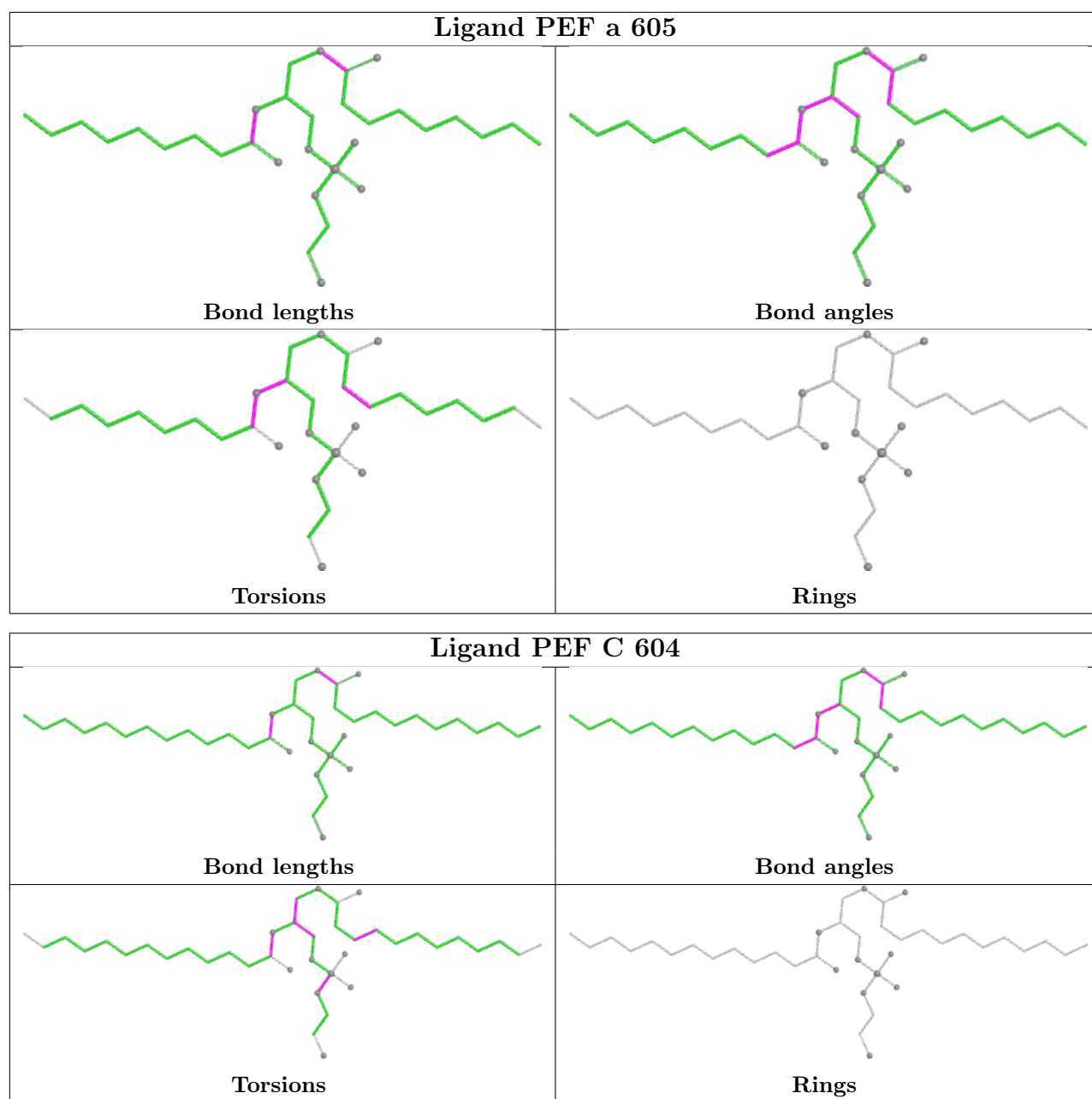


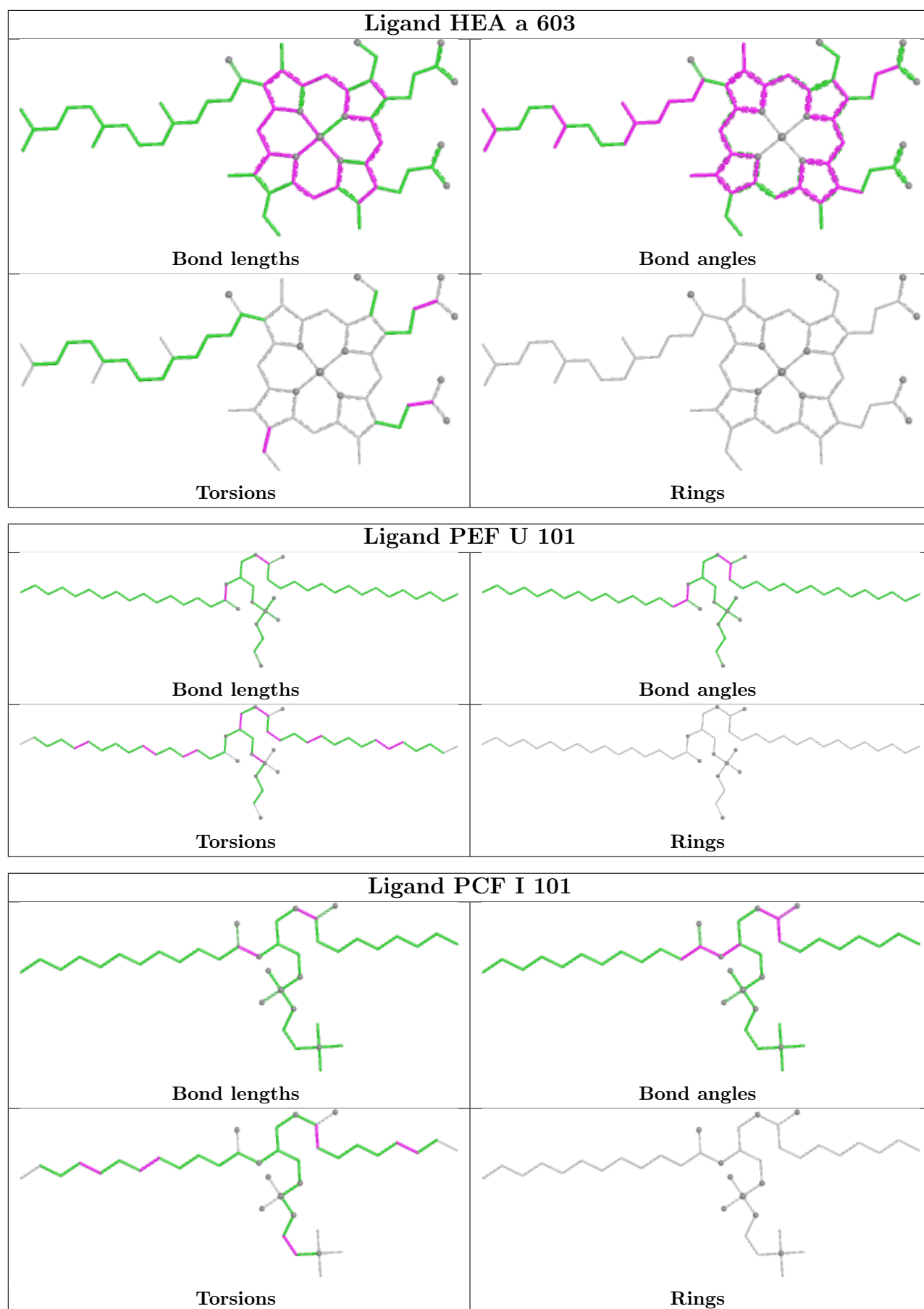


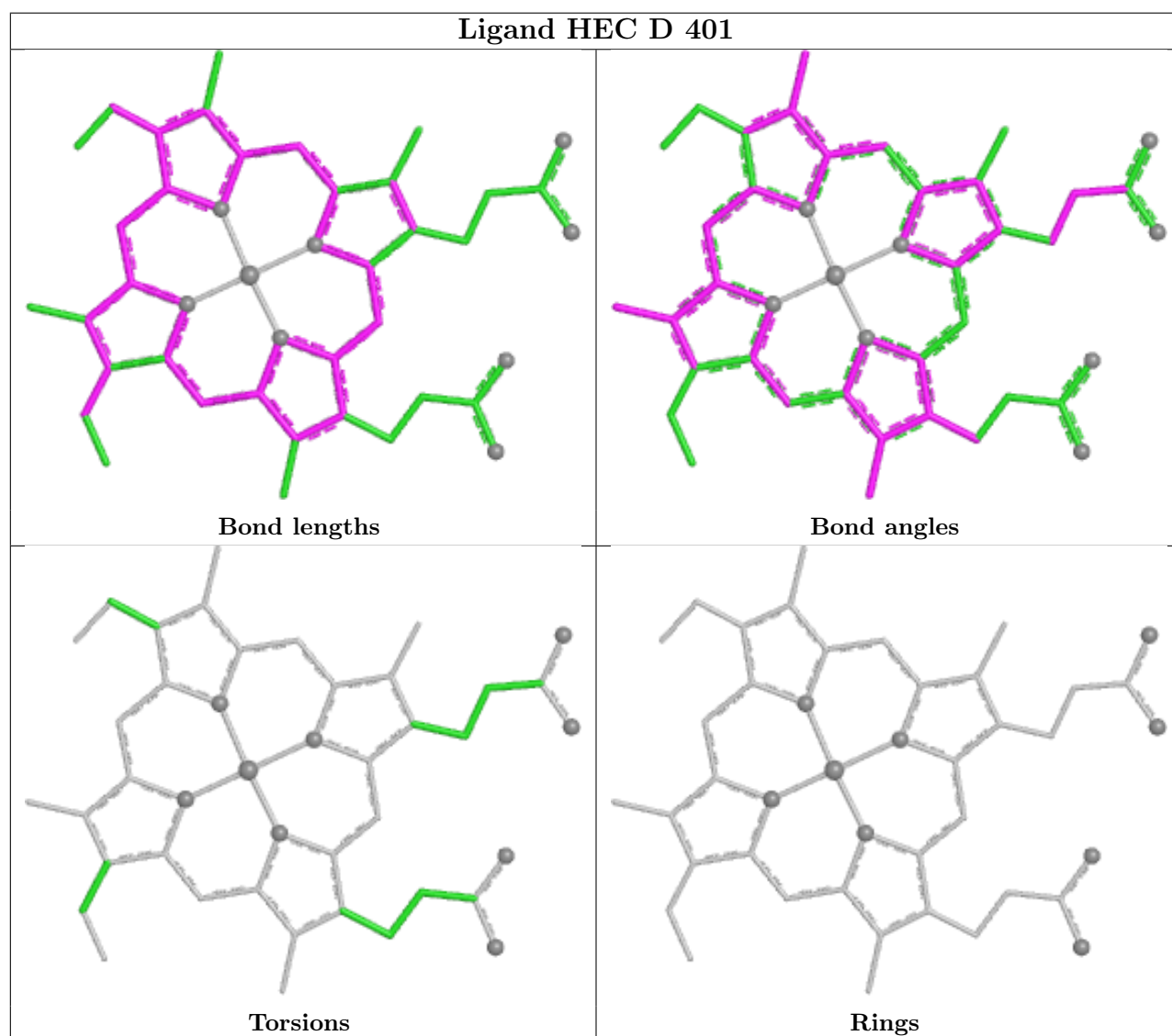
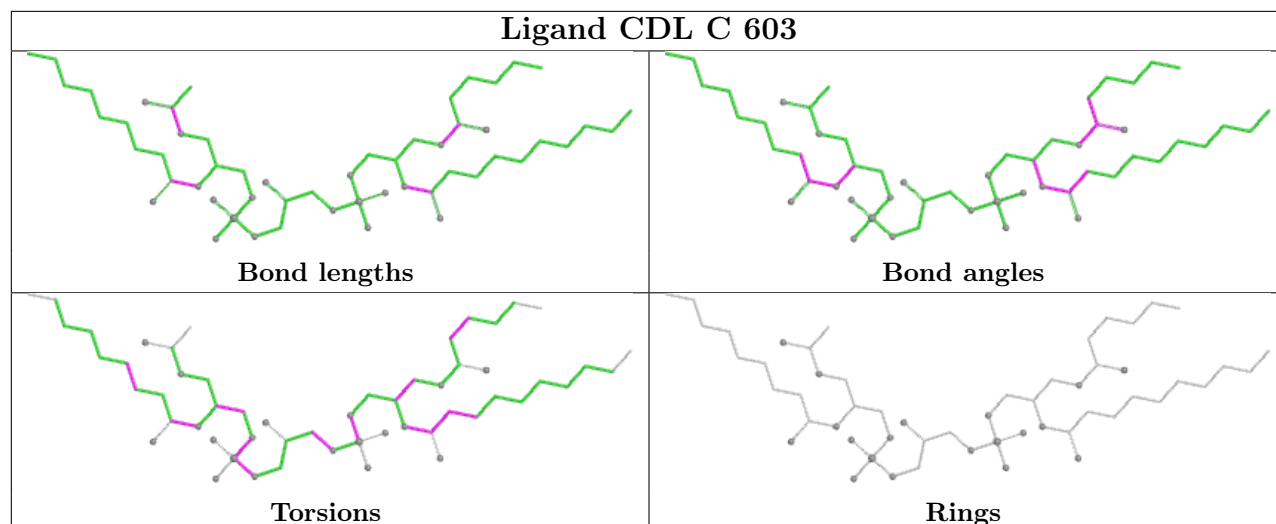


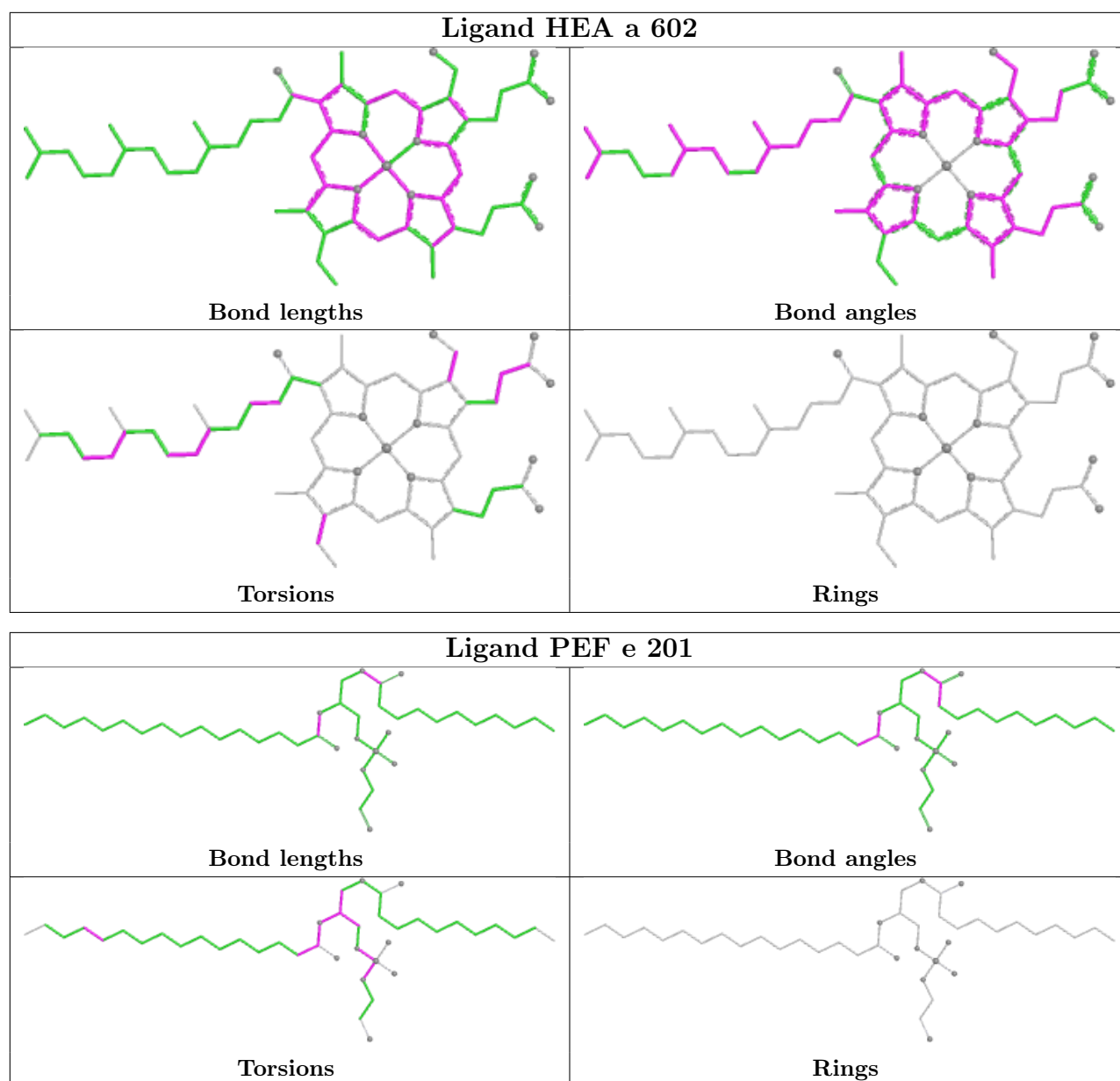


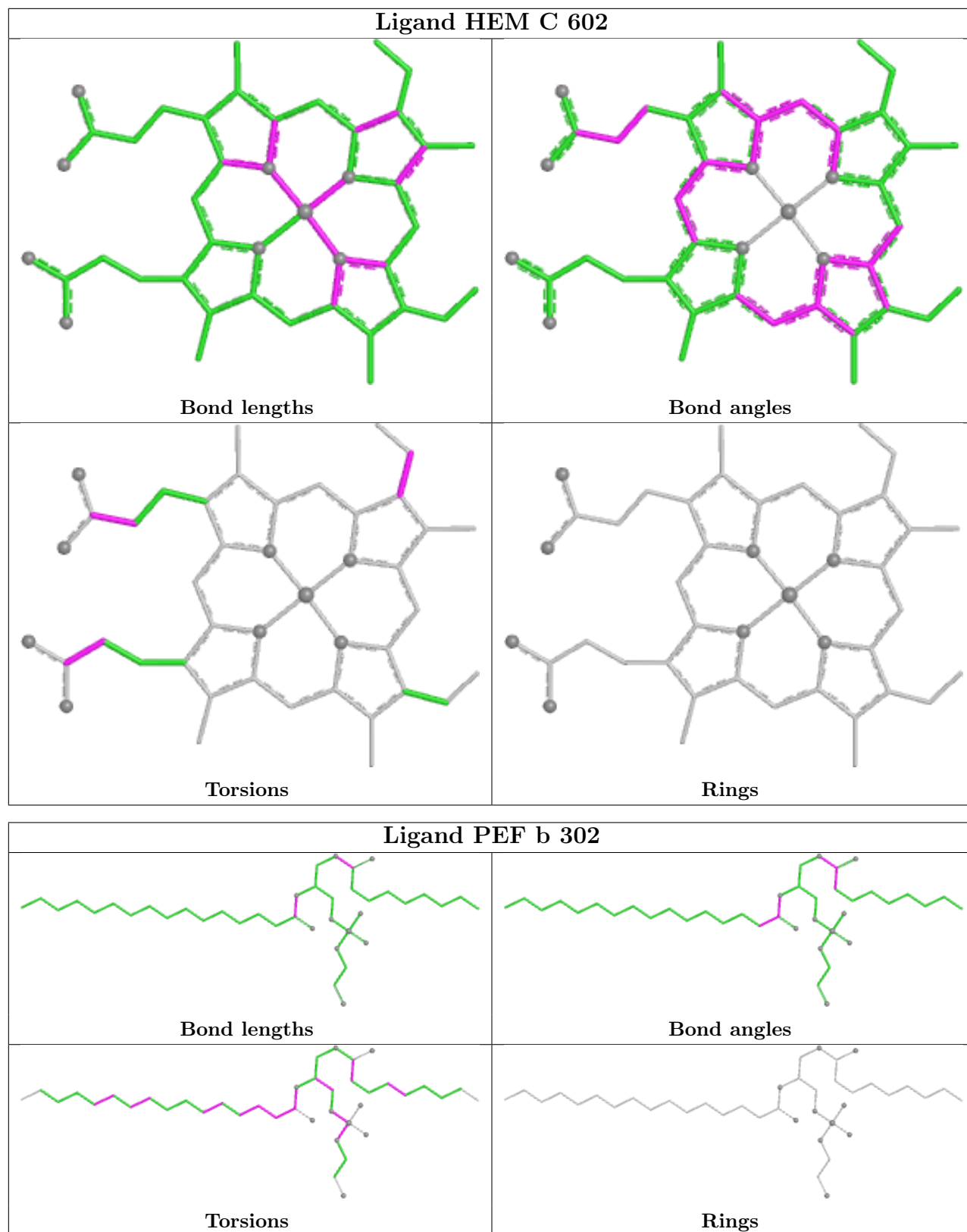


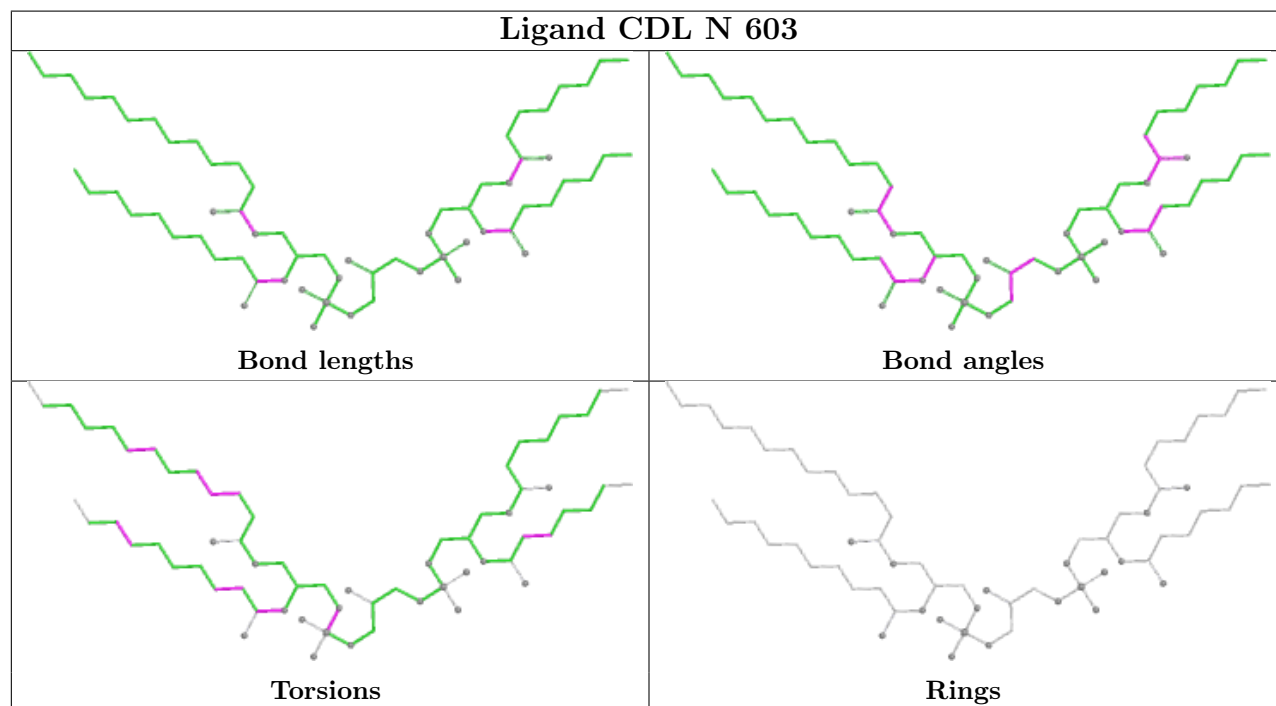
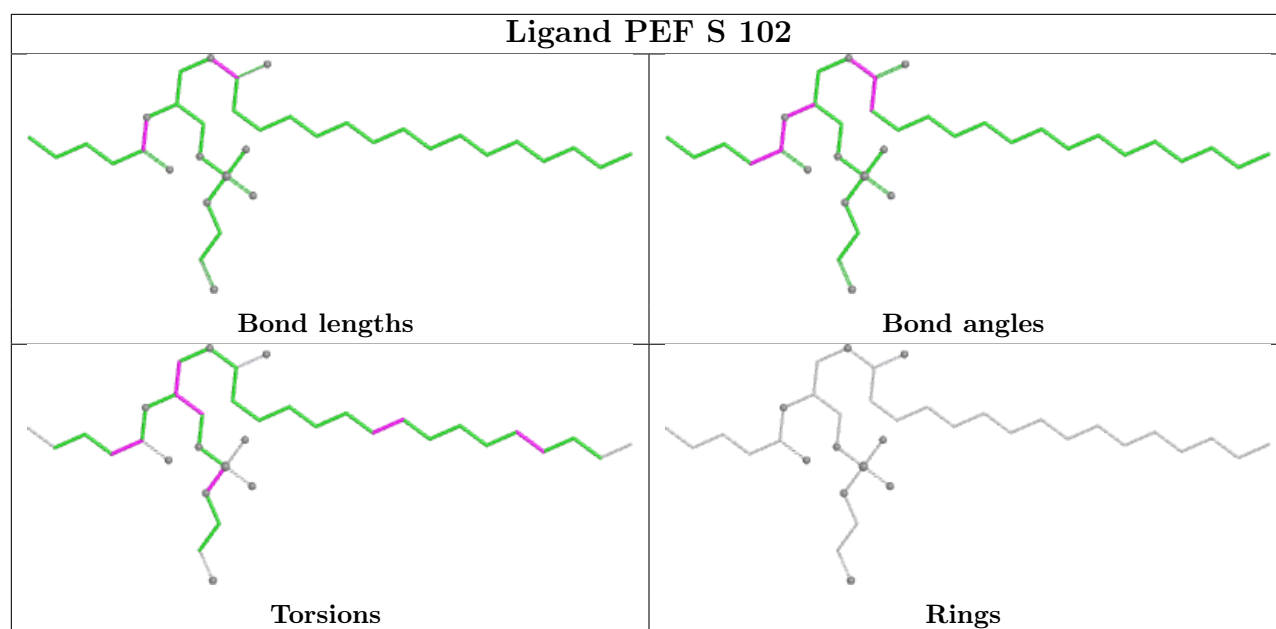


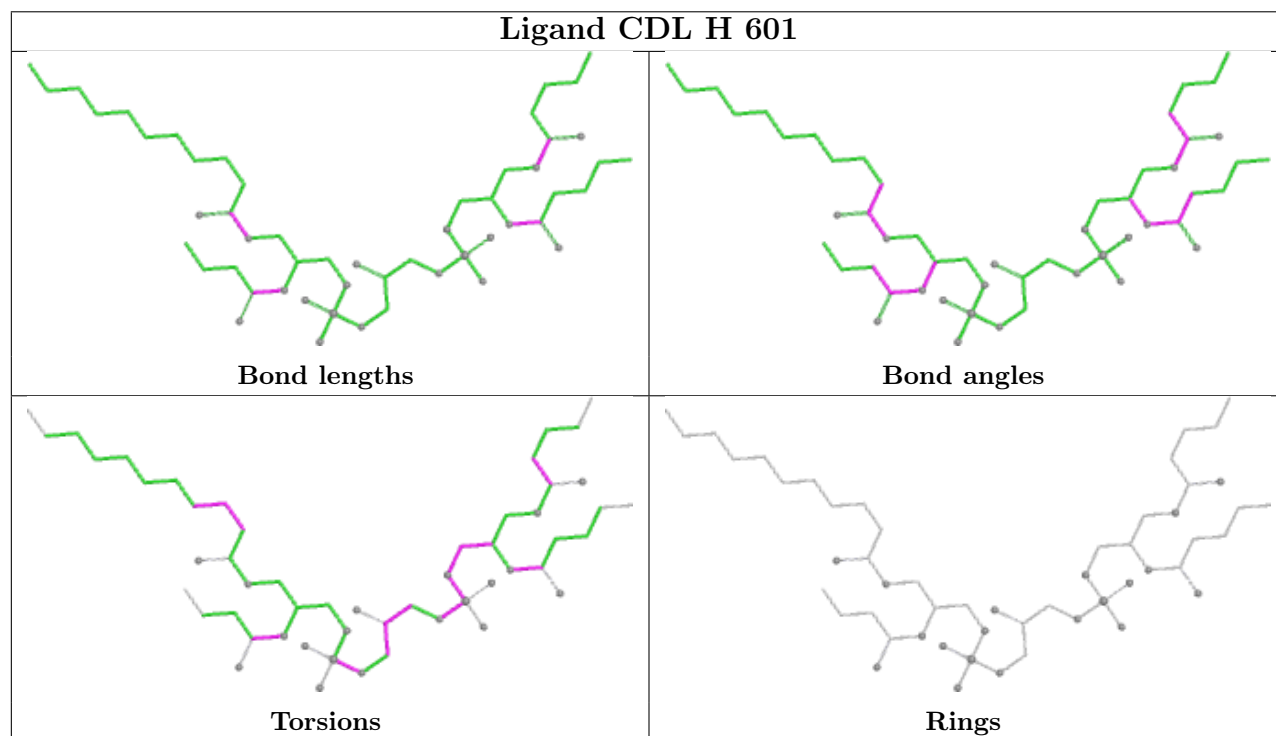
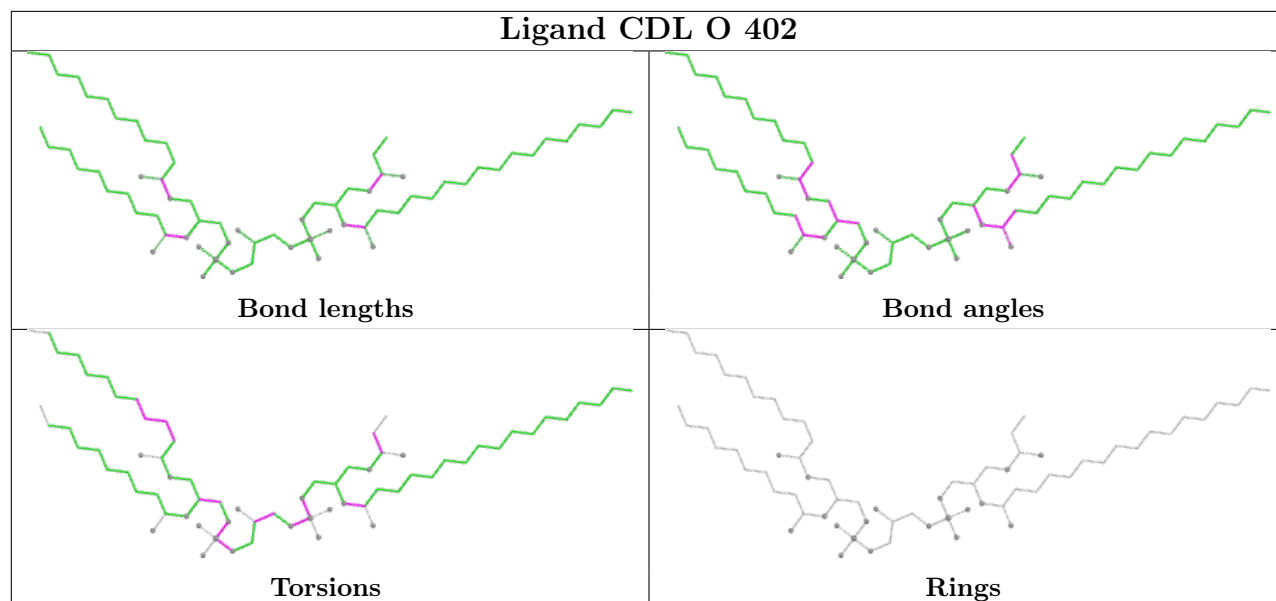


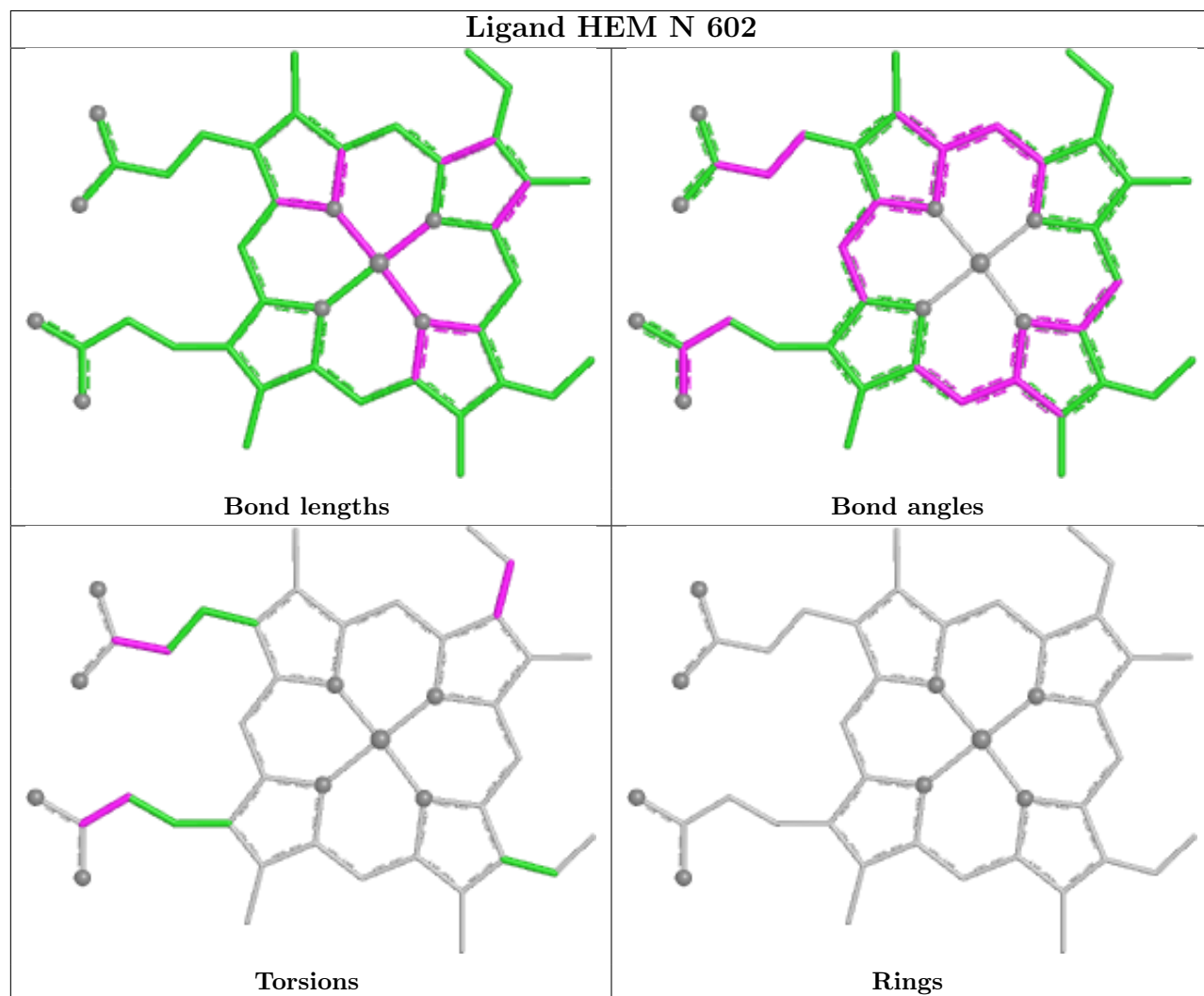
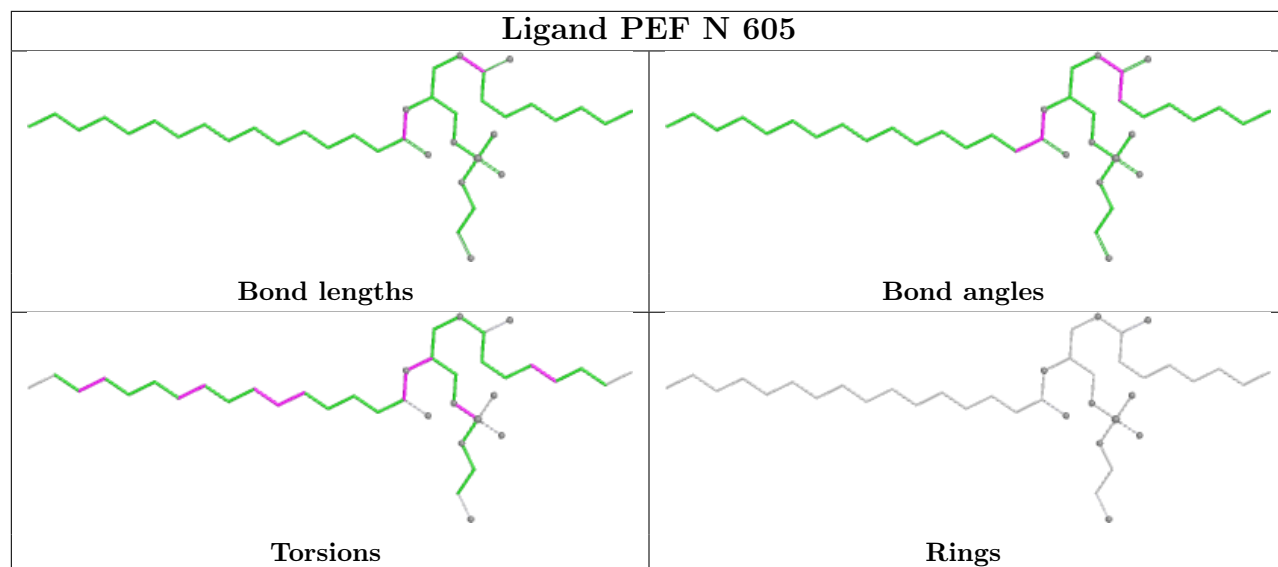


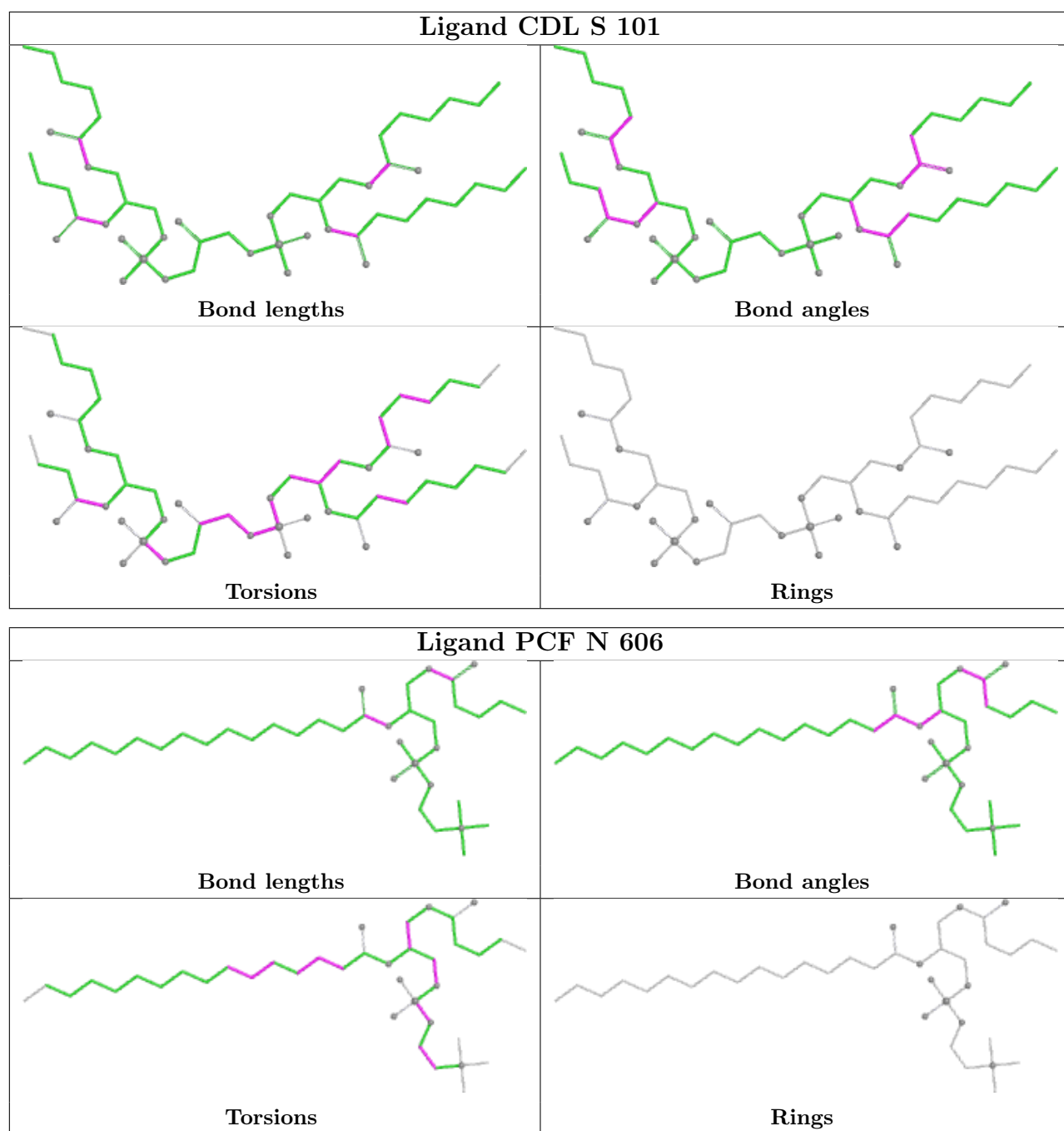


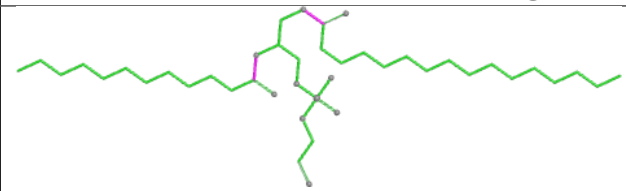
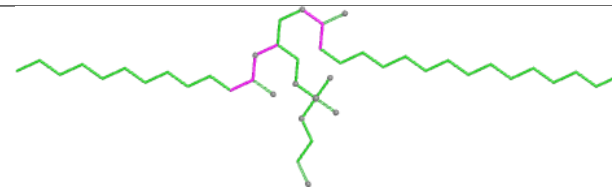
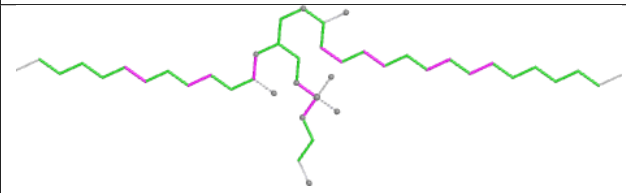
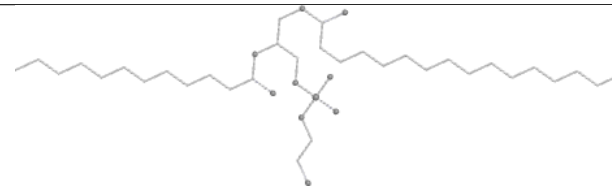


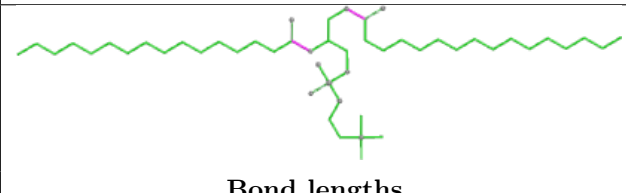
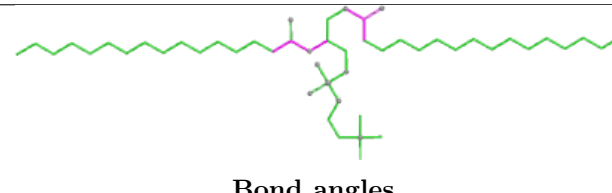
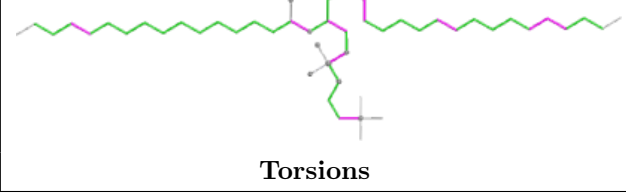
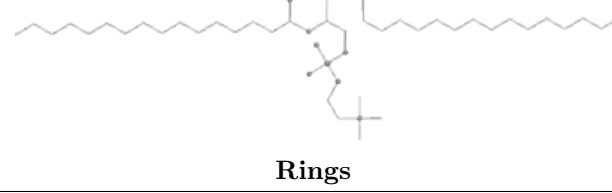


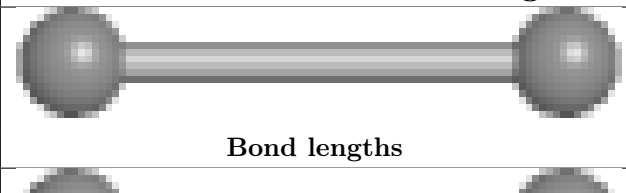
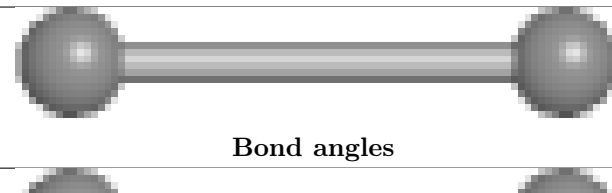


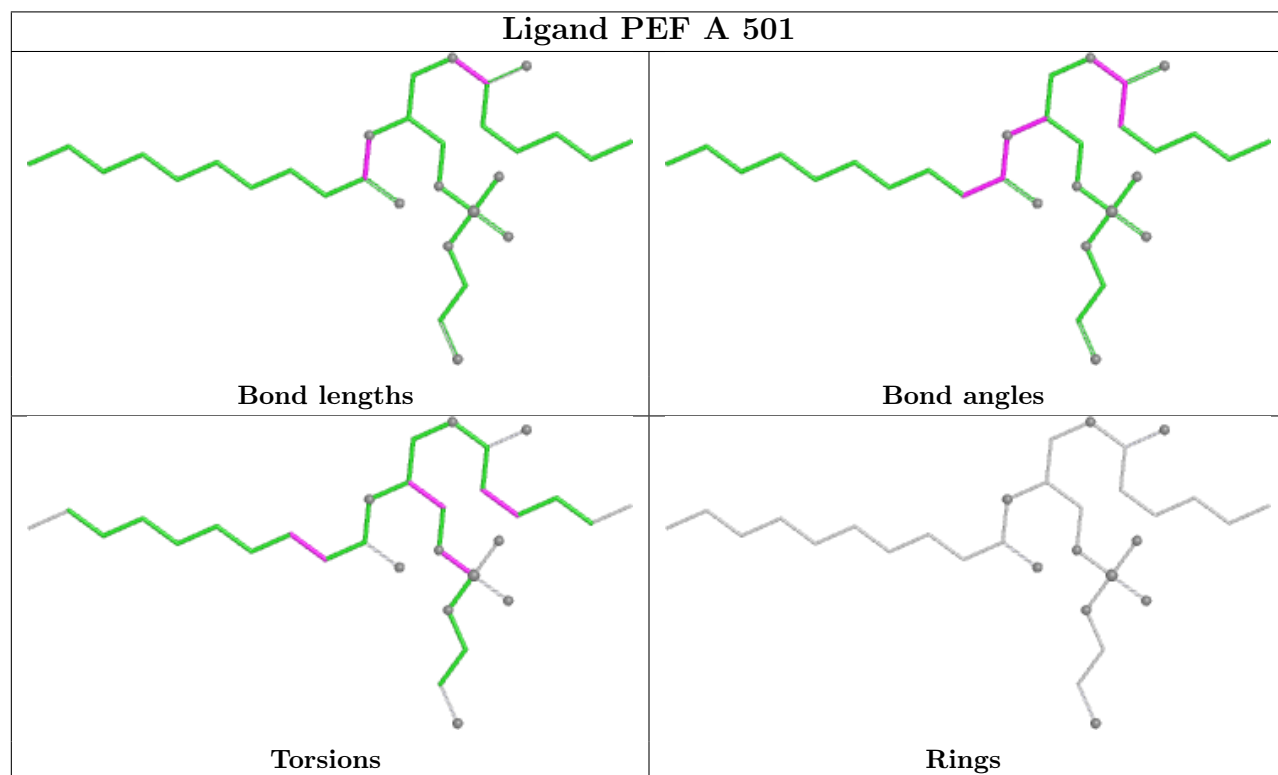
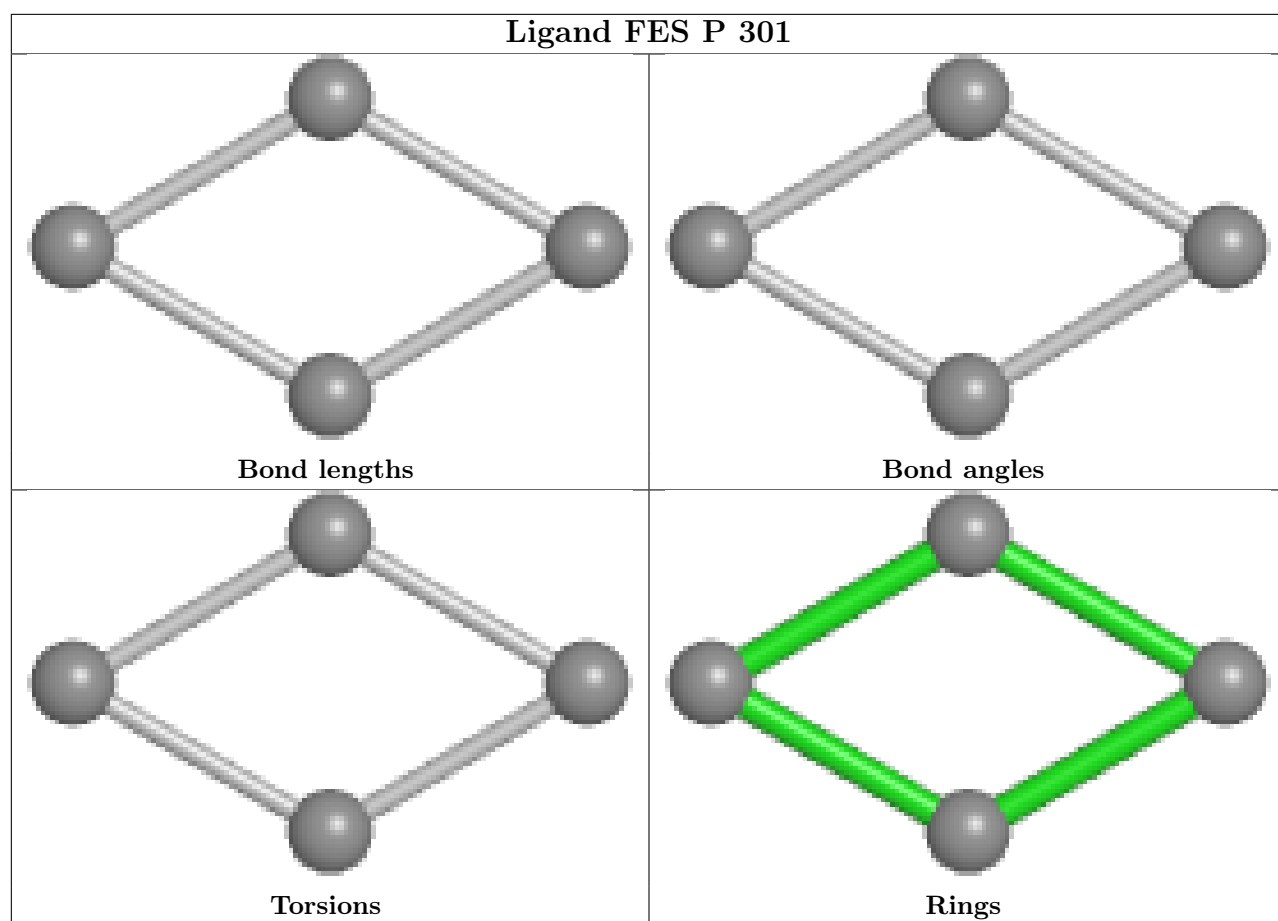


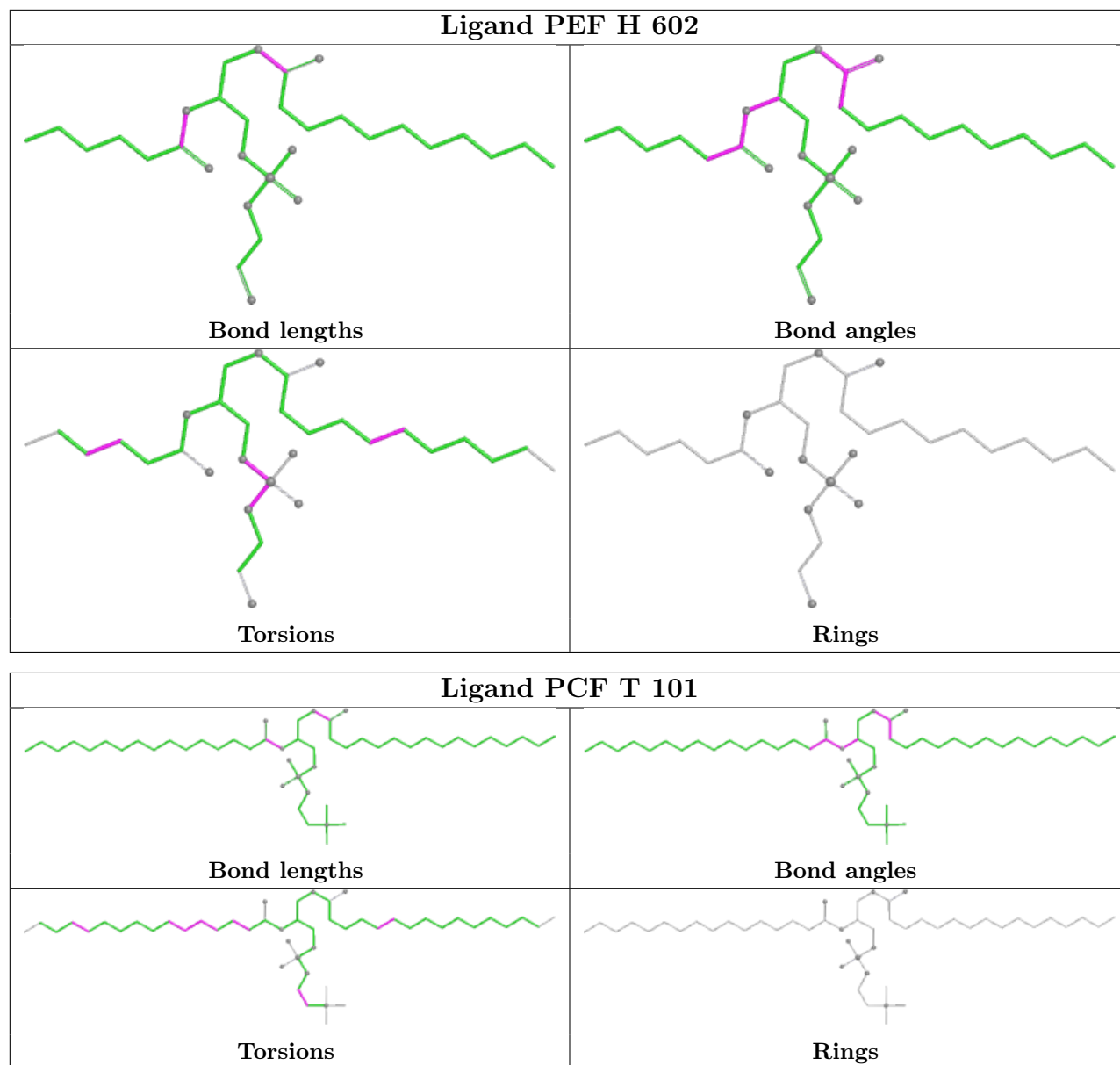


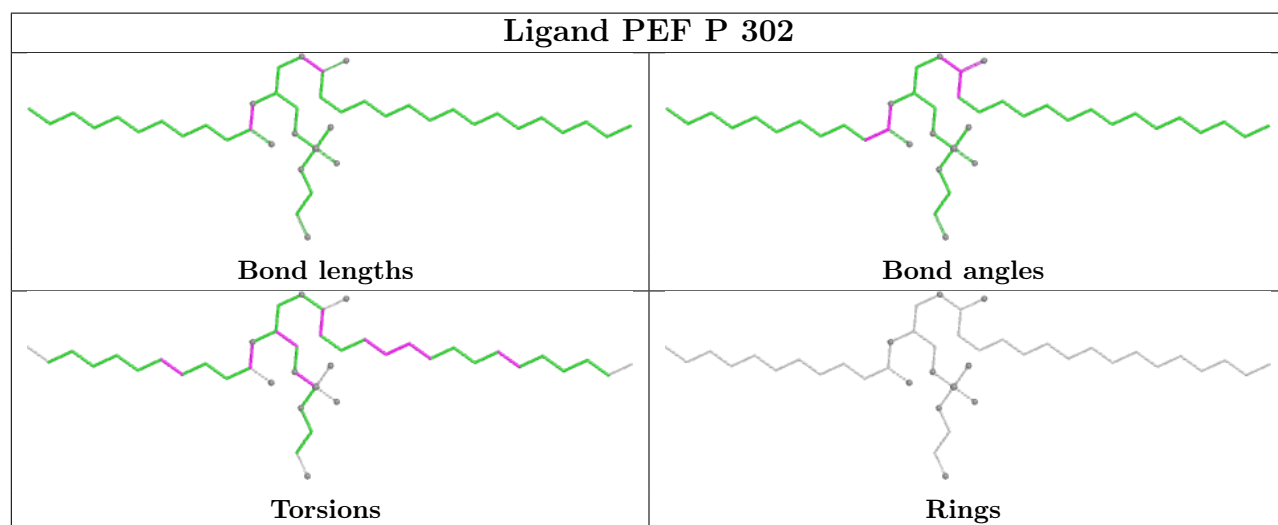
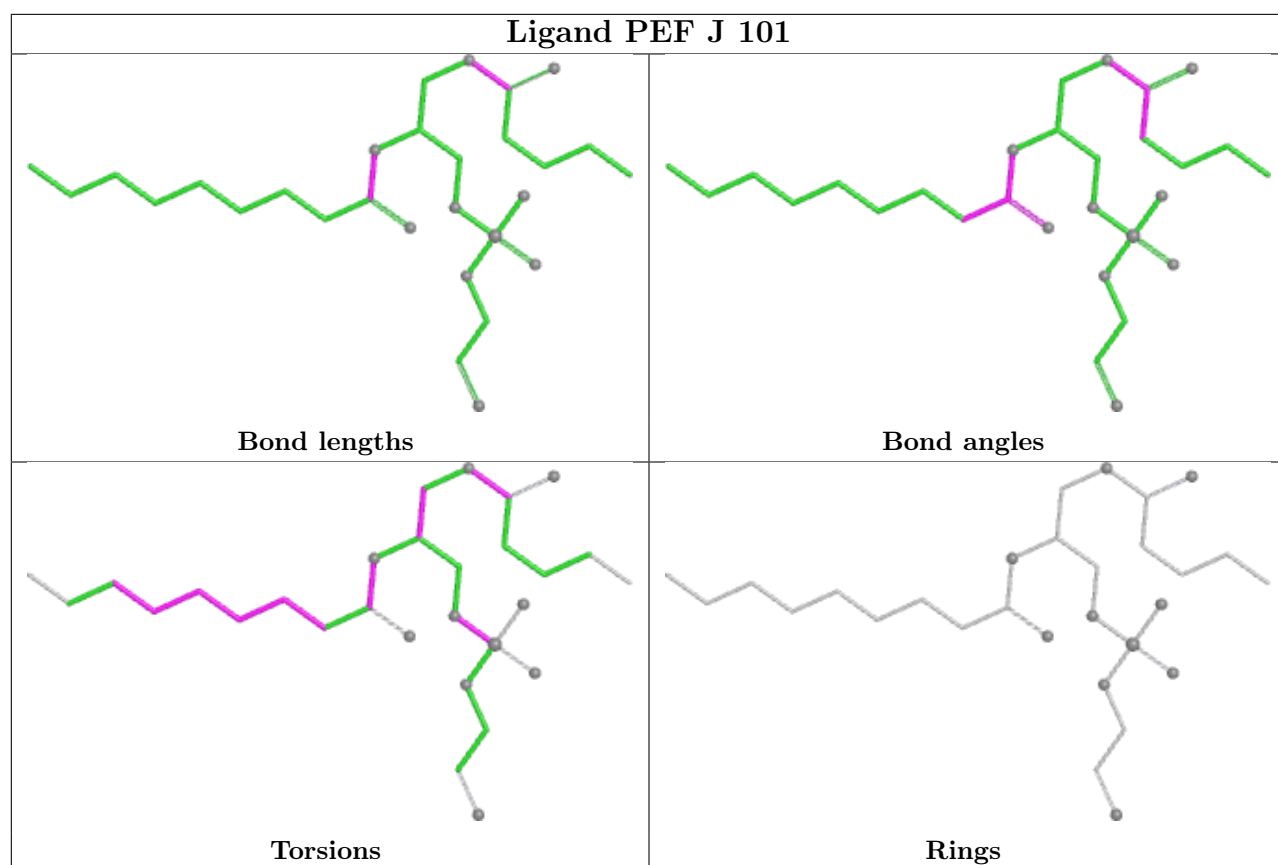
| Ligand PEF E 302                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

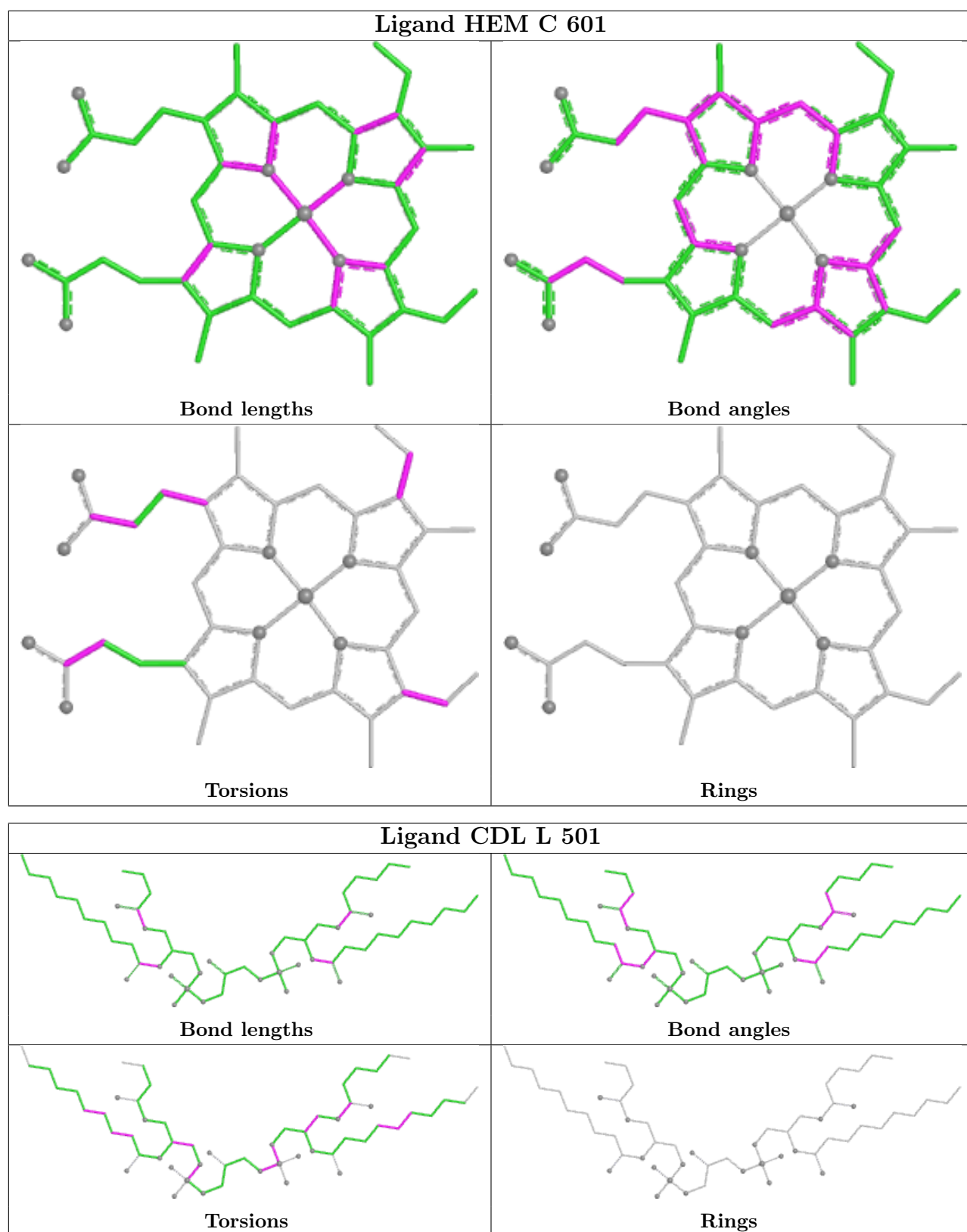
| Ligand PCF C 606                                                                   |                                                                                     |
|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                       | Bond angles                                                                         |
|  |  |
| Torsions                                                                           | Rings                                                                               |

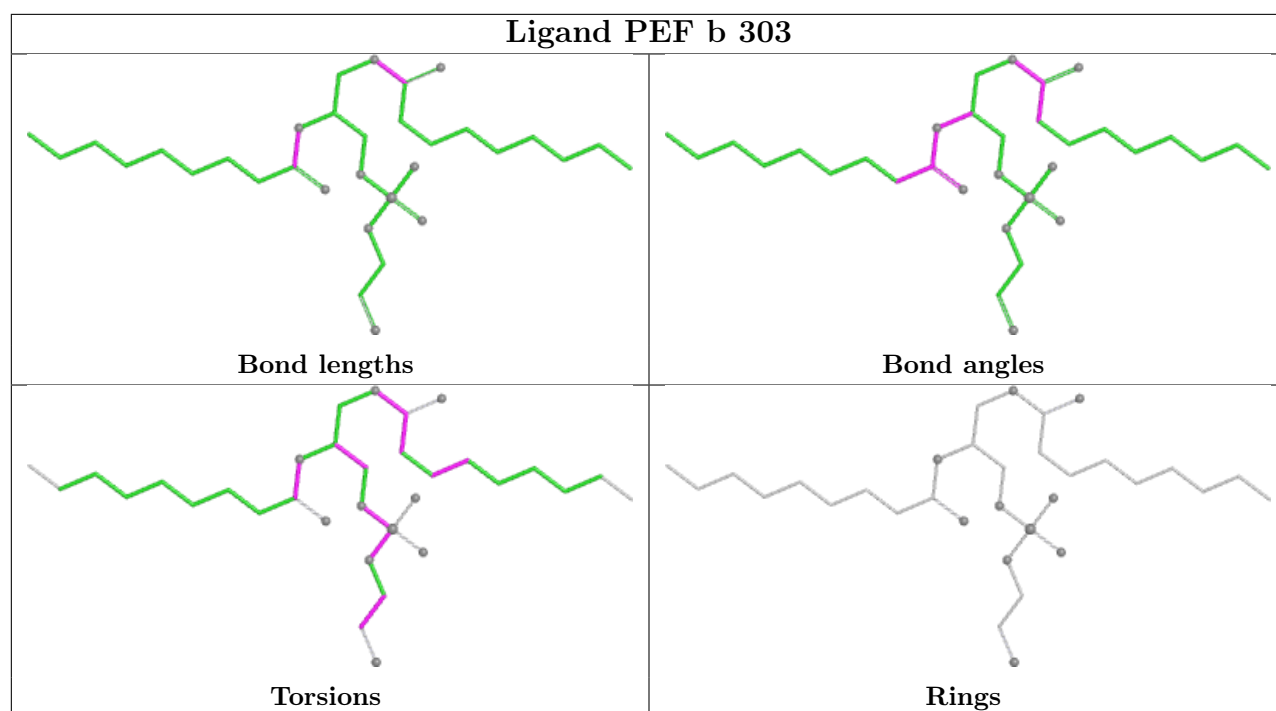
| Ligand CUA b 301                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

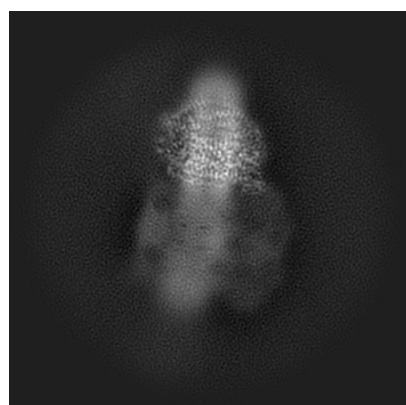
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10318. These allow visual inspection of the internal detail of the map and identification of artifacts.

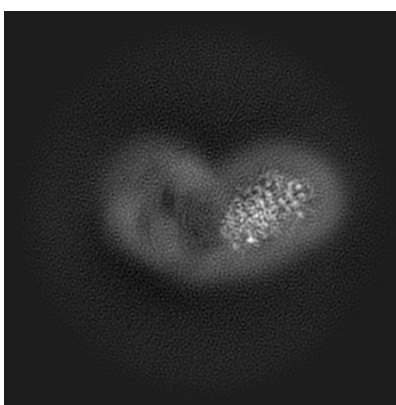
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

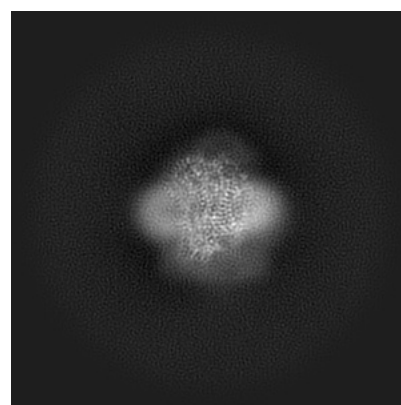
#### 6.1.1 Primary map



X



Y

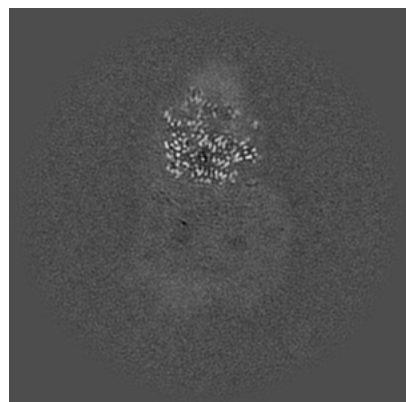


Z

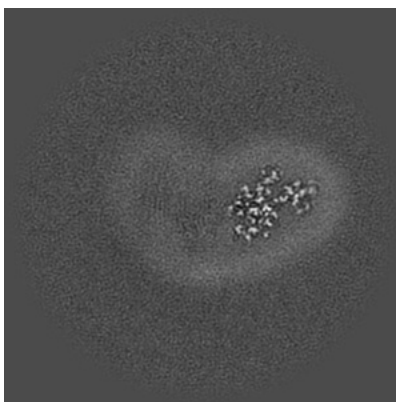
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

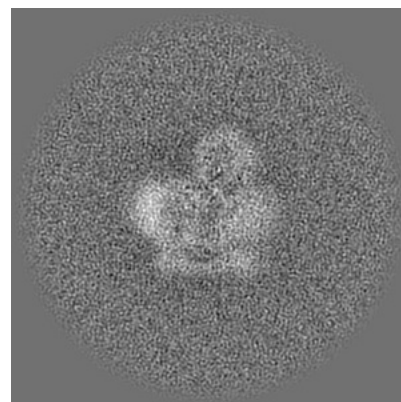
#### 6.2.1 Primary map



X Index: 192



Y Index: 192

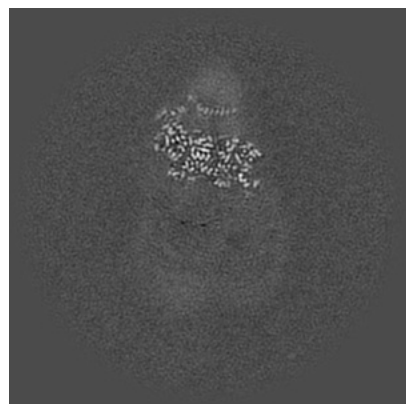


Z Index: 192

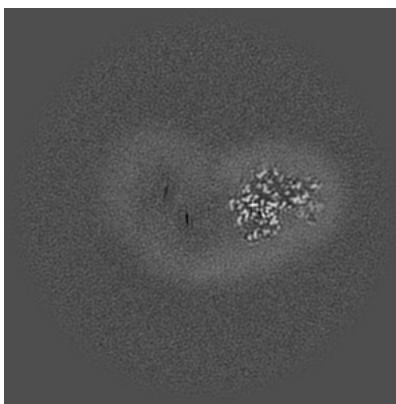
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

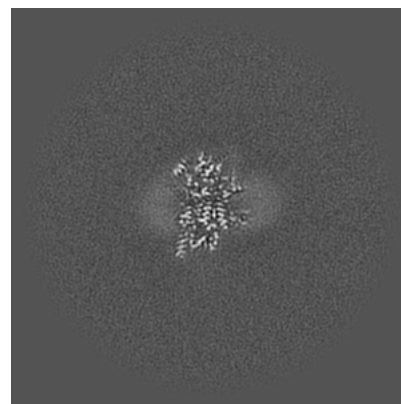
### 6.3.1 Primary map



X Index: 186



Y Index: 184

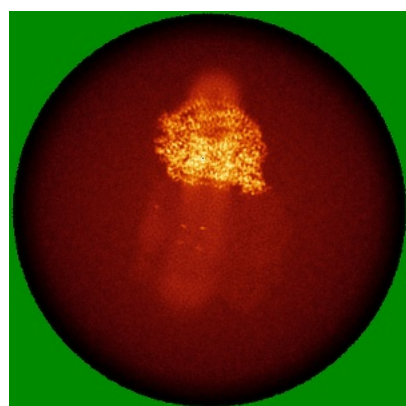


Z Index: 241

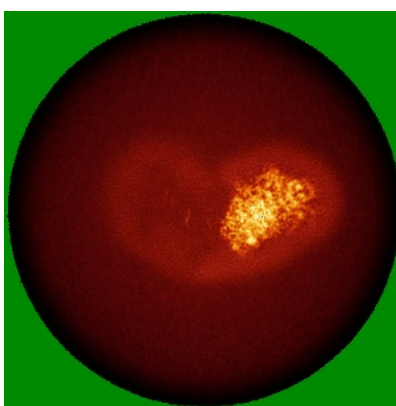
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

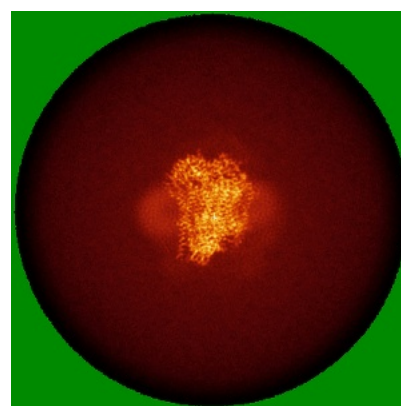
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views

This section was not generated.

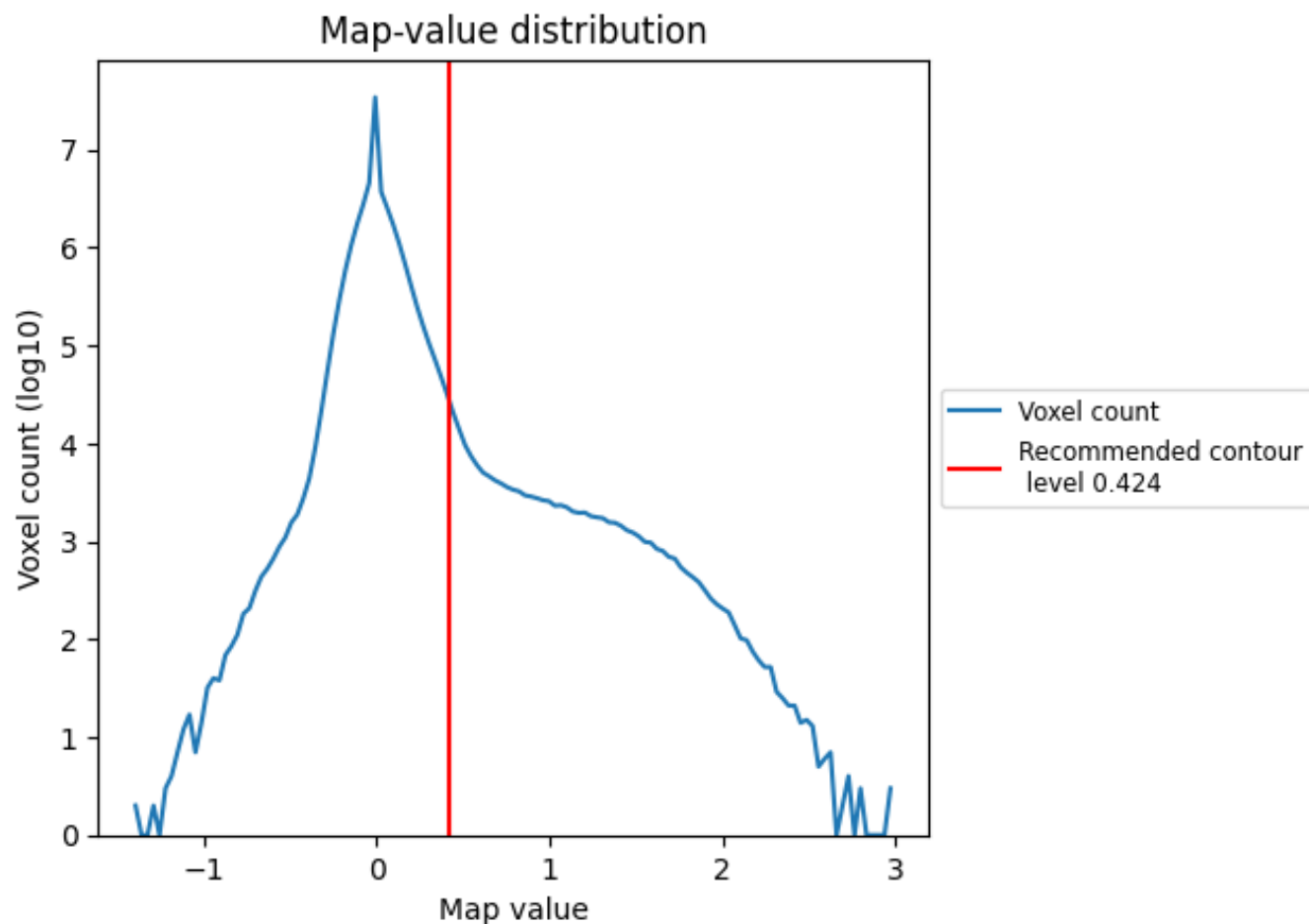
## 6.6 Mask visualisation

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

## 7 Map analysis [i](#)

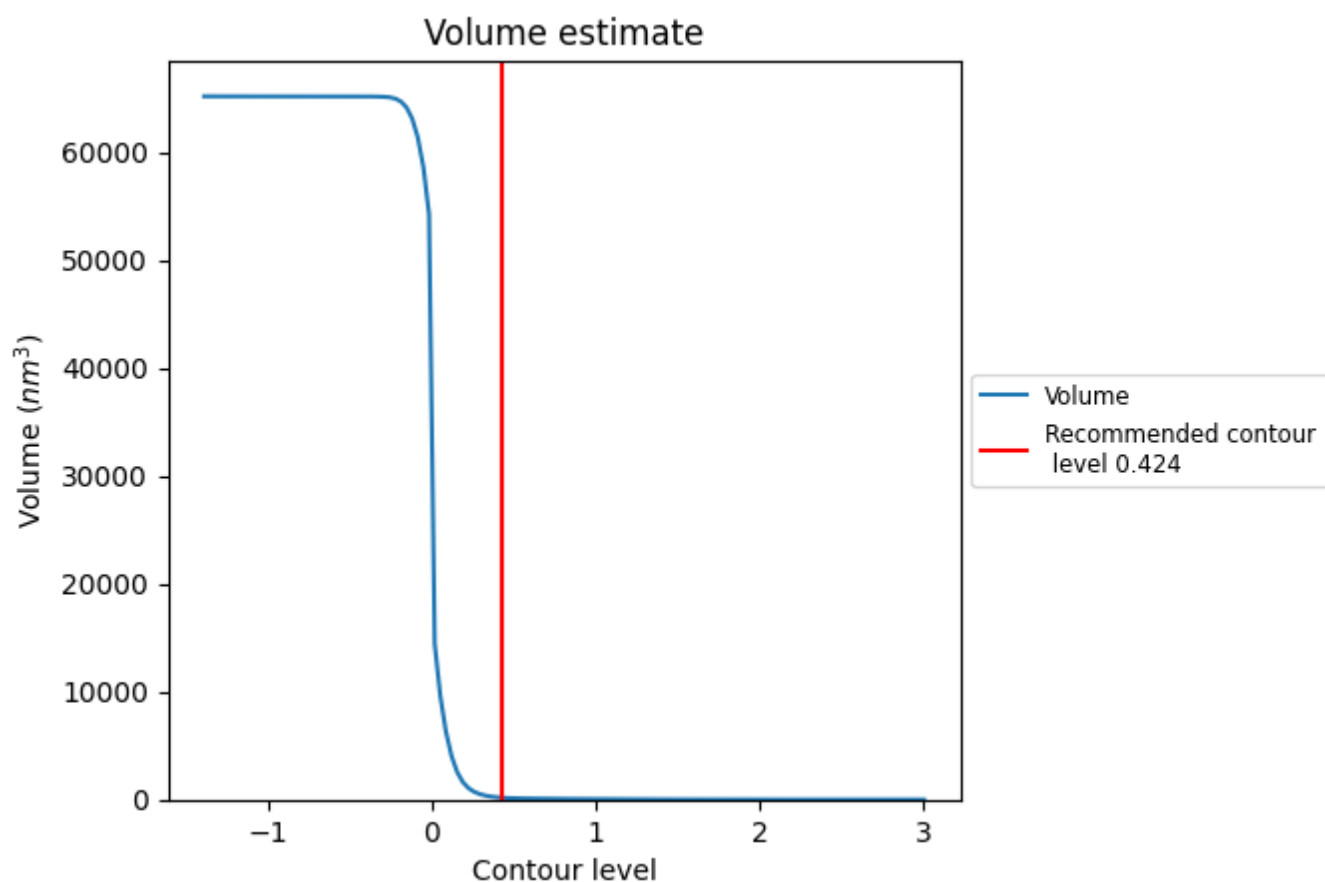
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

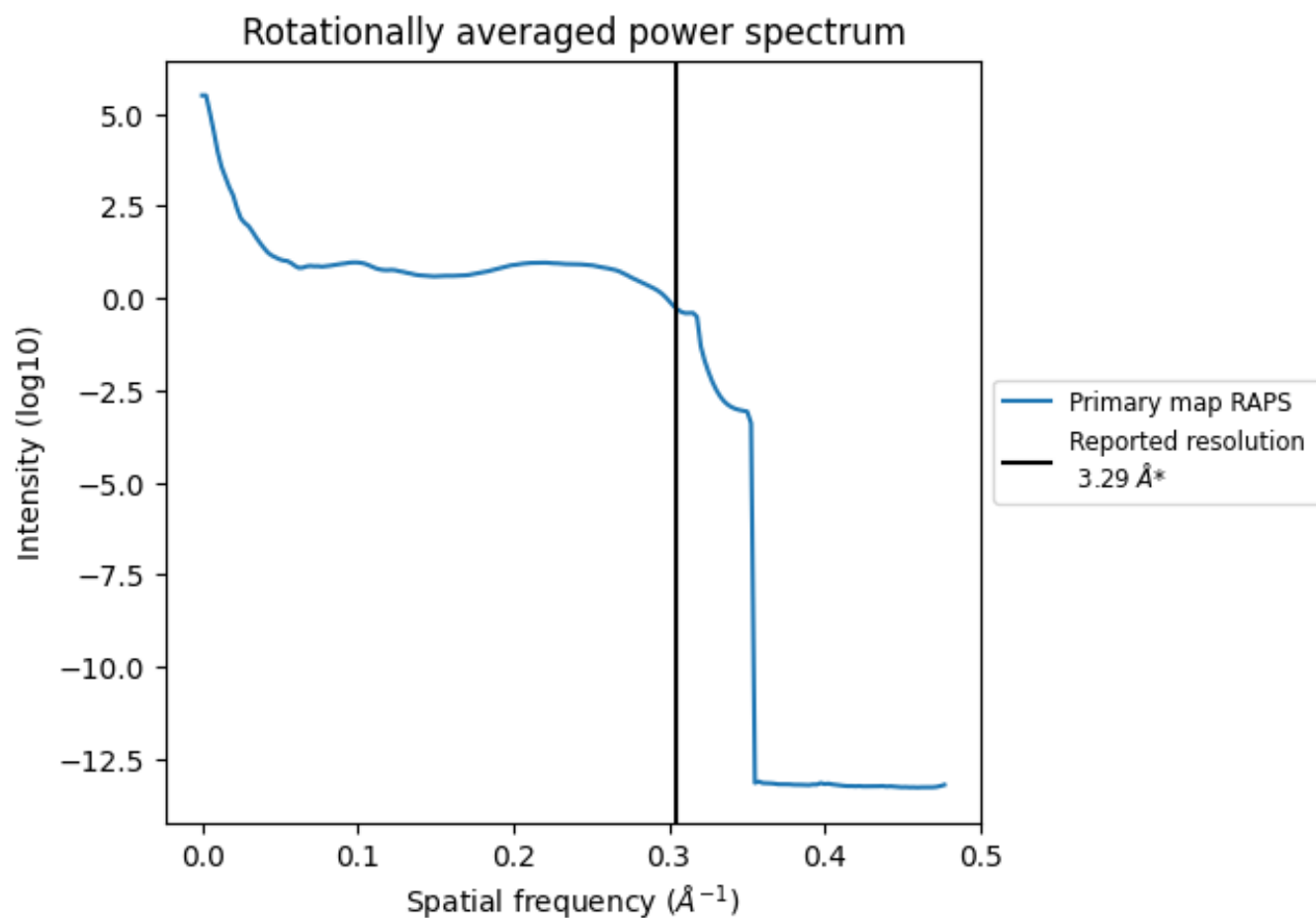
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174 nm<sup>3</sup>; this corresponds to an approximate mass of 158 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 ⓘ

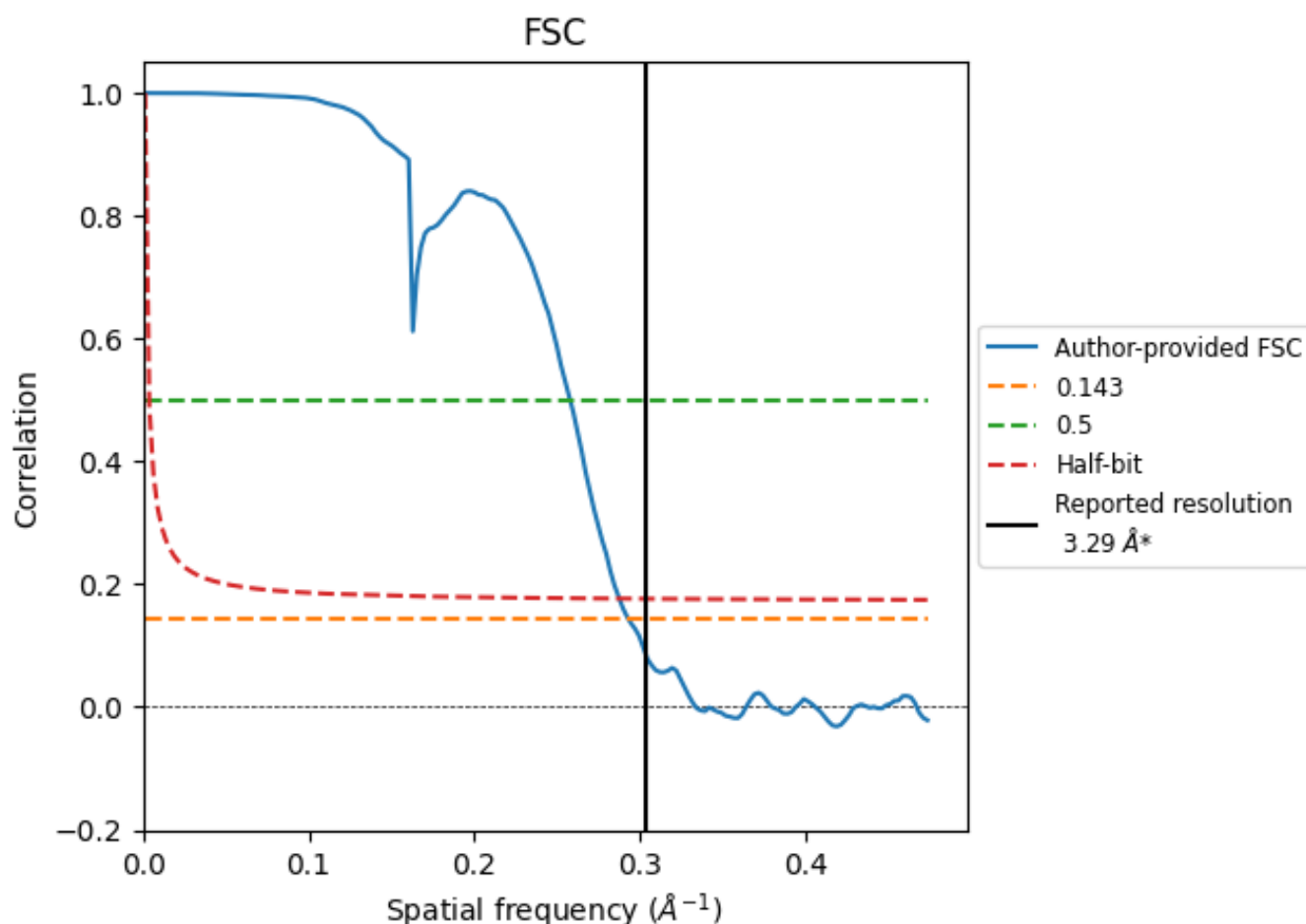


\*Reported resolution corresponds to spatial frequency of 0.304 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.304 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

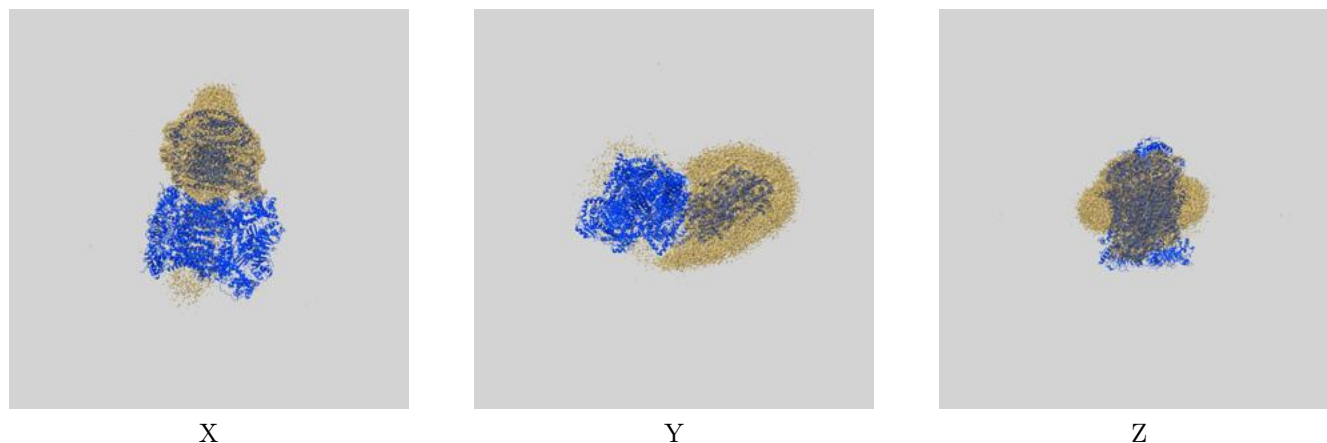
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.29                               | -    | -        |
| Author-provided FSC curve | 3.41                               | 3.88 | 3.48     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

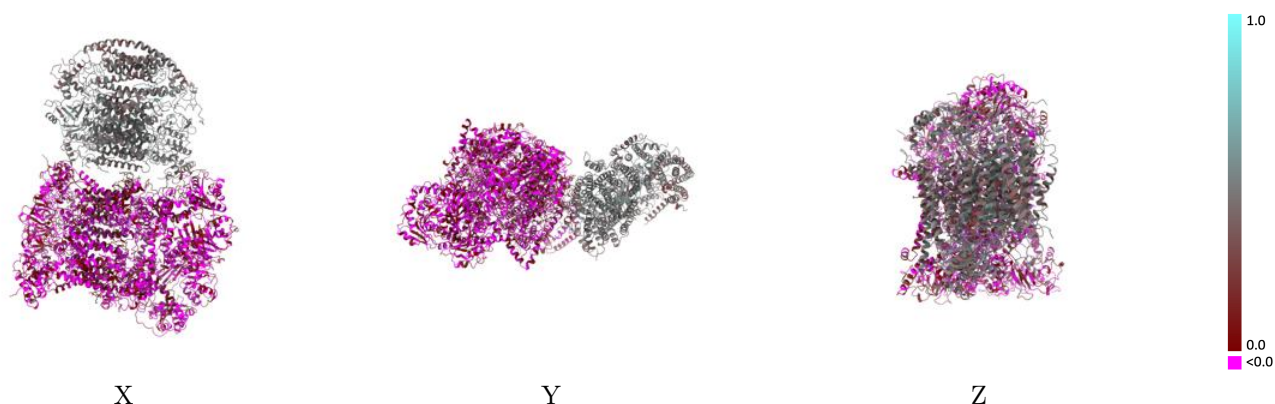
This section contains information regarding the fit between EMDB map EMD-10318 and PDB model 6T15. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.424 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 Q-score mapped to coordinate model [i](#)

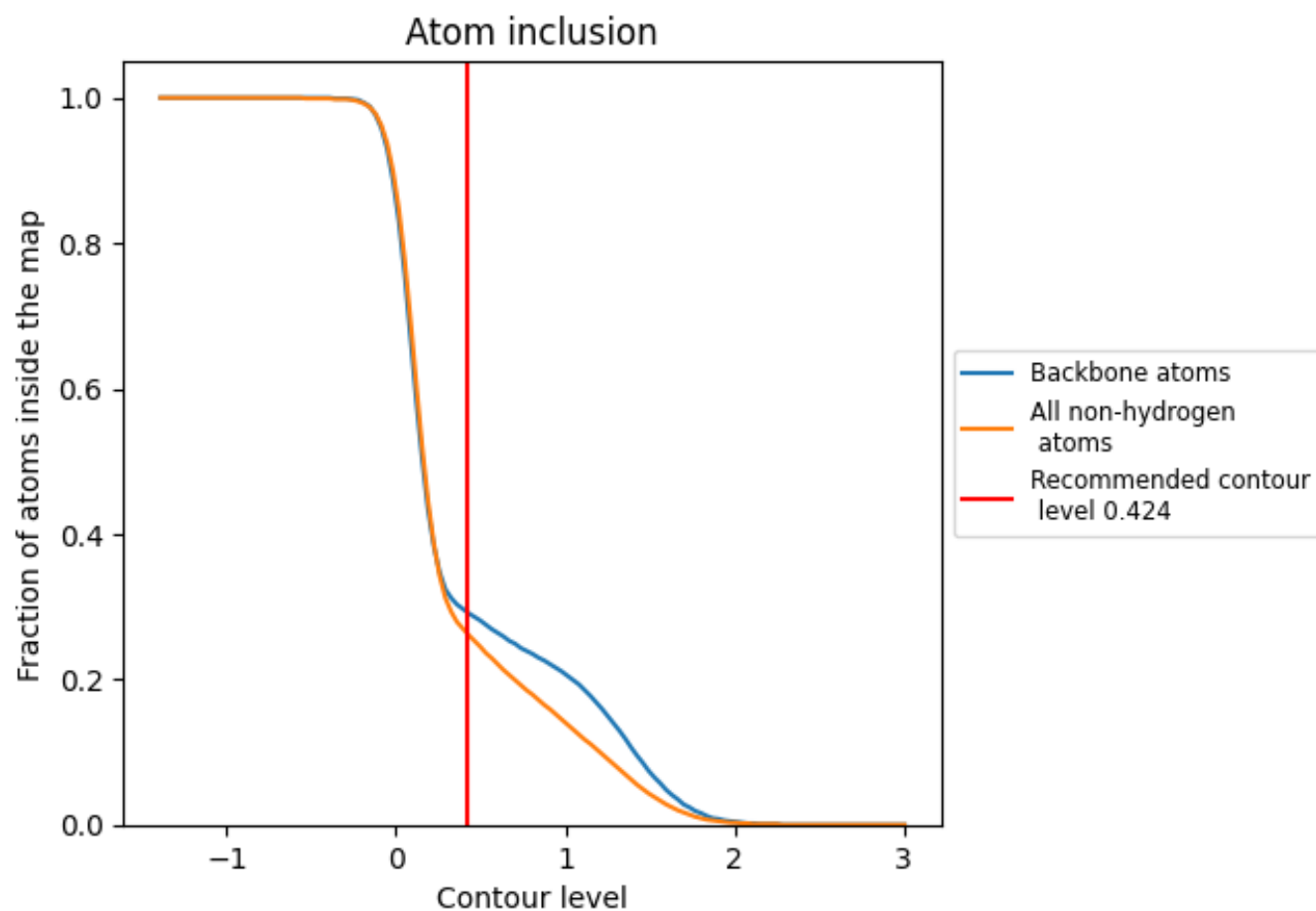


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 26% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.424) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                     |
|-------|--------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| All   |  0.2620   |  0.1510    |
| A     |  0.0000   |  -0.0120   |
| B     |  0.0000   |  -0.0220   |
| C     |  0.0010   |  -0.0200   |
| D     |  0.0000   |  -0.0080   |
| E     |  0.0030   |  0.0720    |
| F     |  0.0000   |  0.0100    |
| G     |  0.0000   |  -0.0100   |
| H     |  0.0000   |  0.0110    |
| I     |  0.0000   |  0.0150    |
| J     |  0.0030   |  0.0320    |
| L     |  0.0020   |  0.0170    |
| M     |  0.0000   |  -0.0140   |
| N     |  0.0010   |  0.0040    |
| O     |  0.0010  |  0.0200   |
| P     |  0.0040 |  0.0560  |
| Q     |  0.0000 |  0.0360  |
| R     |  0.0000 |  -0.0030 |
| S     |  0.0050 |  0.0550  |
| T     |  0.0020 |  0.0320  |
| U     |  0.0080 |  0.0530  |
| a     |  0.8290 |  0.4840  |
| b     |  0.8270 |  0.4750  |
| c     |  0.8200 |  0.4630  |
| d     |  0.8740 |  0.4750  |
| e     |  0.7480 |  0.4390  |
| f     |  0.8390 |  0.4470  |
| g     |  0.8520 |  0.4730  |
| h     |  0.8440 |  0.4610  |
| i     |  0.8260 |  0.4400  |
| j     |  0.8400 |  0.4460  |
| k     |  0.8330 |  0.4310  |
| l     |  0.8220 |  0.4540  |
| m     |  0.7720 |  0.3910  |

