



## Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 02:51 AM EDT

PDB ID : 8EC0 / pdb\_00008ec0  
EMDB ID : EMD-28011  
Title : III2IV respiratory supercomplex from *Saccharomyces cerevisiae* cardiolipin-lacking mutant  
Authors : Hryc, C.F.; Mileykovskaya, E.; Baker, M.; Dowhan, W.  
Deposited on : 2022-08-31  
Resolution : 3.30 Å(reported)

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:

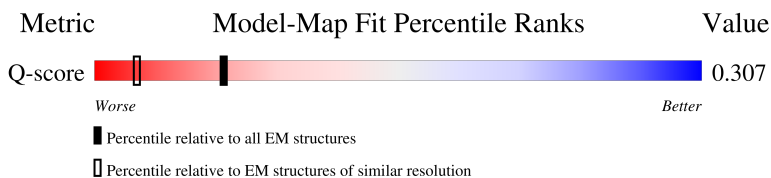
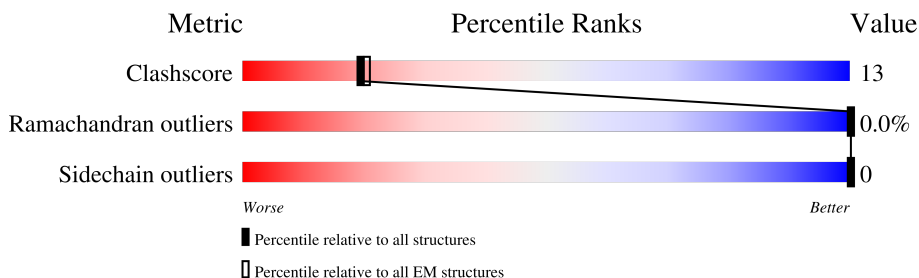
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.50

# 1 Overall quality at a glance

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

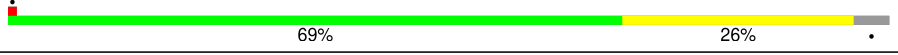
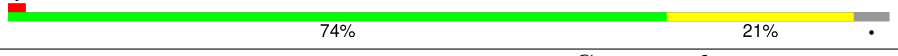
The reported resolution of this entry is 3.30 Å.

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                       | 15087 ( 2.80 - 3.80 )                                    |

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     | 457    |  |
| 1   | a     | 457    |  |
| 2   | B     | 368    |  |
| 2   | b     | 368    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 215    |                  |
| 3   | c     | 215    |                  |
| 4   | E     | 66     |                  |
| 4   | e     | 66     |                  |
| 5   | F     | 127    |                  |
| 5   | f     | 127    |                  |
| 6   | G     | 147    |                  |
| 6   | g     | 147    |                  |
| 7   | H     | 94     |                  |
| 7   | h     | 94     |                  |
| 8   | J     | 385    |                  |
| 8   | j     | 385    |                  |
| 9   | K     | 534    |                  |
| 10  | L     | 309    |                  |
| 10  | l     | 309    |                  |
| 11  | M     | 78     |                  |
| 12  | N     | 60     |                  |
| 13  | O     | 269    |                  |
| 14  | P     | 251    |                  |
| 15  | Q     | 148    |                  |
| 16  | R     | 59     |                  |
| 17  | S     | 129    |                  |
| 18  | T     | 155    |                  |
| 19  | U     | 83     |                  |
| 20  | V     | 66     |                  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 21  | W     | 153    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 24  | FES  | C     | 301 | -         | -        | X       | -                |
| 24  | FES  | c     | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 46624 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.

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

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

- Molecule 3 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 185      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1411  | 893 | 242 | 266 | 10 |         |       |
| 3   | c     | 185      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1411  | 893 | 242 | 266 | 10 |         |       |

- Molecule 4 is a protein called Cytochrome b-c1 complex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 4   | E     | 57       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 465   | 310 | 77 | 78 |         |       |
| 4   | e     | 57       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 465   | 310 | 77 | 78 |         |       |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | F     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 653 | 173 | 191 | 2 |         |       |
| 5   | f     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1019  | 653 | 173 | 191 | 2 |         |       |

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | G     | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 624   | 391 | 108 | 123 | 2 |         |       |
| 6   | g     | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 624   | 391 | 108 | 123 | 2 |         |       |

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 510 | 131 | 130 | 2 |         |       |
| 7   | h     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 773   | 510 | 131 | 130 | 2 |         |       |

- Molecule 8 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | J     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3090  | 2082 | 484 | 503 | 21 |         |       |
| 8   | j     | 385      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3090  | 2082 | 484 | 503 | 21 |         |       |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | K     | 534      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4162  | 2778 | 649 | 713 | 22 |         |       |

- Molecule 10 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 10  | L     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1961  | 1249 | 340 | 363 | 9 |         |       |
| 10  | l     | 248      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1961  | 1249 | 340 | 363 | 9 |         |       |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 11  | M     | 47       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 382   | 261 | 62 | 58 | 1 |         |       |

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 12  | N     | 59       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 484   | 328 | 83 | 73 |  |         |       |

- Molecule 13 is a protein called Cytochrome c oxidase subunit 3.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | P     | 236      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1889  | 1242 | 286 | 351 | 10 |         |       |

- Molecule 15 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | Q     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 545 | 137 | 168 | 1 |         |       |

- Molecule 16 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 16  | R     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 455   | 300 | 79 | 73 | 3 |         |       |

- Molecule 17 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | S     | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 928   | 605 | 160 | 160 | 3 |         |       |

- Molecule 18 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 576 | 151 | 181 | 5 |         |       |

- Molecule 19 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | U     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 410 | 109 | 118 | 5 |         |       |

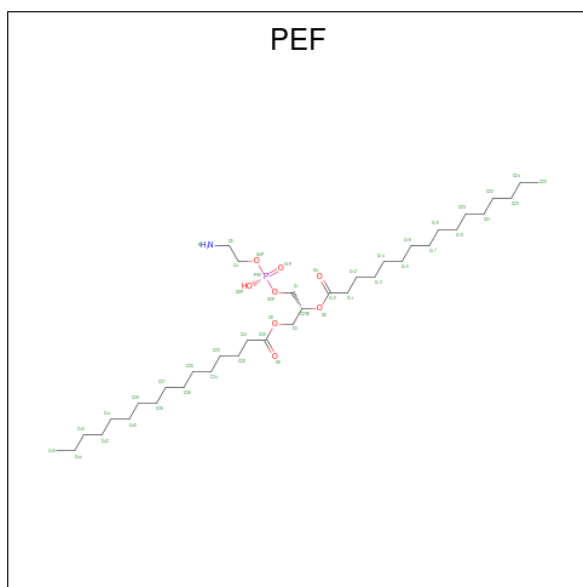
- Molecule 20 is a protein called Cytochrome c oxidase subunit 26, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 20  | V     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 321   | 214 | 53 | 53 | 1 |         |       |

- Molecule 21 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1049  | 663 | 184 | 198 | 4 |         |       |

- Molecule 22 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



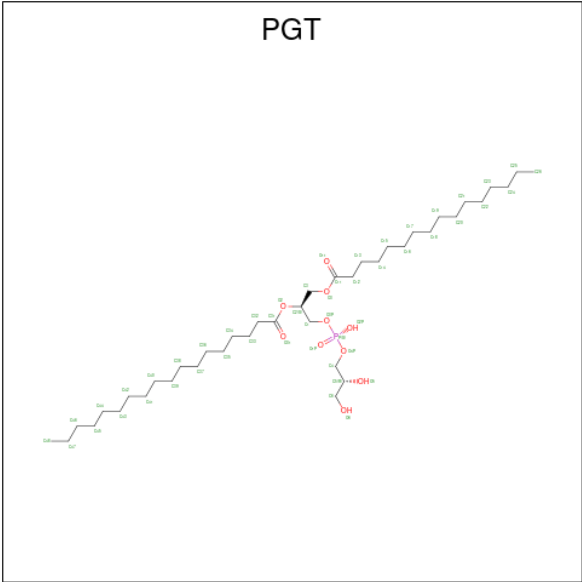
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 22  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |

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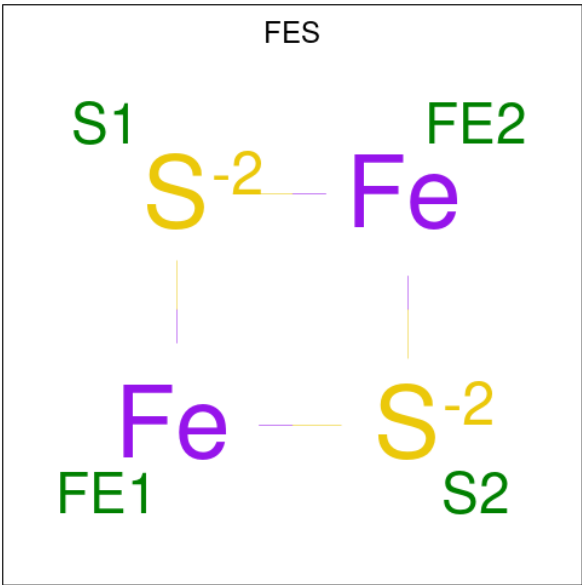
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 22  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 22  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 22  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 22  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 22  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 22  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 22  | V     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 22  | V     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 22  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 22  | c     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 22  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 22  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 22  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 22  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |

- Molecule 23 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



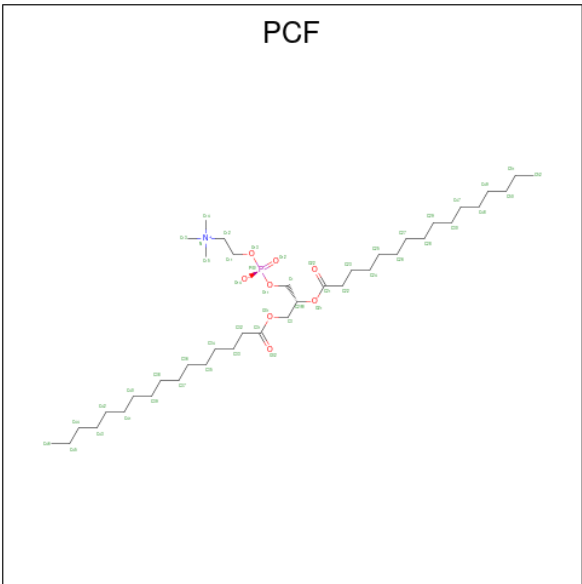
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 23  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 23  | C     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 23  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 23  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 23  | W     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 23  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 23  | j     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |

- Molecule 24 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 24  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 24  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 25 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) (labeled as "Ligand of Interest" by depositor).



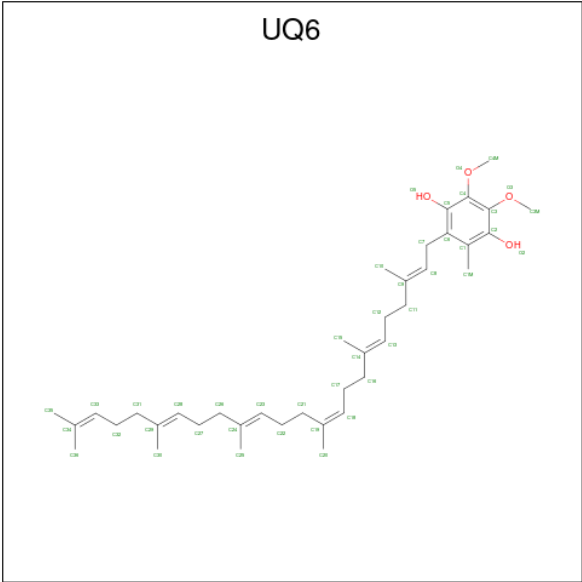
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 25  | E     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms       |         |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 25  | W     | 1        | Total<br>36 | C<br>26 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 25  | W     | 1        | Total<br>50 | C<br>40 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 25  | c     | 1        | Total<br>47 | C<br>37 | N<br>1 | O<br>8 | P<br>1 | 0       |

- # HEM

- Molecule 27 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEXAENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (CCD ID: UQ6) (formula:  $C_{39}H_{60}O_4$ ) (labeled as "Ligand of Interest" by depositor).

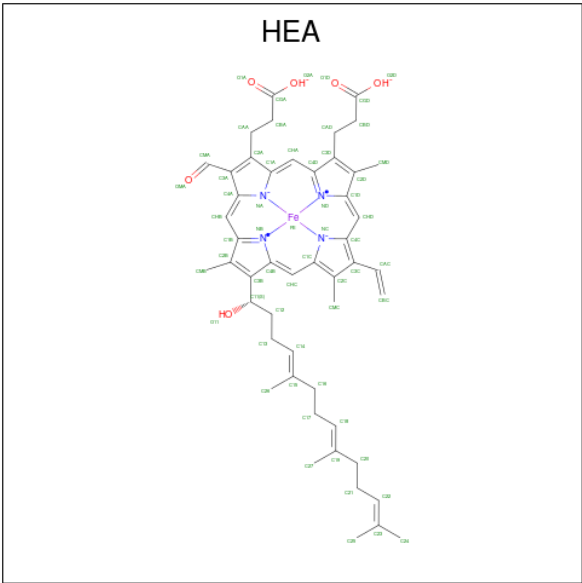


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 27  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 39 | 4 |         |
| 27  | j     | 1        | Total | C  | O | 0       |
|     |       |          | 43    | 39 | 4 |         |

- Molecule 28 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

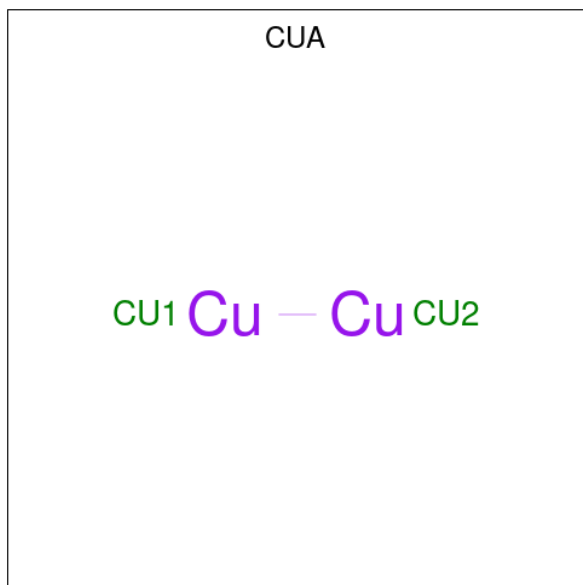
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 28  | K     | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 29 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 29  | K     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |
| 29  | K     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |

- Molecule 30 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).

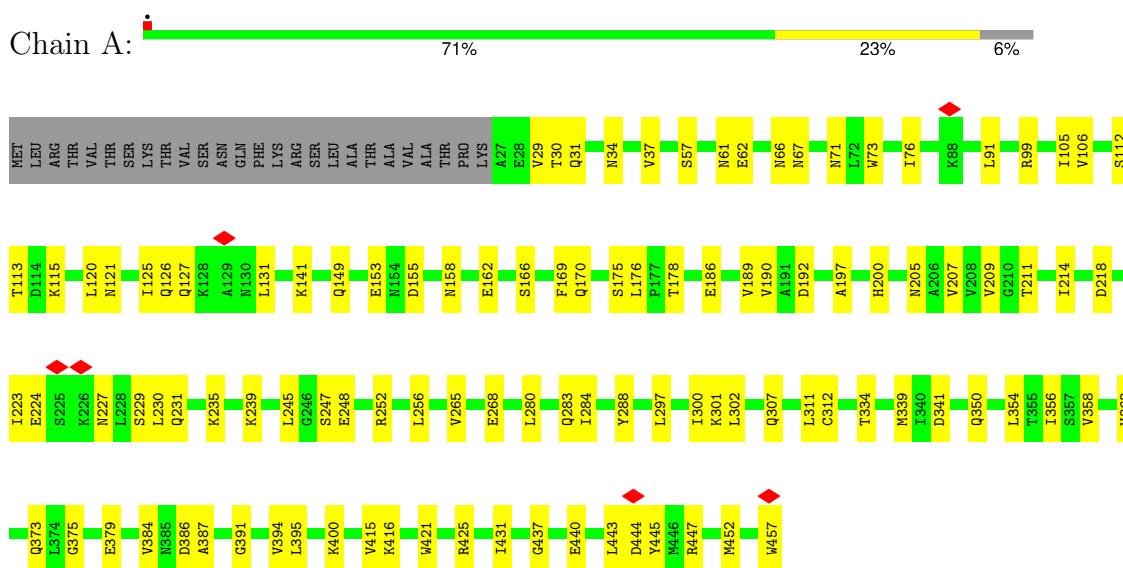


| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 30  | P     | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |
| 30  | P     | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |

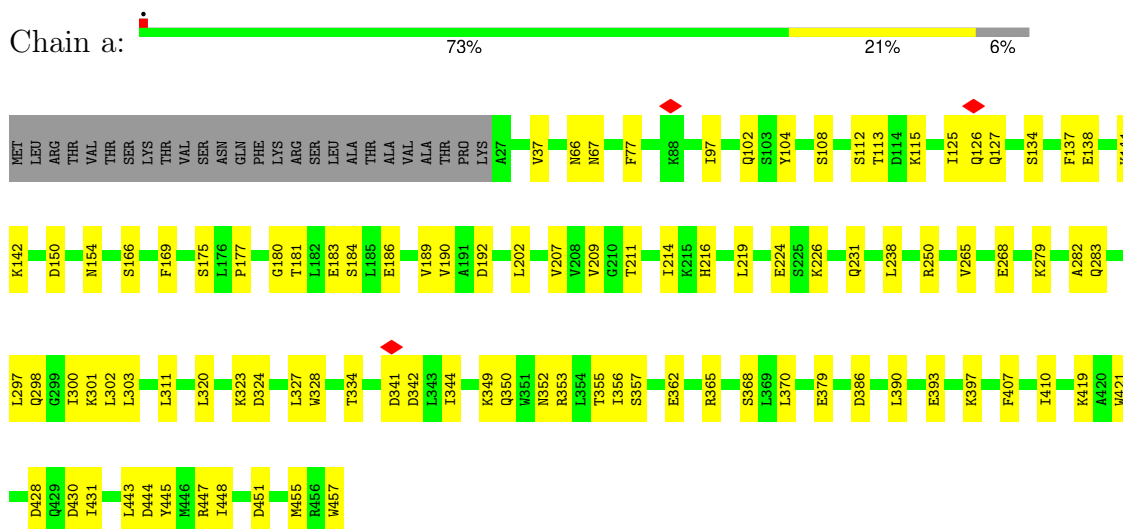
### 3 Residue-property plots

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.

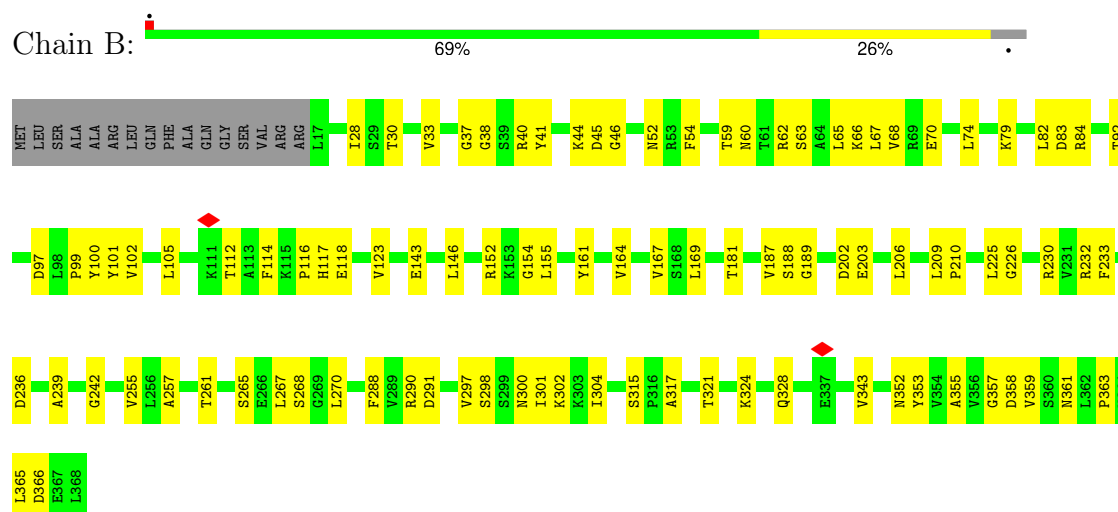
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



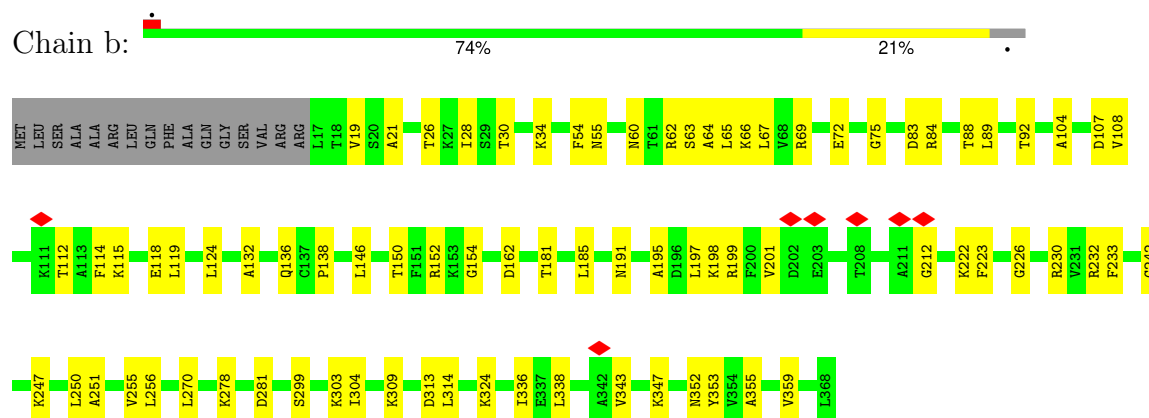
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



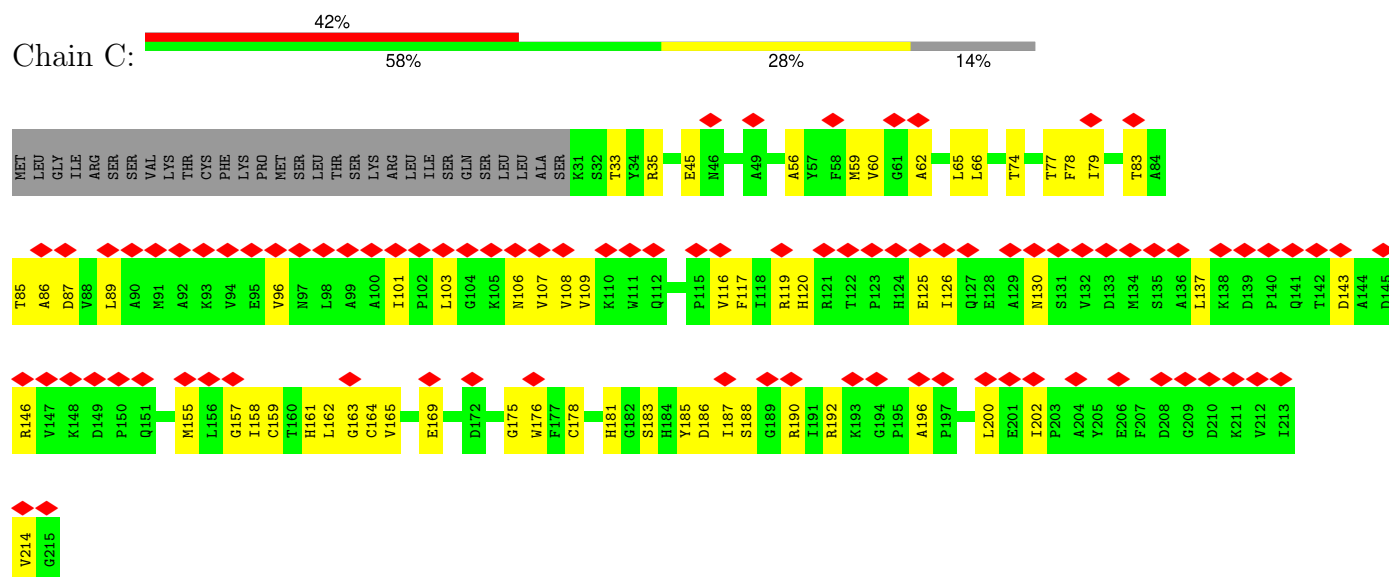
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



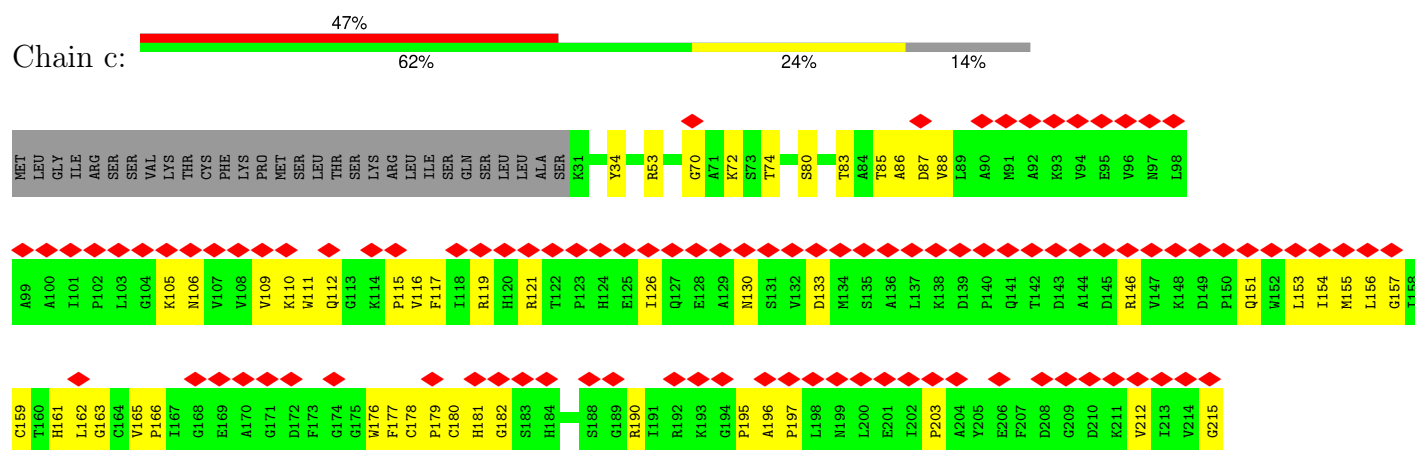
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



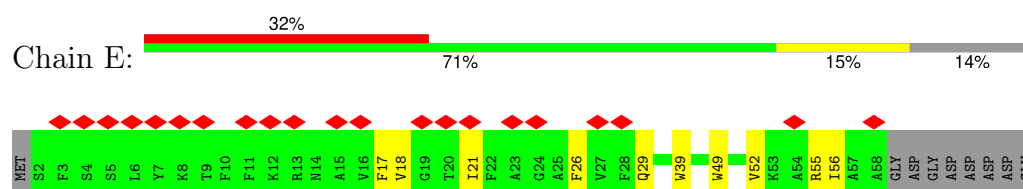
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



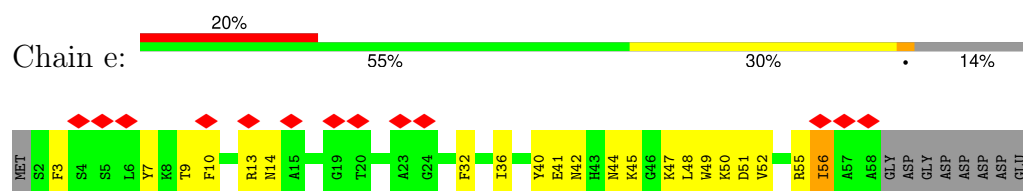
- Molecule 3: Cytochrome b-c1 complex subunit Rieske, mitochondrial



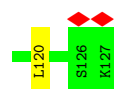
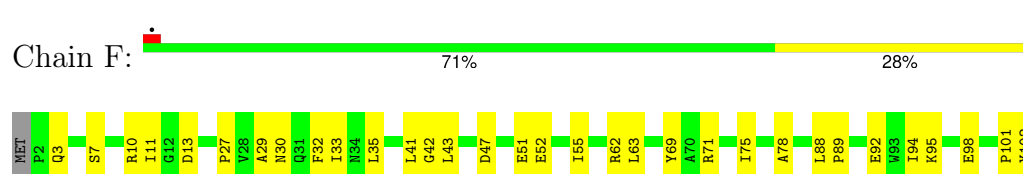
- Molecule 4: Cytochrome b-c1 complex subunit 9, mitochondrial



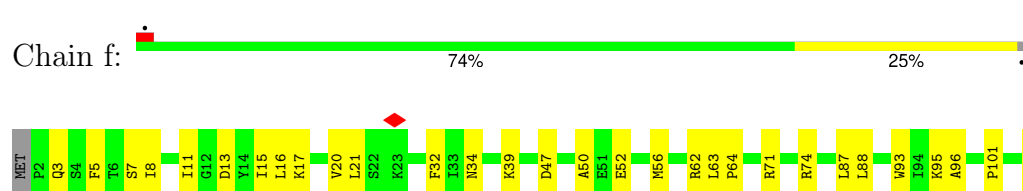
- Molecule 4: Cytochrome b-c1 complex subunit 9, mitochondrial



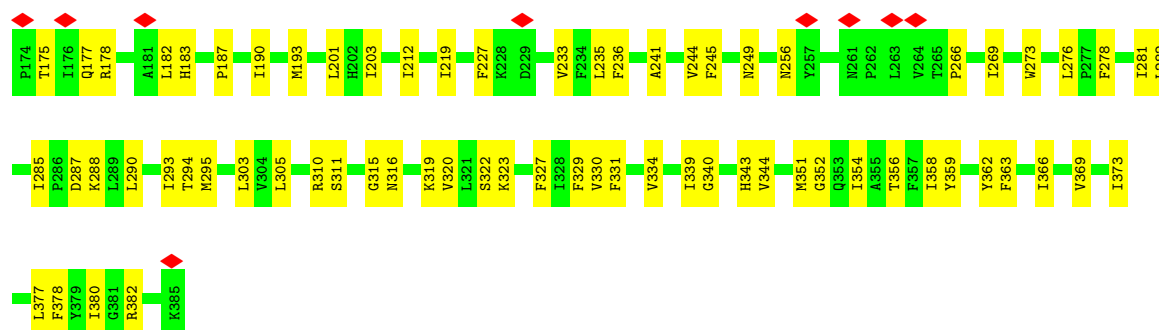
- Molecule 5: Cytochrome b-c1 complex subunit 7, mitochondrial



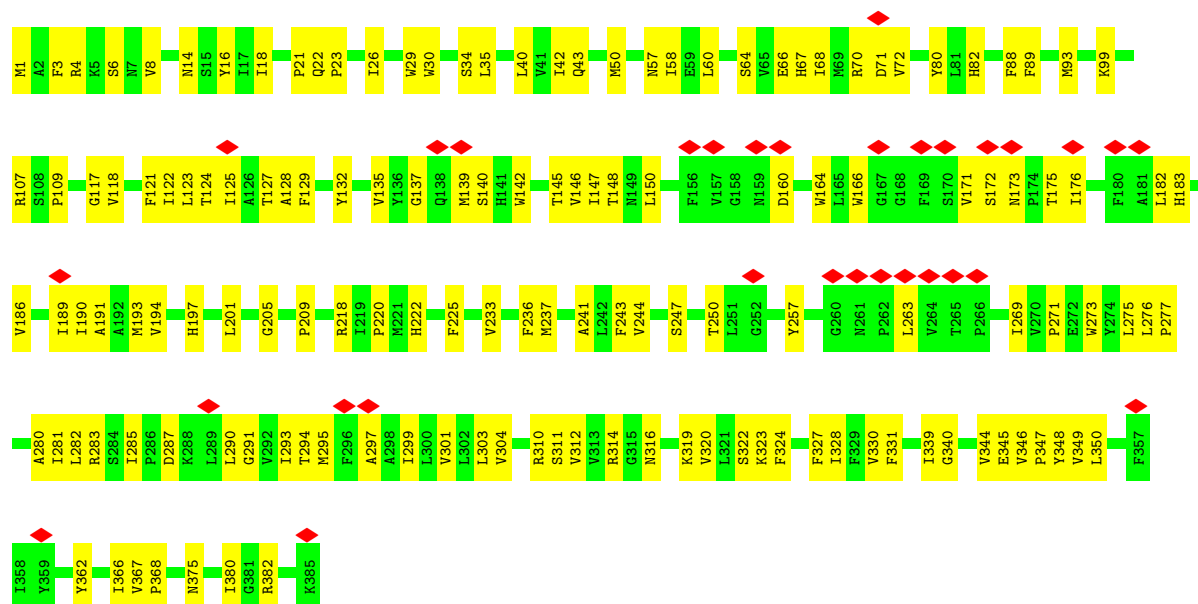
- Molecule 5: Cytochrome b-c1 complex subunit 7, mitochondrial



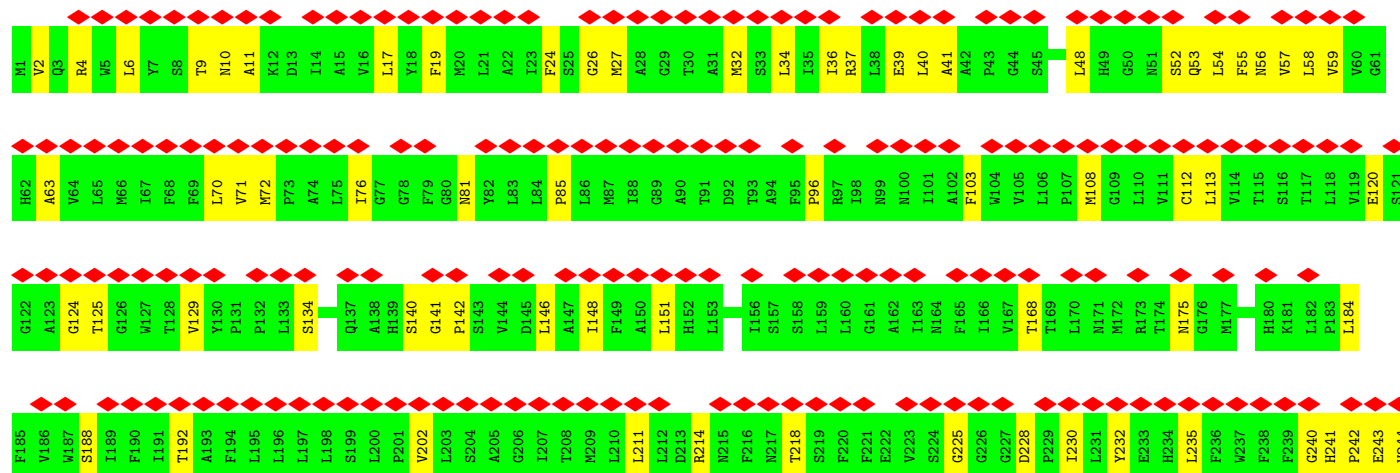


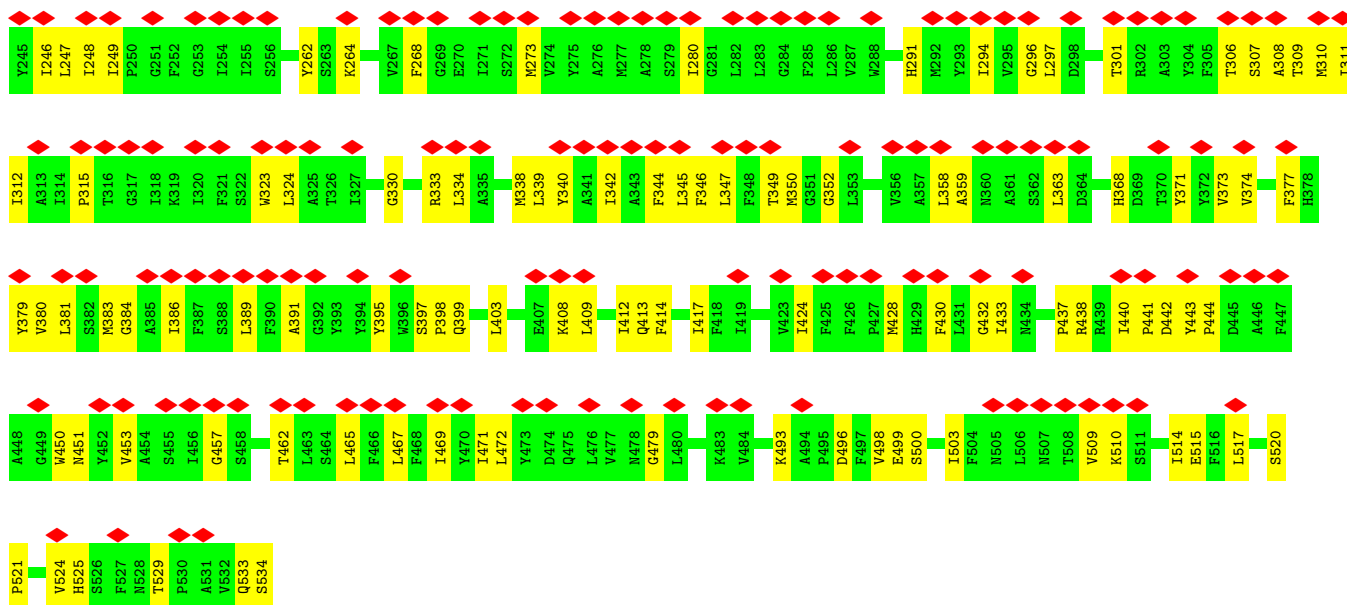


• Molecule 8: Cytochrome b

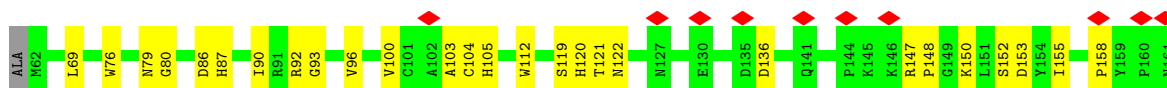


• Molecule 9: Cytochrome c oxidase subunit 1

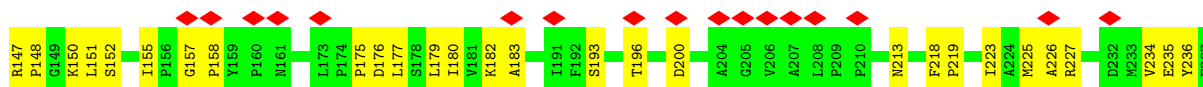
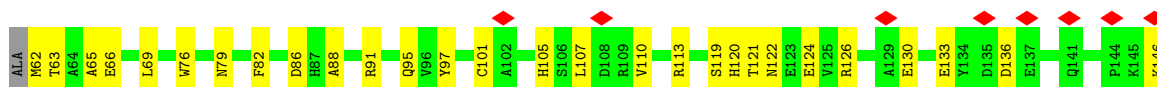




- Molecule 10: Cytochrome c1, heme protein, mitochondrial

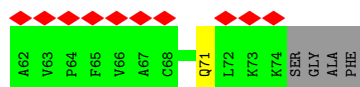
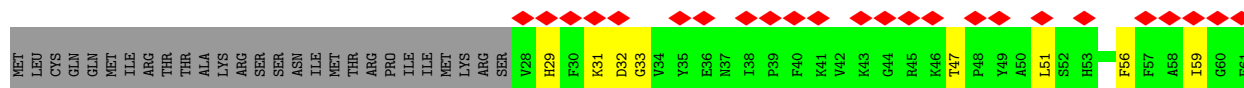
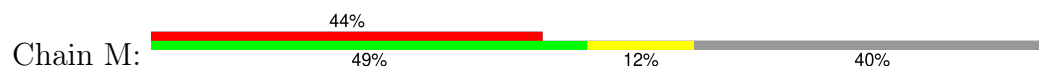


- Molecule 10: Cytochrome c1, heme protein, mitochondrial

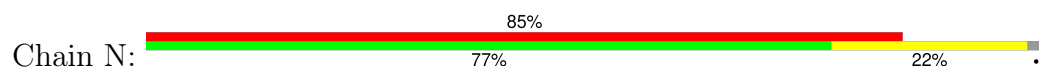




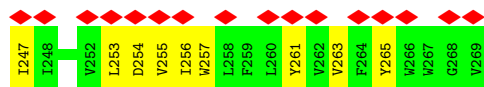
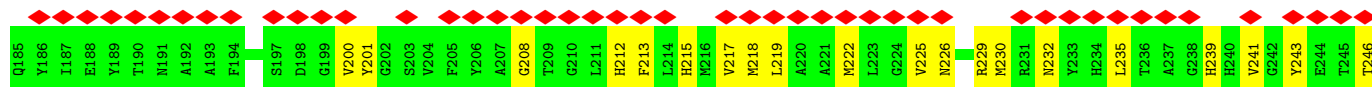
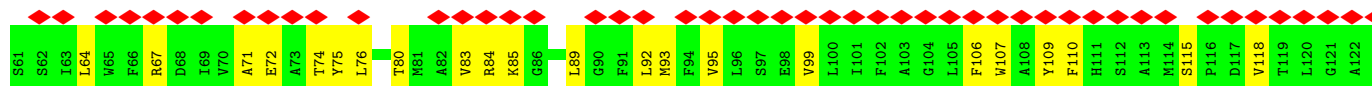
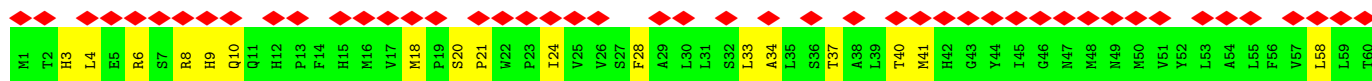
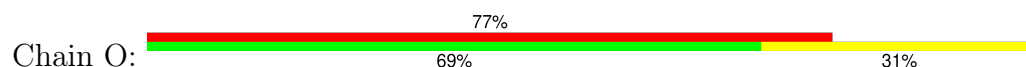
- Molecule 11: Cytochrome c oxidase subunit 8, mitochondrial



- Molecule 12: Cytochrome c oxidase subunit 7, mitochondrial

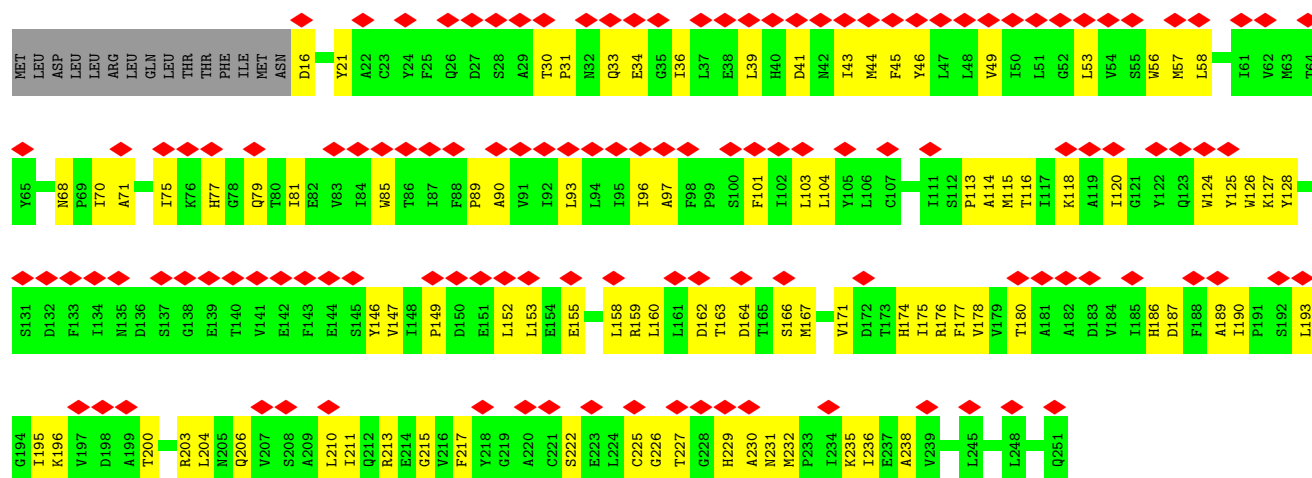


- Molecule 13: Cytochrome c oxidase subunit 3

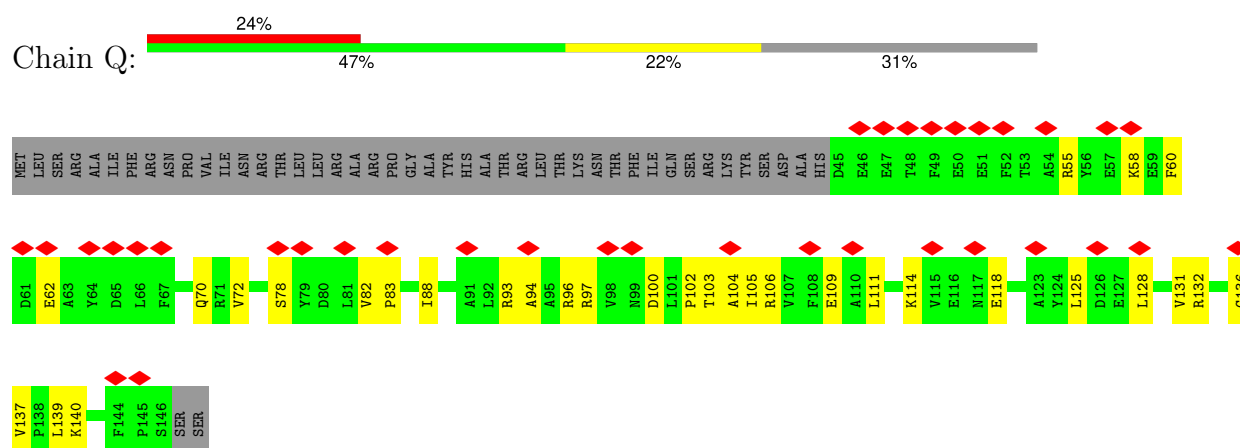


- Molecule 14: Cytochrome c oxidase subunit 2

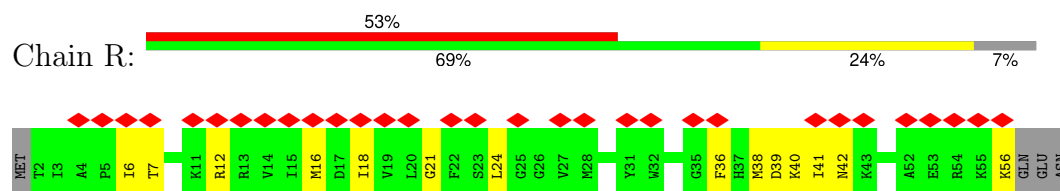




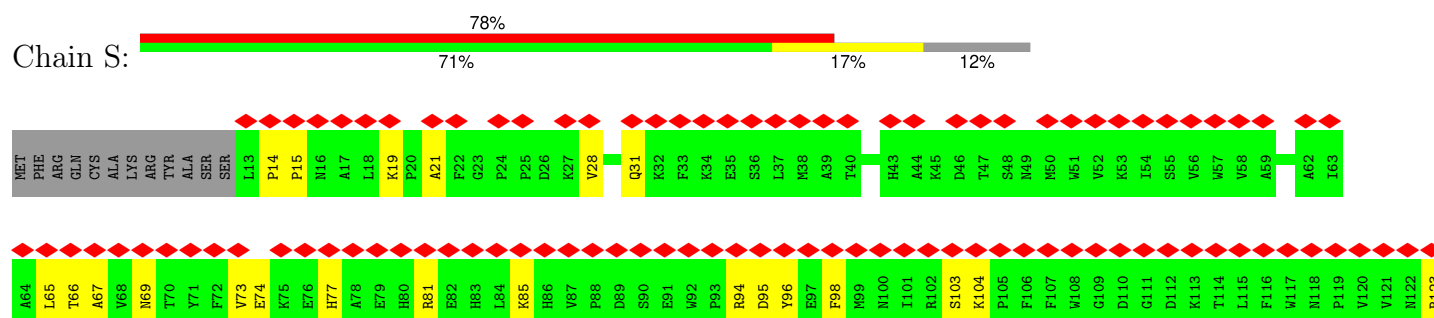
- Molecule 15: Cytochrome c oxidase subunit 6, mitochondrial

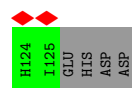


- Molecule 16: Cytochrome c oxidase subunit 9, mitochondrial

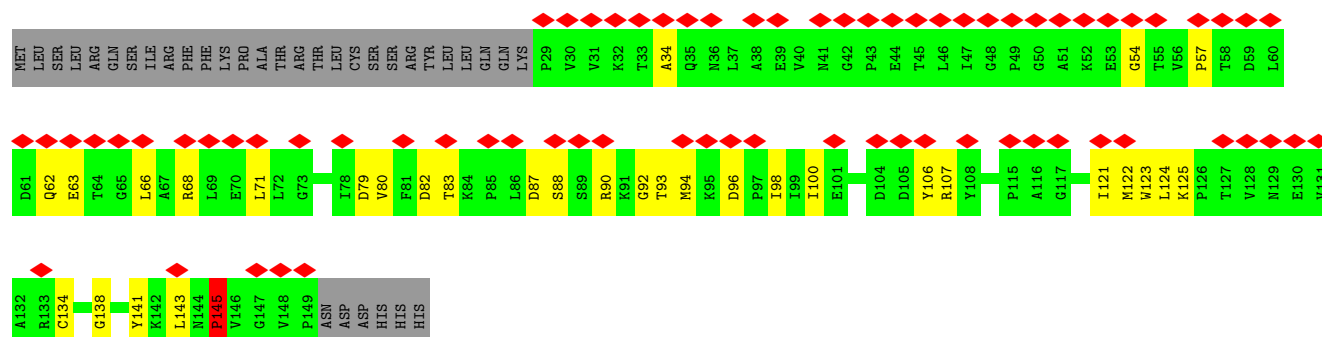


- Molecule 17: Cytochrome c oxidase subunit 13, mitochondrial

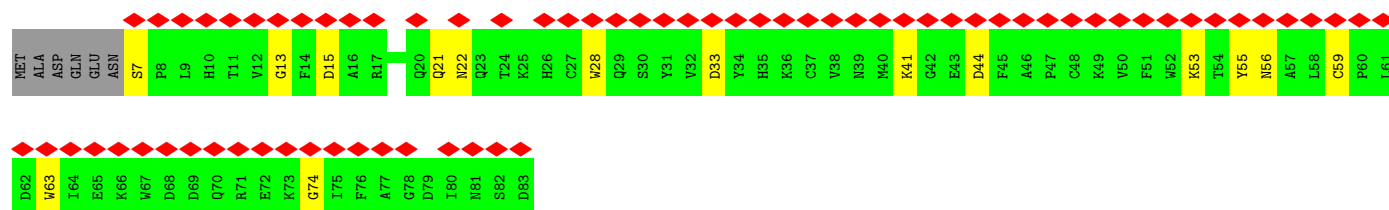
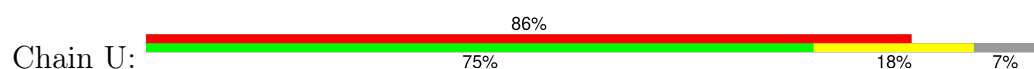




- Molecule 18: Cytochrome c oxidase subunit 4, mitochondrial



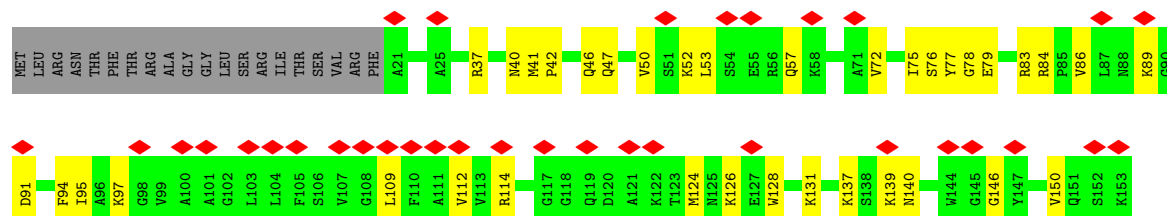
- Molecule 19: Cytochrome c oxidase subunit 12, mitochondrial



- Molecule 20: Cytochrome c oxidase subunit 26, mitochondrial



- Molecule 21: Cytochrome c oxidase subunit 5A, mitochondrial



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 745670                                  | 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 ( $e^-/\text{\AA}^2$ ) | 49                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 3500                                    | Depositor |
| Magnification                        | 130000                                  | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 2.361                                   | Depositor |
| Minimum map value                    | -1.226                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.040                                   | Depositor |
| Recommended contour level            | 0.2                                     | Depositor |
| Map size (Å)                         | 385.2, 385.2, 385.2                     | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.07, 1.07, 1.07                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ6, PEF, CU, CUA, PGT, FES, HEA, HEM, PCF

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     | 0.11         | 0/3406  | 0.30        | 0/4615         |
| 1   | a     | 0.11         | 0/3406  | 0.30        | 0/4615         |
| 2   | B     | 0.11         | 0/2781  | 0.32        | 1/3764 (0.0%)  |
| 2   | b     | 0.10         | 0/2781  | 0.30        | 0/3764         |
| 3   | C     | 0.11         | 0/1444  | 0.31        | 0/1957         |
| 3   | c     | 0.12         | 0/1444  | 0.31        | 0/1957         |
| 4   | E     | 0.09         | 0/479   | 0.24        | 0/646          |
| 4   | e     | 0.13         | 0/479   | 0.43        | 1/646 (0.2%)   |
| 5   | F     | 0.13         | 0/1040  | 0.33        | 0/1408         |
| 5   | f     | 0.12         | 0/1040  | 0.34        | 0/1408         |
| 6   | G     | 0.12         | 0/638   | 0.38        | 0/858          |
| 6   | g     | 0.11         | 0/638   | 0.30        | 0/858          |
| 7   | H     | 0.11         | 0/804   | 0.29        | 0/1088         |
| 7   | h     | 0.12         | 0/804   | 0.36        | 0/1088         |
| 8   | J     | 0.14         | 0/3192  | 0.35        | 0/4354         |
| 8   | j     | 0.14         | 0/3192  | 0.35        | 0/4354         |
| 9   | K     | 0.14         | 0/4290  | 0.37        | 1/5857 (0.0%)  |
| 10  | L     | 0.13         | 0/2022  | 0.35        | 0/2751         |
| 10  | l     | 0.13         | 0/2022  | 0.32        | 0/2751         |
| 11  | M     | 0.11         | 0/396   | 0.30        | 0/533          |
| 12  | N     | 0.10         | 0/500   | 0.28        | 0/681          |
| 13  | O     | 0.11         | 0/2218  | 0.32        | 0/3036         |
| 14  | P     | 0.11         | 0/1941  | 0.32        | 0/2653         |
| 15  | Q     | 0.13         | 0/868   | 0.34        | 0/1174         |
| 16  | R     | 0.15         | 0/467   | 0.38        | 0/626          |
| 17  | S     | 0.10         | 0/962   | 0.26        | 0/1310         |
| 18  | T     | 0.11         | 0/932   | 0.33        | 1/1269 (0.1%)  |
| 19  | U     | 0.09         | 0/664   | 0.23        | 0/899          |
| 20  | V     | 0.09         | 0/332   | 0.28        | 0/452          |
| 21  | W     | 0.12         | 0/1074  | 0.31        | 0/1451         |
| All | All   | 0.12         | 0/46256 | 0.33        | 4/62823 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | e     | 56  | ILE  | N-CA-C  | -5.72 | 108.28      | 113.71   |
| 9   | K     | 437 | PRO  | CA-N-CD | -5.65 | 104.09      | 112.00   |
| 18  | T     | 145 | PRO  | CA-N-CD | -5.54 | 104.24      | 112.00   |
| 2   | B     | 68  | VAL  | N-CA-C  | -5.49 | 108.49      | 113.71   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3345  | 0        | 3323     | 75      | 0            |
| 1   | a     | 3345  | 0        | 3323     | 69      | 0            |
| 2   | B     | 2735  | 0        | 2774     | 69      | 0            |
| 2   | b     | 2735  | 0        | 2774     | 60      | 0            |
| 3   | C     | 1411  | 0        | 1386     | 54      | 0            |
| 3   | c     | 1411  | 0        | 1386     | 45      | 0            |
| 4   | E     | 465   | 0        | 459      | 7       | 0            |
| 4   | e     | 465   | 0        | 459      | 21      | 0            |
| 5   | F     | 1019  | 0        | 1034     | 27      | 0            |
| 5   | f     | 1019  | 0        | 1034     | 30      | 0            |
| 6   | G     | 624   | 0        | 583      | 18      | 0            |
| 6   | g     | 624   | 0        | 583      | 10      | 0            |
| 7   | H     | 773   | 0        | 736      | 21      | 0            |
| 7   | h     | 773   | 0        | 736      | 19      | 0            |
| 8   | J     | 3090  | 0        | 3129     | 102     | 0            |
| 8   | j     | 3090  | 0        | 3129     | 124     | 0            |
| 9   | K     | 4162  | 0        | 4192     | 151     | 0            |
| 10  | L     | 1961  | 0        | 1890     | 53      | 0            |
| 10  | l     | 1961  | 0        | 1890     | 66      | 0            |
| 11  | M     | 382   | 0        | 386      | 7       | 0            |
| 12  | N     | 484   | 0        | 517      | 9       | 0            |
| 13  | O     | 2146  | 0        | 2137     | 60      | 0            |
| 14  | P     | 1889  | 0        | 1866     | 82      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 15  | Q     | 851   | 0        | 822      | 28      | 0            |
| 16  | R     | 455   | 0        | 469      | 13      | 0            |
| 17  | S     | 928   | 0        | 906      | 17      | 0            |
| 18  | T     | 913   | 0        | 912      | 29      | 0            |
| 19  | U     | 642   | 0        | 586      | 11      | 0            |
| 20  | V     | 321   | 0        | 314      | 5       | 0            |
| 21  | W     | 1049  | 0        | 1030     | 33      | 0            |
| 22  | A     | 40    | 0        | 53       | 2       | 0            |
| 22  | C     | 43    | 0        | 62       | 1       | 0            |
| 22  | H     | 36    | 0        | 48       | 4       | 0            |
| 22  | J     | 136   | 0        | 167      | 2       | 0            |
| 22  | V     | 74    | 0        | 97       | 2       | 0            |
| 22  | a     | 40    | 0        | 53       | 1       | 0            |
| 22  | c     | 43    | 0        | 62       | 5       | 0            |
| 22  | j     | 136   | 0        | 167      | 6       | 0            |
| 23  | A     | 51    | 0        | 78       | 4       | 0            |
| 23  | C     | 51    | 0        | 78       | 1       | 0            |
| 23  | H     | 49    | 0        | 71       | 1       | 0            |
| 23  | L     | 51    | 0        | 78       | 0       | 0            |
| 23  | W     | 51    | 0        | 78       | 3       | 0            |
| 23  | a     | 51    | 0        | 78       | 2       | 0            |
| 23  | j     | 49    | 0        | 71       | 1       | 0            |
| 24  | C     | 4     | 0        | 0        | 2       | 0            |
| 24  | c     | 4     | 0        | 0        | 2       | 0            |
| 25  | E     | 47    | 0        | 71       | 0       | 0            |
| 25  | W     | 86    | 0        | 126      | 1       | 0            |
| 25  | c     | 47    | 0        | 71       | 1       | 0            |
| 26  | J     | 86    | 0        | 60       | 9       | 0            |
| 26  | L     | 43    | 0        | 30       | 6       | 0            |
| 26  | j     | 86    | 0        | 60       | 12      | 0            |
| 26  | l     | 43    | 0        | 30       | 13      | 0            |
| 27  | J     | 43    | 0        | 58       | 4       | 0            |
| 27  | j     | 43    | 0        | 58       | 4       | 0            |
| 28  | K     | 1     | 0        | 0        | 0       | 0            |
| 29  | K     | 120   | 0        | 108      | 23      | 0            |
| 30  | P     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 46624 | 0        | 46678    | 1178    | 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 13.

All (1178) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:161:HIS:HE1   | 3:C:181:HIS:ND1   | 1.62                     | 0.97              |
| 10:l:175:PRO:HD3  | 26:l:401:HEM:HAD2 | 1.52                     | 0.90              |
| 1:a:302:LEU:HB3   | 1:a:350:GLN:HG3   | 1.59                     | 0.84              |
| 2:B:52:ASN:HD22   | 2:B:82:LEU:HB2    | 1.42                     | 0.84              |
| 4:e:48:LEU:HD22   | 4:e:50:LYS:HZ3    | 1.42                     | 0.83              |
| 15:Q:82:VAL:H     | 16:R:6:ILE:HG21   | 1.41                     | 0.83              |
| 3:C:178:CYS:HB3   | 3:C:183:SER:H     | 1.45                     | 0.81              |
| 5:F:52:GLU:HG3    | 8:J:109:PRO:HG3   | 1.62                     | 0.81              |
| 4:e:48:LEU:HD23   | 4:e:49:TRP:H      | 1.46                     | 0.80              |
| 1:A:302:LEU:HB3   | 1:A:350:GLN:HG3   | 1.61                     | 0.80              |
| 3:C:161:HIS:CE1   | 3:C:181:HIS:ND1   | 2.51                     | 0.79              |
| 6:G:125:GLU:O     | 6:G:129:HIS:ND1   | 2.17                     | 0.77              |
| 8:J:68:ILE:HD12   | 8:J:72:VAL:HG11   | 1.66                     | 0.77              |
| 1:a:393:GLU:O     | 1:a:397:LYS:HB2   | 1.84                     | 0.77              |
| 5:F:117:LYS:HB2   | 2:b:66:LYS:HE2    | 1.66                     | 0.76              |
| 12:N:23:HIS:HB3   | 12:N:26:SER:HB3   | 1.68                     | 0.76              |
| 3:c:178:CYS:CB    | 24:c:301:FES:S1   | 2.73                     | 0.76              |
| 14:P:114:ALA:HB1  | 19:U:7:SER:HB2    | 1.67                     | 0.76              |
| 10:L:260:GLU:OE2  | 10:L:266:ARG:NH1  | 2.19                     | 0.75              |
| 8:j:345:GLU:OE1   | 10:l:62:MET:N     | 2.21                     | 0.74              |
| 10:L:100:VAL:HG22 | 26:L:401:HEM:HBB1 | 1.70                     | 0.73              |
| 2:B:54:PHE:HE2    | 2:B:114:PHE:HA    | 1.53                     | 0.73              |
| 9:K:371:TYR:OH    | 9:K:428:MET:SD    | 2.47                     | 0.73              |
| 1:A:211:THR:HG21  | 1:A:386:ASP:HB3   | 1.69                     | 0.73              |
| 1:A:62:GLU:HG3    | 1:A:176:LEU:HD11  | 1.70                     | 0.73              |
| 10:L:112:TRP:HE1  | 10:L:155:ILE:HG13 | 1.54                     | 0.72              |
| 10:l:225:MET:HB3  | 10:l:227:ARG:HH22 | 1.52                     | 0.72              |
| 3:c:117:PHE:N     | 3:c:155:MET:O     | 2.22                     | 0.72              |
| 8:J:14:ASN:HA     | 8:J:18:ILE:HB     | 1.72                     | 0.72              |
| 3:c:166:PRO:HB2   | 3:c:176:TRP:HB3   | 1.72                     | 0.71              |
| 1:A:166:SER:HA    | 1:A:175:SER:HB2   | 1.72                     | 0.71              |
| 21:W:53:LEU:O     | 21:W:57:GLN:NE2   | 2.25                     | 0.70              |
| 1:a:108:SER:OG    | 1:a:112:SER:OG    | 2.09                     | 0.70              |
| 8:J:51:ALA:HB2    | 26:J:403:HEM:HBC1 | 1.74                     | 0.70              |
| 2:B:255:VAL:HG23  | 2:B:321:THR:HG21  | 1.73                     | 0.69              |
| 5:F:120:LEU:HD23  | 2:b:66:LYS:HB3    | 1.74                     | 0.69              |
| 19:U:55:TYR:HA    | 19:U:59:CYS:HB3   | 1.75                     | 0.69              |
| 3:C:146:ARG:NH2   | 3:C:188:SER:O     | 2.25                     | 0.69              |
| 14:P:41:ASP:OD2   | 16:R:40:LYS:NZ    | 2.25                     | 0.69              |
| 16:R:6:ILE:HG22   | 16:R:7:THR:H      | 1.56                     | 0.69              |
| 1:A:248:GLU:HB3   | 7:H:28:ALA:HB3    | 1.74                     | 0.69              |
| 26:J:404:HEM:HBD1 | 26:J:404:HEM:HHA  | 1.73                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:529:THR:HG21  | 18:T:107:ARG:HH12 | 1.58                     | 0.69              |
| 10:L:87:HIS:HB3   | 10:L:90:ILE:HD12  | 1.73                     | 0.69              |
| 8:j:183:HIS:HE1   | 26:j:403:HEM:ND   | 1.91                     | 0.68              |
| 10:l:101:CYS:HB3  | 26:l:401:HEM:HAB  | 1.75                     | 0.68              |
| 8:J:169:PHE:HB2   | 3:c:112:GLN:HE22  | 1.59                     | 0.68              |
| 1:a:67:ASN:ND2    | 1:a:177:PRO:O     | 2.27                     | 0.68              |
| 9:K:125:THR:HG21  | 9:K:134:SER:HA    | 1.76                     | 0.68              |
| 29:K:603:HEA:H242 | 14:P:89:PRO:HB3   | 1.76                     | 0.68              |
| 14:P:118:LYS:HG2  | 14:P:178:VAL:HB   | 1.76                     | 0.68              |
| 1:a:216:HIS:HA    | 1:a:219:LEU:HD23  | 1.76                     | 0.67              |
| 2:b:28:ILE:O      | 2:b:191:ASN:ND2   | 2.22                     | 0.67              |
| 1:A:297:LEU:HD12  | 2:B:65:LEU:HB3    | 1.76                     | 0.67              |
| 6:G:129:HIS:HD2   | 10:L:69:LEU:HD23  | 1.59                     | 0.67              |
| 5:F:101:PRO:HB3   | 8:J:382:ARG:HH12  | 1.60                     | 0.67              |
| 9:K:142:PRO:HB3   | 13:O:41:MET:HG3   | 1.76                     | 0.67              |
| 2:b:26:THR:HB     | 2:b:191:ASN:HD21  | 1.59                     | 0.67              |
| 9:K:377:PHE:HB2   | 29:K:603:HEA:HMD2 | 1.76                     | 0.67              |
| 13:O:118:VAL:HG11 | 14:P:203:ARG:HG2  | 1.76                     | 0.67              |
| 1:a:169:PHE:HB2   | 1:a:175:SER:HB3   | 1.76                     | 0.67              |
| 8:J:139:MET:SD    | 8:J:256:ASN:ND2   | 2.67                     | 0.67              |
| 8:j:118:VAL:HG11  | 8:j:303:LEU:HD13  | 1.76                     | 0.67              |
| 9:K:291:HIS:CE1   | 29:K:603:HEA:HBD1 | 2.30                     | 0.67              |
| 1:A:169:PHE:HB2   | 1:A:175:SER:HB3   | 1.76                     | 0.66              |
| 2:b:34:LYS:HG2    | 2:b:88:THR:HG23   | 1.76                     | 0.66              |
| 14:P:215:GLY:H    | 14:P:238:ALA:HB3  | 1.60                     | 0.66              |
| 1:A:230:LEU:HG    | 1:A:231:GLN:HG3   | 1.78                     | 0.66              |
| 15:Q:106:ARG:NH2  | 21:W:76:SER:O     | 2.29                     | 0.66              |
| 8:j:281:ILE:HG23  | 8:j:295:MET:HE1   | 1.78                     | 0.66              |
| 2:B:59:THR:HG23   | 2:B:112:THR:HG21  | 1.76                     | 0.66              |
| 14:P:190:ILE:HD13 | 14:P:236:ILE:HD13 | 1.77                     | 0.66              |
| 10:l:76:TRP:HB2   | 10:l:79:ASN:HB2   | 1.77                     | 0.66              |
| 7:H:34:GLN:HE22   | 10:L:297:THR:HG21 | 1.60                     | 0.66              |
| 3:c:156:LEU:HD22  | 3:c:203:PRO:HD3   | 1.78                     | 0.66              |
| 7:h:62:PRO:HB3    | 8:j:328:ILE:HD13  | 1.78                     | 0.66              |
| 8:J:339:ILE:HD12  | 8:J:351:MET:HE3   | 1.78                     | 0.65              |
| 29:K:603:HEA:HBA2 | 29:K:603:HEA:HMA  | 1.79                     | 0.65              |
| 8:j:247:SER:HG    | 8:j:250:THR:HG1   | 1.43                     | 0.65              |
| 2:B:30:THR:HG22   | 2:B:92:THR:HG22   | 1.77                     | 0.65              |
| 3:C:59:MET:HE1    | 10:L:286:TRP:HE3  | 1.62                     | 0.65              |
| 6:g:107:ILE:O     | 6:g:111:GLN:NE2   | 2.30                     | 0.65              |
| 3:c:110:LYS:HA    | 3:c:115:PRO:HA    | 1.79                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:l:180:ILE:HD13 | 26:l:401:HEM:HMA1 | 1.78                     | 0.65              |
| 10:l:136:ASP:OD1  | 10:l:147:ARG:NH1  | 2.31                     | 0.64              |
| 1:a:37:VAL:HB     | 1:a:207:VAL:HG22  | 1.79                     | 0.64              |
| 14:P:36:ILE:HG22  | 14:P:103:LEU:HD21 | 1.79                     | 0.64              |
| 2:B:324:LYS:O     | 2:B:328:GLN:HG2   | 1.97                     | 0.64              |
| 9:K:374:VAL:HA    | 9:K:377:PHE:CE1   | 2.33                     | 0.64              |
| 3:C:165:VAL:HB    | 8:j:142:TRP:HE1   | 1.63                     | 0.63              |
| 5:F:75:ILE:HG23   | 8:J:212:ILE:HD12  | 1.79                     | 0.63              |
| 13:O:99:VAL:HG13  | 13:O:256:ILE:HG21 | 1.79                     | 0.63              |
| 8:J:241:ALA:HA    | 8:J:244:VAL:HG12  | 1.81                     | 0.63              |
| 5:f:47:ASP:OD2    | 5:f:74:ARG:NH1    | 2.32                     | 0.63              |
| 1:A:265:VAL:HG12  | 1:A:431:ILE:HG22  | 1.79                     | 0.63              |
| 9:K:148:ILE:HG21  | 9:K:211:LEU:HB2   | 1.80                     | 0.63              |
| 15:Q:100:ASP:O    | 15:Q:103:THR:OG1  | 2.16                     | 0.63              |
| 1:a:368:SER:HB2   | 2:b:75:GLY:HA2    | 1.80                     | 0.63              |
| 9:K:371:TYR:HB3   | 9:K:432:GLY:HA2   | 1.81                     | 0.63              |
| 14:P:177:PHE:HE1  | 14:P:195:ILE:HG21 | 1.63                     | 0.62              |
| 1:A:112:SER:HB2   | 1:A:115:LYS:HE2   | 1.81                     | 0.62              |
| 9:K:381:LEU:HB3   | 29:K:602:HEA:HAC  | 1.80                     | 0.62              |
| 8:j:310:ARG:O     | 8:j:375:ASN:ND2   | 2.33                     | 0.62              |
| 2:B:298:SER:OG    | 2:B:302:LYS:NZ    | 2.32                     | 0.62              |
| 8:J:29:TRP:HB3    | 8:J:99:LYS:HG3    | 1.81                     | 0.62              |
| 5:f:20:VAL:HG13   | 5:f:21:LEU:HD12   | 1.80                     | 0.62              |
| 2:B:62:ARG:NH1    | 2:B:67:LEU:O      | 2.32                     | 0.62              |
| 1:A:312:CYS:HA    | 1:A:334:THR:HG22  | 1.82                     | 0.62              |
| 8:j:148:THR:HG21  | 8:j:166:TRP:HE1   | 1.65                     | 0.62              |
| 15:Q:132:ARG:HH22 | 15:Q:140:LYS:HE2  | 1.65                     | 0.62              |
| 1:A:91:LEU:HD13   | 1:A:106:VAL:HG13  | 1.81                     | 0.62              |
| 9:K:441:PRO:HD2   | 14:P:230:ALA:HB2  | 1.82                     | 0.61              |
| 2:b:19:VAL:HG11   | 2:b:201:VAL:HG11  | 1.82                     | 0.61              |
| 13:O:163:ASN:O    | 13:O:164:ARG:NH1  | 2.33                     | 0.61              |
| 1:a:209:VAL:HG13  | 1:a:390:LEU:HD22  | 1.81                     | 0.61              |
| 1:A:155:ASP:OD2   | 1:A:158:ASN:ND2   | 2.33                     | 0.61              |
| 1:a:268:GLU:OE2   | 1:a:421:TRP:NE1   | 2.26                     | 0.61              |
| 8:j:123:LEU:HD13  | 8:j:193:MET:HE1   | 1.83                     | 0.61              |
| 14:P:166:SER:HB3  | 14:P:235:LYS:HE2  | 1.82                     | 0.61              |
| 2:b:150:THR:HG22  | 2:b:352:ASN:HD22  | 1.66                     | 0.61              |
| 8:J:111:VAL:O     | 8:J:115:ASN:ND2   | 2.33                     | 0.61              |
| 9:K:399:GLN:NE2   | 9:K:515:GLU:O     | 2.34                     | 0.61              |
| 14:P:187:ASP:OD2  | 14:P:222:SER:OG   | 2.19                     | 0.61              |
| 8:j:21:PRO:O      | 8:j:218:ARG:NH1   | 2.33                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:j:67:HIS:ND1    | 8:j:71:ASP:OD2    | 2.34                     | 0.61              |
| 8:j:287:ASP:HB2   | 8:j:290:LEU:HB2   | 1.83                     | 0.61              |
| 7:H:6:GLY:HA2     | 8:j:1:MET:HE1     | 1.82                     | 0.61              |
| 1:A:283:GLN:NE2   | 1:A:373:GLN:OE1   | 2.34                     | 0.61              |
| 14:P:57:MET:HE1   | 16:R:18:ILE:HA    | 1.83                     | 0.61              |
| 10:l:150:LYS:HD2  | 10:l:152:SER:H    | 1.66                     | 0.61              |
| 8:J:287:ASP:HB3   | 8:J:290:LEU:HB3   | 1.81                     | 0.61              |
| 26:J:403:HEM:HBC2 | 26:J:403:HEM:HHD  | 1.83                     | 0.61              |
| 9:K:503:ILE:HG13  | 15:Q:70:GLN:HG3   | 1.82                     | 0.61              |
| 1:A:268:GLU:OE2   | 1:A:421:TRP:NE1   | 2.31                     | 0.60              |
| 9:K:268:PHE:HE1   | 14:P:75:ILE:HG22  | 1.66                     | 0.60              |
| 14:P:39:LEU:HD13  | 14:P:103:LEU:HD22 | 1.82                     | 0.60              |
| 3:c:146:ARG:HH11  | 3:c:155:MET:HE3   | 1.66                     | 0.60              |
| 3:C:161:HIS:HB2   | 3:C:196:ALA:HB2   | 1.83                     | 0.60              |
| 18:T:143:LEU:HD23 | 18:T:145:PRO:HD3  | 1.84                     | 0.60              |
| 3:C:116:VAL:HG11  | 3:C:214:VAL:HG11  | 1.82                     | 0.60              |
| 26:J:404:HEM:HHC  | 26:J:404:HEM:HBB2 | 1.82                     | 0.60              |
| 9:K:11:ALA:O      | 9:K:81:ASN:ND2    | 2.35                     | 0.60              |
| 10:l:63:THR:HG22  | 10:l:65:ALA:H     | 1.67                     | 0.60              |
| 10:l:225:MET:HG2  | 26:l:401:HEM:C4C  | 2.36                     | 0.60              |
| 1:A:288:TYR:OH    | 1:A:307:GLN:NE2   | 2.33                     | 0.60              |
| 2:B:118:GLU:OE2   | 5:f:62:ARG:NH1    | 2.34                     | 0.60              |
| 8:J:126:ALA:O     | 8:J:130:LEU:HG    | 2.02                     | 0.60              |
| 8:J:290:LEU:HA    | 8:J:293:ILE:HG12  | 1.83                     | 0.60              |
| 9:K:346:PHE:O     | 9:K:349:THR:OG1   | 2.17                     | 0.60              |
| 9:K:368:HIS:CE1   | 14:P:196:LYS:HB3  | 2.36                     | 0.60              |
| 1:a:166:SER:HA    | 1:a:175:SER:HB2   | 1.83                     | 0.60              |
| 1:a:447:ARG:NH2   | 8:j:222:HIS:O     | 2.35                     | 0.60              |
| 21:W:72:VAL:HA    | 21:W:75:ILE:HG12  | 1.83                     | 0.60              |
| 2:b:21:ALA:HB2    | 2:b:197:LEU:HD13  | 1.84                     | 0.59              |
| 8:j:123:LEU:HD22  | 8:j:190:ILE:HD11  | 1.85                     | 0.59              |
| 8:j:123:LEU:HD21  | 8:j:186:VAL:HG22  | 1.84                     | 0.59              |
| 14:P:149:PRO:HD2  | 14:P:152:LEU:HB2  | 1.84                     | 0.59              |
| 9:K:244:VAL:CG1   | 29:K:603:HEA:HAC  | 2.32                     | 0.59              |
| 1:a:451:ASP:HA    | 22:a:501:PEF:HN2  | 1.67                     | 0.59              |
| 7:h:77:ASN:O      | 7:h:81:TYR:N      | 2.24                     | 0.59              |
| 8:j:88:PHE:HB3    | 8:j:236:PHE:HZ    | 1.68                     | 0.59              |
| 21:W:139:LYS:HG2  | 21:W:140:ASN:H    | 1.68                     | 0.59              |
| 8:J:266:PRO:HD2   | 8:J:269:ILE:HD11  | 1.85                     | 0.59              |
| 29:K:603:HEA:HHC  | 29:K:603:HEA:H122 | 1.84                     | 0.59              |
| 2:b:226:GLY:N     | 2:b:352:ASN:OD1   | 2.33                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:70:GLY:HA3    | 22:c:303:PEF:H142 | 1.84                     | 0.59              |
| 1:A:300:ILE:HG12  | 1:A:301:LYS:H     | 1.68                     | 0.58              |
| 23:A:502:PGT:H472 | 27:J:405:UQ6:H71  | 1.84                     | 0.58              |
| 9:K:175:ASN:ND2   | 18:T:83:THR:O     | 2.36                     | 0.58              |
| 15:Q:94:ALA:HA    | 15:Q:97:ARG:HD2   | 1.84                     | 0.58              |
| 7:h:92:VAL:HG11   | 8:j:346:VAL:HG11  | 1.84                     | 0.58              |
| 8:J:201:LEU:HD21  | 27:J:405:UQ6:H3M3 | 1.85                     | 0.58              |
| 13:O:139:LEU:HA   | 13:O:142:THR:HG22 | 1.84                     | 0.58              |
| 5:f:52:GLU:OE1    | 8:j:314:ARG:NH2   | 2.36                     | 0.58              |
| 8:j:124:THR:HA    | 8:j:127:THR:HG22  | 1.84                     | 0.58              |
| 9:K:430:PHE:HA    | 9:K:433:ILE:HG12  | 1.84                     | 0.58              |
| 13:O:74:THR:HA    | 13:O:239:HIS:HE2  | 1.68                     | 0.58              |
| 3:C:165:VAL:HB    | 8:j:142:TRP:NE1   | 2.18                     | 0.58              |
| 9:K:85:PRO:HB3    | 9:K:168:THR:HG21  | 1.86                     | 0.58              |
| 9:K:377:PHE:HA    | 9:K:380:VAL:HG22  | 1.86                     | 0.58              |
| 2:B:38:GLY:H      | 2:B:41:TYR:HD2    | 1.50                     | 0.58              |
| 2:b:222:LYS:NZ    | 2:b:223:PHE:O     | 2.36                     | 0.58              |
| 4:e:44:ASN:HB3    | 4:e:47:LYS:HE2    | 1.85                     | 0.58              |
| 13:O:226:ASN:O    | 13:O:230:MET:HG2  | 2.04                     | 0.58              |
| 8:J:320:VAL:HA    | 8:J:323:LYS:HE2   | 1.86                     | 0.58              |
| 8:j:349:VAL:HG13  | 8:j:350:LEU:HD12  | 1.86                     | 0.57              |
| 10:l:133:GLU:N    | 10:l:133:GLU:OE1  | 2.36                     | 0.57              |
| 2:b:230:ARG:HB3   | 2:b:359:VAL:HG21  | 1.85                     | 0.57              |
| 13:O:67:ARG:HB2   | 13:O:229:ARG:HH21 | 1.69                     | 0.57              |
| 1:a:447:ARG:HH21  | 8:j:220:PRO:HB2   | 1.69                     | 0.57              |
| 8:j:172:SER:O     | 8:j:175:THR:OG1   | 2.20                     | 0.57              |
| 2:B:230:ARG:NH2   | 2:B:363:PRO:O     | 2.37                     | 0.57              |
| 3:c:161:HIS:HA    | 3:c:196:ALA:HB2   | 1.87                     | 0.57              |
| 13:O:107:TRP:HA   | 13:O:110:PHE:HB3  | 1.87                     | 0.57              |
| 3:c:166:PRO:HA    | 3:c:178:CYS:HA    | 1.85                     | 0.57              |
| 14:P:200:THR:HB   | 14:P:203:ARG:HB2  | 1.87                     | 0.57              |
| 7:h:43:ASN:OD1    | 7:h:47:ASN:ND2    | 2.38                     | 0.57              |
| 14:P:155:GLU:HG3  | 21:W:131:LYS:HE2  | 1.85                     | 0.57              |
| 3:C:143:ASP:H     | 3:C:190:ARG:HH21  | 1.53                     | 0.57              |
| 9:K:134:SER:O     | 9:K:214:ARG:NH1   | 2.38                     | 0.57              |
| 16:R:36:PHE:CE2   | 16:R:40:LYS:HD2   | 2.40                     | 0.57              |
| 2:B:230:ARG:HH11  | 2:B:359:VAL:HG13  | 1.69                     | 0.57              |
| 8:J:80:TYR:O      | 8:J:84:ASN:ND2    | 2.27                     | 0.57              |
| 3:c:121:ARG:HG3   | 3:c:153:LEU:HB2   | 1.87                     | 0.56              |
| 5:f:7:SER:O       | 5:f:11:ILE:HG13   | 2.04                     | 0.56              |
| 8:J:127:THR:HA    | 8:J:130:LEU:HD12  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:310:MET:HG2   | 14:P:93:LEU:HD13  | 1.87                     | 0.56              |
| 3:C:159:CYS:SG    | 3:C:161:HIS:HB3   | 2.46                     | 0.56              |
| 5:F:43:LEU:HD21   | 5:F:78:ALA:HB2    | 1.88                     | 0.56              |
| 8:J:13:VAL:HG13   | 8:J:17:ILE:HD13   | 1.87                     | 0.56              |
| 8:J:57:ASN:O      | 8:J:61:ALA:N      | 2.38                     | 0.56              |
| 8:J:121:PHE:HA    | 8:J:124:THR:HG22  | 1.87                     | 0.56              |
| 21:W:83:ARG:HB2   | 21:W:83:ARG:NH1   | 2.20                     | 0.56              |
| 2:b:63:SER:HB3    | 2:b:67:LEU:HD23   | 1.86                     | 0.56              |
| 8:j:316:ASN:ND2   | 8:j:322:SER:OG    | 2.37                     | 0.56              |
| 2:B:46:GLY:HA3    | 2:B:161:TYR:HB2   | 1.88                     | 0.56              |
| 2:B:60:ASN:H      | 2:B:112:THR:HB    | 1.70                     | 0.56              |
| 14:P:186:HIS:ND1  | 14:P:232:MET:HE1  | 2.21                     | 0.56              |
| 15:Q:118:GLU:HB3  | 20:V:27:SER:HA    | 1.87                     | 0.56              |
| 8:j:118:VAL:O     | 8:j:122:ILE:HG12  | 2.05                     | 0.56              |
| 8:j:137:GLY:H     | 8:j:140:SER:HB3   | 1.71                     | 0.56              |
| 1:A:37:VAL:HB     | 1:A:207:VAL:HG12  | 1.88                     | 0.56              |
| 17:S:19:LYS:HD2   | 17:S:21:ALA:H     | 1.70                     | 0.56              |
| 2:b:195:ALA:HB1   | 2:b:199:ARG:HH12  | 1.70                     | 0.56              |
| 8:j:71:ASP:HA     | 10:l:113:ARG:HH21 | 1.71                     | 0.56              |
| 6:G:101:CYS:HA    | 6:G:104:ARG:HG2   | 1.88                     | 0.56              |
| 14:P:16:ASP:OD1   | 14:P:213:ARG:NH2  | 2.39                     | 0.56              |
| 2:B:66:LYS:HA     | 5:f:120:LEU:HD22  | 1.88                     | 0.56              |
| 1:A:311:LEU:HG    | 1:A:339:MET:HB3   | 1.88                     | 0.56              |
| 8:J:273:TRP:HA    | 8:J:276:LEU:HD23  | 1.88                     | 0.56              |
| 9:K:469:ILE:HA    | 9:K:472:LEU:HD12  | 1.87                     | 0.56              |
| 3:c:178:CYS:HB3   | 24:c:301:FES:S1   | 2.42                     | 0.56              |
| 4:e:48:LEU:HD23   | 4:e:49:TRP:N      | 2.17                     | 0.56              |
| 5:f:88:LEU:HB2    | 5:f:93:TRP:HE1    | 1.70                     | 0.56              |
| 2:B:206:LEU:HA    | 2:B:209:LEU:HD23  | 1.88                     | 0.56              |
| 8:J:130:LEU:HD13  | 8:J:182:LEU:HD13  | 1.88                     | 0.56              |
| 9:K:389:LEU:HD21  | 29:K:602:HEA:H253 | 1.87                     | 0.56              |
| 18:T:57:PRO:HG2   | 18:T:62:GLN:HB3   | 1.88                     | 0.56              |
| 3:c:109:VAL:O     | 3:c:116:VAL:N     | 2.36                     | 0.55              |
| 6:G:129:HIS:CD2   | 10:L:69:LEU:HD23  | 2.39                     | 0.55              |
| 14:P:174:HIS:HA   | 14:P:210:LEU:HB3  | 1.88                     | 0.55              |
| 1:a:211:THR:HG21  | 1:a:386:ASP:HB3   | 1.87                     | 0.55              |
| 2:B:52:ASN:ND2    | 2:B:82:LEU:HB2    | 2.18                     | 0.55              |
| 3:C:86:ALA:HA     | 3:C:89:LEU:HD12   | 1.88                     | 0.55              |
| 10:L:121:THR:HG23 | 10:L:122:ASN:H    | 1.70                     | 0.55              |
| 4:e:55:ARG:HG2    | 4:e:56:ILE:HG13   | 1.88                     | 0.55              |
| 8:j:88:PHE:HZ     | 8:j:243:PHE:HD2   | 1.54                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:315:GLY:O     | 8:J:319:LYS:NZ    | 2.40                     | 0.55              |
| 13:O:215:HIS:HA   | 13:O:218:MET:HE3  | 1.89                     | 0.55              |
| 22:c:303:PEF:H351 | 8:j:241:ALA:HB2   | 1.89                     | 0.55              |
| 13:O:131:ALA:HB3  | 13:O:201:TYR:HD2  | 1.72                     | 0.55              |
| 1:a:428:ASP:O     | 3:c:53:ARG:NH1    | 2.40                     | 0.55              |
| 2:b:309:LYS:O     | 2:b:347:LYS:NZ    | 2.40                     | 0.55              |
| 8:j:171:VAL:HA    | 8:j:175:THR:HG21  | 1.89                     | 0.55              |
| 6:G:90:GLU:HA     | 6:G:93:ALA:HB2    | 1.88                     | 0.54              |
| 1:a:362:GLU:HA    | 1:a:365:ARG:HG2   | 1.88                     | 0.54              |
| 5:f:3:GLN:HB2     | 8:j:310:ARG:HB3   | 1.89                     | 0.54              |
| 8:J:278:PHE:HA    | 8:J:281:ILE:HG22  | 1.89                     | 0.54              |
| 14:P:53:LEU:O     | 14:P:57:MET:HG2   | 2.08                     | 0.54              |
| 26:j:403:HEM:HHA  | 26:j:403:HEM:HBD1 | 1.88                     | 0.54              |
| 4:E:55:ARG:HH21   | 4:E:56:ILE:HG22   | 1.72                     | 0.54              |
| 13:O:243:TYR:HA   | 13:O:246:THR:HG22 | 1.89                     | 0.54              |
| 14:P:93:LEU:HA    | 14:P:96:ILE:HG12  | 1.89                     | 0.54              |
| 2:b:195:ALA:HB1   | 2:b:199:ARG:NH1   | 2.22                     | 0.54              |
| 3:C:162:LEU:HD13  | 8:j:146:VAL:HG13  | 1.88                     | 0.54              |
| 7:H:62:PRO:HB2    | 8:J:331:PHE:HD2   | 1.72                     | 0.54              |
| 8:J:38:LEU:HD23   | 8:J:233:VAL:HG21  | 1.89                     | 0.54              |
| 9:K:27:MET:HA     | 9:K:465:LEU:HD11  | 1.89                     | 0.54              |
| 13:O:138:PRO:HG2  | 13:O:265:TYR:HE1  | 1.72                     | 0.54              |
| 14:P:125:TYR:HE2  | 14:P:127:LYS:HZ1  | 1.55                     | 0.54              |
| 6:g:132:HIS:HB3   | 10:l:69:LEU:HD21  | 1.88                     | 0.54              |
| 9:K:19:PHE:CZ     | 29:K:602:HEA:H241 | 2.43                     | 0.54              |
| 9:K:306:THR:HA    | 9:K:309:THR:HG22  | 1.88                     | 0.54              |
| 2:b:256:LEU:HA    | 2:b:314:LEU:HD11  | 1.89                     | 0.54              |
| 8:j:57:ASN:HB2    | 8:j:60:LEU:HB2    | 1.90                     | 0.54              |
| 8:j:80:TYR:OH     | 10:l:182:LYS:NZ   | 2.39                     | 0.54              |
| 10:l:225:MET:HG2  | 26:l:401:HEM:NC   | 2.23                     | 0.54              |
| 9:K:19:PHE:HZ     | 29:K:602:HEA:H241 | 1.72                     | 0.54              |
| 10:L:281:TYR:O    | 10:L:285:ILE:HG12 | 2.07                     | 0.54              |
| 13:O:126:PRO:HG2  | 13:O:201:TYR:HE1  | 1.73                     | 0.54              |
| 2:b:62:ARG:NH2    | 2:b:107:ASP:OD2   | 2.41                     | 0.54              |
| 2:b:250:LEU:HD21  | 2:b:278:LYS:HE3   | 1.90                     | 0.54              |
| 8:j:301:VAL:HA    | 8:j:304:VAL:HG12  | 1.90                     | 0.54              |
| 9:K:34:LEU:HD22   | 9:K:462:THR:HG21  | 1.90                     | 0.54              |
| 2:B:358:ASP:OD2   | 2:B:361:ASN:ND2   | 2.40                     | 0.54              |
| 9:K:380:VAL:HB    | 29:K:603:HEA:HBC1 | 1.90                     | 0.54              |
| 10:L:92:ARG:HB3   | 10:L:236:TYR:HE2  | 1.72                     | 0.54              |
| 10:L:103:ALA:HA   | 10:L:158:PRO:HG2  | 1.89                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:120:ILE:HD12 | 14:P:180:THR:HG23 | 1.90                     | 0.54              |
| 8:j:160:ASP:OD1   | 8:j:164:TRP:NE1   | 2.41                     | 0.54              |
| 1:A:30:THR:O      | 1:A:31:GLN:NE2    | 2.41                     | 0.54              |
| 9:K:241:HIS:HB3   | 9:K:242:PRO:HD3   | 1.90                     | 0.54              |
| 5:f:95:LYS:HE3    | 5:f:96:ALA:H      | 1.72                     | 0.54              |
| 9:K:413:GLN:HE22  | 9:K:467:LEU:HB3   | 1.73                     | 0.54              |
| 9:K:498:VAL:HG23  | 9:K:499:GLU:HG2   | 1.89                     | 0.54              |
| 10:L:184:ARG:NH1  | 26:L:401:HEM:O2A  | 2.41                     | 0.53              |
| 3:c:166:PRO:HA    | 3:c:179:PRO:HD3   | 1.89                     | 0.53              |
| 1:A:209:VAL:HG21  | 1:A:387:ALA:HB1   | 1.90                     | 0.53              |
| 14:P:30:THR:HG23  | 14:P:33:GLN:H     | 1.73                     | 0.53              |
| 2:B:63:SER:HB2    | 2:B:66:LYS:HG2    | 1.90                     | 0.53              |
| 8:J:344:VAL:H     | 3:c:182:GLY:HA3   | 1.72                     | 0.53              |
| 2:b:146:LEU:HD21  | 2:b:242:GLY:HA3   | 1.89                     | 0.53              |
| 5:f:3:GLN:HE22    | 5:f:8:ILE:HG12    | 1.73                     | 0.53              |
| 8:J:183:HIS:NE2   | 26:J:403:HEM:NC   | 2.55                     | 0.53              |
| 9:K:403:LEU:HD12  | 9:K:479:GLY:HA3   | 1.90                     | 0.53              |
| 11:M:47:THR:HG23  | 11:M:51:LEU:HB3   | 1.90                     | 0.53              |
| 2:B:65:LEU:HD13   | 5:f:117:LYS:HZ2   | 1.73                     | 0.53              |
| 9:K:324:LEU:HD21  | 14:P:57:MET:HB3   | 1.89                     | 0.53              |
| 17:S:94:ARG:NH2   | 19:U:74:GLY:O     | 2.42                     | 0.53              |
| 1:a:150:ASP:OD2   | 1:a:154:ASN:ND2   | 2.42                     | 0.53              |
| 8:j:70:ARG:NH2    | 10:l:258:CYS:O    | 2.41                     | 0.53              |
| 8:j:197:HIS:CE1   | 26:j:404:HEM:NA   | 2.77                     | 0.53              |
| 2:B:232:ARG:NH2   | 2:b:162:ASP:OD2   | 2.41                     | 0.53              |
| 5:F:29:ALA:O      | 5:F:33:ILE:HG12   | 2.09                     | 0.53              |
| 6:g:106:LYS:NZ    | 6:g:122:ASP:OD1   | 2.42                     | 0.53              |
| 3:C:45:GLU:HB3    | 23:C:302:PGT:H62  | 1.91                     | 0.53              |
| 9:K:330:GLY:O     | 14:P:68:ASN:ND2   | 2.40                     | 0.53              |
| 14:P:190:ILE:HD12 | 14:P:195:ILE:HD11 | 1.91                     | 0.53              |
| 15:Q:60:PHE:CE1   | 15:Q:72:VAL:HG21  | 2.44                     | 0.53              |
| 26:j:403:HEM:HBC2 | 26:j:403:HEM:HHD  | 1.89                     | 0.53              |
| 2:B:70:GLU:OE2    | 2:B:100:TYR:OH    | 2.24                     | 0.53              |
| 5:F:55:ILE:HD11   | 5:F:110:ALA:HB1   | 1.91                     | 0.53              |
| 8:J:35:LEU:HD11   | 8:J:236:PHE:CD2   | 2.44                     | 0.53              |
| 9:K:202:VAL:HG12  | 9:K:235:LEU:HG    | 1.89                     | 0.53              |
| 2:b:313:ASP:OD1   | 2:b:314:LEU:N     | 2.41                     | 0.53              |
| 23:A:502:PGT:H62  | 8:J:4:ARG:HH22    | 1.73                     | 0.53              |
| 22:H:101:PEF:N    | 21:W:89:LYS:O     | 2.41                     | 0.53              |
| 8:J:40:LEU:O      | 8:J:44:ILE:HG12   | 2.09                     | 0.53              |
| 8:j:16:TYR:O      | 27:j:405:UQ6:O2   | 2.26                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:J:404:HEM:HHC  | 26:J:404:HEM:CBB  | 2.38                     | 0.53              |
| 14:P:158:LEU:H    | 14:P:162:ASP:HB2  | 1.73                     | 0.53              |
| 10:I:176:ASP:N    | 10:I:176:ASP:OD1  | 2.41                     | 0.53              |
| 9:K:148:ILE:HA    | 9:K:151:LEU:HD12  | 1.91                     | 0.52              |
| 10:L:119:SER:O    | 10:L:120:HIS:ND1  | 2.41                     | 0.52              |
| 18:T:100:ILE:HG21 | 18:T:107:ARG:HD2  | 1.90                     | 0.52              |
| 8:j:147:ILE:HA    | 8:j:150:LEU:HD23  | 1.89                     | 0.52              |
| 2:B:366:ASP:OD2   | 2:b:152:ARG:NH2   | 2.31                     | 0.52              |
| 13:O:84:ARG:HD3   | 13:O:239:HIS:HA   | 1.91                     | 0.52              |
| 8:j:29:TRP:HB3    | 8:j:99:LYS:HG3    | 1.90                     | 0.52              |
| 26:J:404:HEM:HBD1 | 26:J:404:HEM:CHA  | 2.40                     | 0.52              |
| 9:K:374:VAL:HB    | 9:K:438:ARG:HH11  | 1.75                     | 0.52              |
| 21:W:78:GLY:HA3   | 21:W:83:ARG:HH11  | 1.73                     | 0.52              |
| 8:j:26:ILE:HG23   | 8:j:30:TRP:HB2    | 1.90                     | 0.52              |
| 1:A:66:ASN:ND2    | 1:A:192:ASP:OD1   | 2.42                     | 0.52              |
| 15:Q:96:ARG:HE    | 15:Q:104:ALA:HB2  | 1.74                     | 0.52              |
| 3:c:177:PHE:CZ    | 3:c:182:GLY:HA2   | 2.44                     | 0.52              |
| 5:f:16:LEU:HD21   | 8:j:380:ILE:HG13  | 1.90                     | 0.52              |
| 10:I:235:GLU:H    | 10:I:241:PRO:HG2  | 1.75                     | 0.52              |
| 5:F:3:GLN:HB2     | 8:J:310:ARG:HB2   | 1.90                     | 0.52              |
| 12:N:22:ARG:NH2   | 13:O:72:GLU:OE2   | 2.43                     | 0.52              |
| 19:U:41:LYS:HE2   | 19:U:44:ASP:H     | 1.74                     | 0.52              |
| 1:A:375:GLY:O     | 1:A:379:GLU:HB2   | 2.10                     | 0.52              |
| 8:J:285:ILE:O     | 3:c:195:PRO:HB3   | 2.10                     | 0.52              |
| 10:I:101:CYS:HB3  | 26:I:401:HEM:CAB  | 2.39                     | 0.52              |
| 13:O:6:ARG:HA     | 13:O:9:HIS:CE1    | 2.45                     | 0.52              |
| 14:P:70:ILE:HD11  | 15:Q:78:SER:HA    | 1.91                     | 0.52              |
| 15:Q:62:GLU:OE2   | 18:T:93:THR:OG1   | 2.28                     | 0.52              |
| 5:f:3:GLN:NE2     | 5:f:7:SER:OG      | 2.43                     | 0.52              |
| 10:I:180:ILE:CD1  | 26:I:401:HEM:HAA2 | 2.39                     | 0.52              |
| 3:C:85:THR:OG1    | 3:C:87:ASP:OD1    | 2.26                     | 0.52              |
| 3:C:106:ASN:OD1   | 3:C:119:ARG:NH1   | 2.37                     | 0.52              |
| 8:J:249:ASN:O     | 10:L:182:LYS:NZ   | 2.38                     | 0.52              |
| 9:K:40:LEU:O      | 9:K:443:TYR:OH    | 2.26                     | 0.52              |
| 9:K:72:MET:O      | 9:K:76:ILE:HG12   | 2.10                     | 0.52              |
| 9:K:218:THR:HA    | 13:O:200:VAL:HG11 | 1.91                     | 0.52              |
| 13:O:212:HIS:HB3  | 13:O:257:TRP:HH2  | 1.75                     | 0.52              |
| 15:Q:137:VAL:HG12 | 15:Q:139:LEU:HD23 | 1.90                     | 0.52              |
| 1:A:61:ASN:ND2    | 1:A:235:LYS:HD2   | 2.25                     | 0.51              |
| 12:N:38:ALA:HB1   | 13:O:28:PHE:HE2   | 1.75                     | 0.51              |
| 14:P:81:ILE:HG22  | 14:P:85:TRP:CZ3   | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:225:CYS:H    | 14:P:229:HIS:HB2  | 1.75                     | 0.51              |
| 17:S:66:THR:HA    | 17:S:69:ASN:HD21  | 1.76                     | 0.51              |
| 5:f:87:LEU:HD23   | 7:h:50:ARG:HD2    | 1.92                     | 0.51              |
| 8:J:203:ILE:HG13  | 8:j:8:VAL:HG11    | 1.92                     | 0.51              |
| 1:a:323:LYS:NZ    | 1:a:324:ASP:OD1   | 2.41                     | 0.51              |
| 4:e:40:TYR:CE1    | 10:l:268:ARG:HB3  | 2.46                     | 0.51              |
| 2:B:117:HIS:HB3   | 5:f:62:ARG:HB3    | 1.93                     | 0.51              |
| 1:A:444:ASP:OD1   | 1:A:445:TYR:N     | 2.40                     | 0.51              |
| 2:B:265:SER:O     | 2:B:268:SER:OG    | 2.24                     | 0.51              |
| 9:K:192:THR:HG23  | 9:K:246:ILE:HA    | 1.92                     | 0.51              |
| 10:L:175:PRO:HB2  | 10:L:180:ILE:HD11 | 1.93                     | 0.51              |
| 10:l:218:PHE:HD1  | 10:l:219:PRO:HD2  | 1.75                     | 0.51              |
| 5:F:3:GLN:HG3     | 8:J:310:ARG:HD3   | 1.92                     | 0.51              |
| 8:J:249:ASN:HB2   | 10:L:182:LYS:HE2  | 1.91                     | 0.51              |
| 3:c:115:PRO:HG2   | 3:c:157:GLY:HA3   | 1.92                     | 0.51              |
| 10:l:225:MET:SD   | 26:l:401:HEM:C4D  | 3.04                     | 0.51              |
| 15:Q:83:PRO:HB2   | 15:Q:88:ILE:HG13  | 1.91                     | 0.51              |
| 1:a:125:ILE:HG13  | 1:a:126:GLN:H     | 1.76                     | 0.51              |
| 8:j:58:ILE:HG22   | 8:j:176:ILE:HD12  | 1.93                     | 0.51              |
| 1:A:71:ASN:ND2    | 1:A:178:THR:O     | 2.29                     | 0.51              |
| 1:A:113:THR:HG21  | 1:A:214:ILE:HG21  | 1.92                     | 0.51              |
| 8:J:46:THR:HG23   | 8:J:82:HIS:CE1    | 2.45                     | 0.51              |
| 9:K:36:ILE:HD11   | 9:K:58:LEU:HB2    | 1.93                     | 0.51              |
| 9:K:359:ALA:HB2   | 29:K:603:HEA:HMB3 | 1.92                     | 0.51              |
| 9:K:9:THR:HA      | 9:K:96:PRO:HB3    | 1.93                     | 0.51              |
| 9:K:11:ALA:HB1    | 9:K:81:ASN:HB2    | 1.92                     | 0.51              |
| 9:K:230:ILE:HD11  | 14:P:203:ARG:HD2  | 1.93                     | 0.51              |
| 14:P:147:VAL:HG11 | 14:P:231:ASN:HB2  | 1.92                     | 0.51              |
| 1:A:189:VAL:HG23  | 1:A:190:VAL:H     | 1.76                     | 0.51              |
| 3:C:59:MET:HE1    | 10:L:286:TRP:CE3  | 2.43                     | 0.51              |
| 9:K:228:ASP:OD2   | 9:K:228:ASP:N     | 2.44                     | 0.51              |
| 9:K:363:LEU:HD11  | 14:P:43:ILE:HD12  | 1.93                     | 0.51              |
| 14:P:116:THR:HG22 | 14:P:176:ARG:HB2  | 1.93                     | 0.51              |
| 1:A:252:ARG:HH21  | 7:H:21:GLN:HE21   | 1.59                     | 0.51              |
| 3:C:176:TRP:HB2   | 3:C:185:TYR:HB2   | 1.93                     | 0.51              |
| 8:J:117:GLY:O     | 26:J:404:HEM:HMC2 | 2.10                     | 0.51              |
| 8:J:142:TRP:HZ2   | 3:c:165:VAL:HB    | 1.76                     | 0.51              |
| 8:j:285:ILE:HD12  | 8:j:290:LEU:HB3   | 1.93                     | 0.51              |
| 9:K:4:ARG:HD2     | 11:M:31:LYS:HE3   | 1.93                     | 0.50              |
| 5:f:101:PRO:HB3   | 8:j:382:ARG:HH21  | 1.76                     | 0.50              |
| 8:j:271:PRO:HB3   | 8:j:275:LEU:HD22  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:44:ILE:O      | 8:J:48:ILE:HG12   | 2.12                     | 0.50              |
| 8:J:170:SER:HB3   | 3:c:112:GLN:NE2   | 2.26                     | 0.50              |
| 9:K:17:LEU:HD21   | 9:K:103:PHE:CE2   | 2.47                     | 0.50              |
| 9:K:409:LEU:HD23  | 9:K:412:ILE:HD11  | 1.93                     | 0.50              |
| 15:Q:83:PRO:HD3   | 15:Q:114:LYS:HE2  | 1.94                     | 0.50              |
| 18:T:98:ILE:HG12  | 18:T:141:TYR:CE1  | 2.46                     | 0.50              |
| 1:a:297:LEU:HB3   | 2:b:65:LEU:HD13   | 1.94                     | 0.50              |
| 8:J:146:VAL:HG13  | 3:c:162:LEU:HB3   | 1.93                     | 0.50              |
| 11:M:32:ASP:OD1   | 11:M:32:ASP:N     | 2.44                     | 0.50              |
| 10:l:200:ASP:OD1  | 10:l:200:ASP:N    | 2.44                     | 0.50              |
| 8:J:378:PHE:O     | 8:J:382:ARG:HG3   | 2.12                     | 0.50              |
| 23:a:502:PGT:H221 | 23:a:502:PGT:H432 | 1.92                     | 0.50              |
| 3:c:87:ASP:OD1    | 3:c:88:VAL:N      | 2.45                     | 0.50              |
| 8:j:201:LEU:CD1   | 26:j:404:HEM:HAA1 | 2.41                     | 0.50              |
| 2:B:202:ASP:OD1   | 2:B:203:GLU:N     | 2.44                     | 0.50              |
| 5:F:71:ARG:O      | 5:F:75:ILE:HG12   | 2.11                     | 0.50              |
| 9:K:63:ALA:HB2    | 29:K:602:HEA:HBD2 | 1.94                     | 0.50              |
| 9:K:517:LEU:HD13  | 18:T:123:TRP:HZ2  | 1.76                     | 0.50              |
| 14:P:147:VAL:HG21 | 14:P:231:ASN:HB2  | 1.94                     | 0.50              |
| 8:j:58:ILE:HG21   | 8:j:173:ASN:HA    | 1.93                     | 0.50              |
| 8:j:290:LEU:HA    | 8:j:293:ILE:HG12  | 1.93                     | 0.50              |
| 1:A:57:SER:HB3    | 1:A:200:HIS:HD2   | 1.76                     | 0.50              |
| 1:A:375:GLY:HA3   | 2:B:28:ILE:HG13   | 1.93                     | 0.50              |
| 6:G:114:TYR:HE2   | 6:G:117:LEU:HD13  | 1.76                     | 0.50              |
| 9:K:264:LYS:HE2   | 9:K:493:LYS:HD2   | 1.93                     | 0.50              |
| 10:L:93:GLY:HA2   | 10:L:96:VAL:HG12  | 1.94                     | 0.50              |
| 13:O:72:GLU:HB3   | 13:O:76:LEU:HD13  | 1.94                     | 0.50              |
| 15:Q:88:ILE:HG21  | 15:Q:111:LEU:HD21 | 1.94                     | 0.50              |
| 8:j:93:MET:HG3    | 26:j:404:HEM:HBB2 | 1.93                     | 0.50              |
| 1:A:363:VAL:HG21  | 1:A:415:VAL:HG12  | 1.92                     | 0.50              |
| 8:J:35:LEU:HD21   | 8:J:236:PHE:HB2   | 1.94                     | 0.50              |
| 13:O:213:PHE:O    | 13:O:217:VAL:HG23 | 2.12                     | 0.50              |
| 15:Q:109:GLU:OE1  | 15:Q:140:LYS:NZ   | 2.44                     | 0.50              |
| 10:l:126:ARG:HH12 | 10:l:151:LEU:HA   | 1.76                     | 0.50              |
| 3:C:159:CYS:HB3   | 3:C:163:GLY:H     | 1.75                     | 0.50              |
| 6:G:139:ALA:O     | 6:G:141:ARG:N     | 2.41                     | 0.50              |
| 8:J:62:PHE:HA     | 8:J:65:VAL:HG12   | 1.93                     | 0.50              |
| 9:K:120:GLU:HA    | 11:M:71:GLN:HE21  | 1.76                     | 0.50              |
| 14:P:126:TRP:CE2  | 14:P:232:MET:HE2  | 2.47                     | 0.50              |
| 14:P:186:HIS:CG   | 14:P:232:MET:HE1  | 2.46                     | 0.50              |
| 21:W:137:LYS:HD2  | 21:W:146:GLY:HA3  | 1.94                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:125:ILE:HG13  | 1:A:126:GLN:HG3   | 1.94                     | 0.49              |
| 1:A:247:SER:HA    | 7:H:29:VAL:HA     | 1.93                     | 0.49              |
| 9:K:339:LEU:HD13  | 9:K:414:PHE:CG    | 2.47                     | 0.49              |
| 14:P:16:ASP:HA    | 14:P:217:PHE:HD1  | 1.76                     | 0.49              |
| 3:c:159:CYS:SG    | 3:c:161:HIS:HB3   | 2.52                     | 0.49              |
| 7:h:37:LEU:HD12   | 7:h:40:ILE:HB     | 1.93                     | 0.49              |
| 10:l:223:ILE:HG22 | 10:l:225:MET:H    | 1.76                     | 0.49              |
| 2:B:83:ASP:OD1    | 2:B:84:ARG:N      | 2.41                     | 0.49              |
| 9:K:140:SER:OG    | 9:K:141:GLY:N     | 2.45                     | 0.49              |
| 10:L:147:ARG:NH1  | 10:L:148:PRO:O    | 2.45                     | 0.49              |
| 18:T:90:ARG:HG3   | 18:T:92:GLY:H     | 1.77                     | 0.49              |
| 8:j:14:ASN:HA     | 8:j:18:ILE:HB     | 1.94                     | 0.49              |
| 7:H:39:GLY:O      | 7:H:43:ASN:ND2    | 2.46                     | 0.49              |
| 9:K:262:TYR:HB3   | 9:K:338:MET:CE    | 2.42                     | 0.49              |
| 13:O:164:ARG:NE   | 18:T:54:GLY:O     | 2.39                     | 0.49              |
| 13:O:222:MET:HA   | 13:O:225:VAL:HG12 | 1.92                     | 0.49              |
| 15:Q:105:ILE:HG12 | 15:Q:139:LEU:HD22 | 1.94                     | 0.49              |
| 19:U:28:TRP:HE1   | 19:U:63:TRP:HZ3   | 1.60                     | 0.49              |
| 8:J:118:VAL:HG11  | 8:J:303:LEU:HG    | 1.94                     | 0.49              |
| 15:Q:128:LEU:HA   | 15:Q:131:VAL:HG22 | 1.93                     | 0.49              |
| 17:S:103:SER:OG   | 17:S:104:LYS:N    | 2.44                     | 0.49              |
| 2:b:30:THR:HG22   | 2:b:92:THR:HG22   | 1.94                     | 0.49              |
| 4:e:10:PHE:HA     | 4:e:13:ARG:HH22   | 1.77                     | 0.49              |
| 7:h:53:LYS:HA     | 7:h:56:PHE:CE1    | 2.47                     | 0.49              |
| 8:j:128:ALA:HB2   | 26:j:403:HEM:HMB1 | 1.93                     | 0.49              |
| 8:j:324:PHE:O     | 8:j:328:ILE:HG12  | 2.12                     | 0.49              |
| 22:j:406:PEF:H312 | 22:j:406:PEF:H141 | 1.93                     | 0.49              |
| 2:B:65:LEU:HD22   | 5:f:117:LYS:HZ3   | 1.77                     | 0.49              |
| 7:H:41:PHE:HZ     | 22:H:101:PEF:H392 | 1.77                     | 0.49              |
| 8:J:107:ARG:NH2   | 8:J:311:SER:O     | 2.40                     | 0.49              |
| 9:K:280:ILE:HD11  | 9:K:315:PRO:HB2   | 1.93                     | 0.49              |
| 9:K:291:HIS:ND1   | 29:K:603:HEA:O1D  | 2.45                     | 0.49              |
| 9:K:308:ALA:HA    | 9:K:311:ILE:HG22  | 1.95                     | 0.49              |
| 10:L:212:SER:OG   | 10:L:222:SER:OG   | 2.24                     | 0.49              |
| 14:P:163:THR:HG22 | 14:P:164:ASP:H    | 1.77                     | 0.49              |
| 1:a:97:ILE:HG13   | 1:a:102:GLN:HA    | 1.95                     | 0.49              |
| 2:b:247:LYS:HD2   | 2:b:336:ILE:HD11  | 1.94                     | 0.49              |
| 1:A:443:LEU:HD13  | 1:A:447:ARG:HG3   | 1.94                     | 0.49              |
| 3:C:74:THR:O      | 3:C:78:PHE:HD1    | 1.95                     | 0.49              |
| 8:J:245:PHE:O     | 10:L:266:ARG:NE   | 2.45                     | 0.49              |
| 8:J:354:ILE:O     | 8:J:358:ILE:HG12  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:181:THR:HG22  | 3:c:34:TYR:HD2    | 1.77                     | 0.49              |
| 2:b:251:ALA:HB2   | 2:b:338:LEU:HB3   | 1.95                     | 0.49              |
| 5:f:50:ALA:O      | 5:f:56:MET:HG3    | 2.12                     | 0.49              |
| 14:P:180:THR:HB   | 14:P:204:LEU:HD12 | 1.93                     | 0.49              |
| 7:h:50:ARG:HH12   | 7:h:51:ARG:HE     | 1.60                     | 0.49              |
| 8:j:241:ALA:HA    | 8:j:244:VAL:HG22  | 1.95                     | 0.49              |
| 5:F:62:ARG:NH1    | 2:b:118:GLU:OE2   | 2.45                     | 0.49              |
| 9:K:296:GLY:O     | 19:U:22:ASN:ND2   | 2.46                     | 0.49              |
| 1:a:297:LEU:HD22  | 2:b:65:LEU:HD22   | 1.95                     | 0.49              |
| 3:c:195:PRO:O     | 3:c:197:PRO:HD3   | 2.12                     | 0.49              |
| 2:B:188:SER:OG    | 2:B:189:GLY:N     | 2.44                     | 0.49              |
| 5:F:41:LEU:HB3    | 5:F:43:LEU:HD23   | 1.94                     | 0.49              |
| 7:H:62:PRO:HA     | 7:H:65:ILE:HG22   | 1.93                     | 0.49              |
| 9:K:294:ILE:HG13  | 9:K:368:HIS:CD2   | 2.48                     | 0.49              |
| 8:j:117:GLY:C     | 26:j:404:HEM:HBC2 | 2.38                     | 0.49              |
| 10:l:260:GLU:HB2  | 10:l:262:GLU:HG3  | 1.95                     | 0.49              |
| 1:A:73:TRP:CZ2    | 1:A:197:ALA:HB2   | 2.48                     | 0.49              |
| 2:B:54:PHE:HD1    | 2:B:123:VAL:HG11  | 1.77                     | 0.49              |
| 9:K:19:PHE:CZ     | 29:K:602:HEA:H251 | 2.48                     | 0.49              |
| 9:K:500:SER:HA    | 15:Q:106:ARG:NH2  | 2.28                     | 0.49              |
| 10:l:120:HIS:HB3  | 10:l:124:GLU:HG3  | 1.95                     | 0.49              |
| 5:F:88:LEU:HD23   | 5:F:92:GLU:HB3    | 1.95                     | 0.48              |
| 8:J:377:LEU:HA    | 8:J:380:ILE:HG22  | 1.94                     | 0.48              |
| 14:P:153:LEU:HD21 | 21:W:124:MET:HE3  | 1.93                     | 0.48              |
| 21:W:78:GLY:HA3   | 21:W:83:ARG:HD2   | 1.96                     | 0.48              |
| 1:a:443:LEU:HD13  | 1:a:447:ARG:HB3   | 1.95                     | 0.48              |
| 2:b:69:ARG:O      | 2:b:72:GLU:HG3    | 2.13                     | 0.48              |
| 10:l:107:LEU:HG   | 10:l:177:LEU:HB2  | 1.95                     | 0.48              |
| 1:A:149:GLN:O     | 1:A:153:GLU:HG3   | 2.12                     | 0.48              |
| 3:C:164:CYS:HB2   | 8:j:142:TRP:HD1   | 1.78                     | 0.48              |
| 7:H:36:PRO:HG2    | 10:L:286:TRP:CZ2  | 2.48                     | 0.48              |
| 8:J:343:HIS:HB3   | 3:c:182:GLY:HA3   | 1.95                     | 0.48              |
| 9:K:500:SER:N     | 15:Q:70:GLN:OE1   | 2.44                     | 0.48              |
| 9:K:533:GLN:HG3   | 18:T:121:ILE:HD13 | 1.94                     | 0.48              |
| 23:a:502:PGT:O1P  | 8:j:4:ARG:NH1     | 2.46                     | 0.48              |
| 5:f:47:ASP:OD1    | 5:f:71:ARG:NE     | 2.46                     | 0.48              |
| 1:A:239:LYS:HG2   | 21:W:42:PRO:HB3   | 1.94                     | 0.48              |
| 6:G:95:VAL:HB     | 6:G:127:PHE:HE1   | 1.77                     | 0.48              |
| 14:P:97:ALA:O     | 14:P:101:PHE:N    | 2.38                     | 0.48              |
| 14:P:171:VAL:HA   | 14:P:211:ILE:HG23 | 1.95                     | 0.48              |
| 19:U:33:ASP:N     | 19:U:33:ASP:OD1   | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:j:280:ALA:HB2   | 8:j:340:GLY:HA3   | 1.94                     | 0.48              |
| 10:l:193:SER:HA   | 10:l:196:THR:HG22 | 1.94                     | 0.48              |
| 8:J:141:HIS:NE2   | 8:J:171:VAL:HG21  | 2.29                     | 0.48              |
| 9:K:225:GLY:HA2   | 17:S:98:PHE:HE1   | 1.77                     | 0.48              |
| 1:a:265:VAL:HG22  | 1:a:431:ILE:HG22  | 1.95                     | 0.48              |
| 8:j:139:MET:HB3   | 8:j:269:ILE:HD12  | 1.95                     | 0.48              |
| 1:A:34:ASN:HB3    | 1:A:223:ILE:HD12  | 1.95                     | 0.48              |
| 1:A:224:GLU:HB2   | 1:A:227:ASN:HB2   | 1.96                     | 0.48              |
| 5:F:47:ASP:OD2    | 5:F:102:TYR:OH    | 2.30                     | 0.48              |
| 9:K:330:GLY:HA2   | 14:P:71:ALA:HA    | 1.95                     | 0.48              |
| 13:O:143:ILE:HG12 | 17:S:67:ALA:HB2   | 1.96                     | 0.48              |
| 16:R:6:ILE:HG22   | 16:R:7:THR:N      | 2.27                     | 0.48              |
| 2:b:55:ASN:HD21   | 2:b:89:LEU:HD11   | 1.78                     | 0.48              |
| 3:c:161:HIS:CD2   | 3:c:195:PRO:HD2   | 2.49                     | 0.48              |
| 7:h:61:ILE:O      | 7:h:65:ILE:HG23   | 2.13                     | 0.48              |
| 9:K:24:PHE:HA     | 9:K:27:MET:HE2    | 1.94                     | 0.48              |
| 1:a:356:ILE:HD12  | 1:a:457:TRP:CZ3   | 2.48                     | 0.48              |
| 8:j:330:VAL:HG21  | 22:j:401:PEF:H361 | 1.95                     | 0.48              |
| 2:B:40:ARG:HG3    | 2:B:155:LEU:HA    | 1.94                     | 0.48              |
| 3:C:56:ALA:O      | 3:C:60:VAL:HG23   | 2.14                     | 0.48              |
| 3:C:146:ARG:HB3   | 3:C:202:ILE:HG13  | 1.96                     | 0.48              |
| 8:J:124:THR:HA    | 8:J:127:THR:HG22  | 1.95                     | 0.48              |
| 1:a:430:ASP:OD1   | 1:a:430:ASP:N     | 2.46                     | 0.48              |
| 5:f:13:ASP:OD1    | 5:f:17:LYS:NZ     | 2.46                     | 0.48              |
| 8:j:43:GLN:OE1    | 8:j:82:HIS:ND1    | 2.46                     | 0.48              |
| 1:A:252:ARG:HH21  | 7:H:21:GLN:NE2    | 2.11                     | 0.48              |
| 5:F:69:TYR:OH     | 7:H:22:LYS:NZ     | 2.46                     | 0.48              |
| 8:J:282:LEU:HB2   | 8:J:295:MET:HE3   | 1.96                     | 0.48              |
| 10:L:173:LEU:HD23 | 10:L:173:LEU:H    | 1.78                     | 0.48              |
| 3:c:133:ASP:OD1   | 3:c:133:ASP:N     | 2.44                     | 0.48              |
| 3:C:162:LEU:HD12  | 3:C:181:HIS:CE1   | 2.49                     | 0.48              |
| 5:F:27:PRO:HA     | 5:F:30:ASN:HD21   | 1.79                     | 0.48              |
| 9:K:534:SER:HB3   | 18:T:88:SER:HB3   | 1.96                     | 0.48              |
| 13:O:208:GLY:O    | 13:O:212:HIS:ND1  | 2.47                     | 0.48              |
| 2:B:270:LEU:HD23  | 2:B:270:LEU:H     | 1.77                     | 0.47              |
| 3:C:74:THR:O      | 3:C:77:THR:OG1    | 2.24                     | 0.47              |
| 8:J:327:PHE:HA    | 8:J:330:VAL:HG12  | 1.96                     | 0.47              |
| 9:K:496:ASP:HB3   | 9:K:498:VAL:HG22  | 1.96                     | 0.47              |
| 10:L:177:LEU:HA   | 10:L:180:ILE:HG12 | 1.96                     | 0.47              |
| 13:O:235:LEU:HD11 | 13:O:241:VAL:H    | 1.79                     | 0.47              |
| 21:W:109:LEU:HA   | 21:W:112:VAL:HG22 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:47:LYS:HG3    | 10:l:86:ASP:HA    | 1.95                     | 0.47              |
| 1:A:170:GLN:HB2   | 1:A:245:LEU:HD21  | 1.95                     | 0.47              |
| 9:K:509:VAL:HG12  | 18:T:123:TRP:HH2  | 1.79                     | 0.47              |
| 10:L:243:THR:HG23 | 10:L:246:GLN:HG2  | 1.95                     | 0.47              |
| 13:O:10:GLN:HG2   | 18:T:80:VAL:HB    | 1.96                     | 0.47              |
| 18:T:34:ALA:HB1   | 18:T:68:ARG:HH22  | 1.79                     | 0.47              |
| 1:a:189:VAL:HG23  | 1:a:190:VAL:H     | 1.78                     | 0.47              |
| 3:C:126:ILE:O     | 3:C:130:ASN:ND2   | 2.47                     | 0.47              |
| 6:G:124:VAL:HG21  | 10:L:204:ALA:HB3  | 1.96                     | 0.47              |
| 8:J:227:PHE:HD1   | 10:L:291:LYS:HD2  | 1.79                     | 0.47              |
| 29:K:602:HEA:H271 | 29:K:602:HEA:H212 | 1.69                     | 0.47              |
| 13:O:71:ALA:O     | 13:O:75:TYR:HB3   | 2.14                     | 0.47              |
| 14:P:177:PHE:O    | 14:P:206:GLN:HA   | 2.15                     | 0.47              |
| 15:Q:60:PHE:HE1   | 15:Q:72:VAL:HG21  | 1.79                     | 0.47              |
| 1:A:341:ASP:OD1   | 23:A:502:PGT:O5   | 2.32                     | 0.47              |
| 8:J:91:MET:O      | 8:J:95:MET:HG3    | 2.14                     | 0.47              |
| 15:Q:93:ARG:HD2   | 15:Q:94:ALA:N     | 2.29                     | 0.47              |
| 21:W:41:MET:HE2   | 21:W:46:GLN:HG3   | 1.95                     | 0.47              |
| 1:a:444:ASP:OD1   | 1:a:445:TYR:N     | 2.42                     | 0.47              |
| 3:C:79:ILE:O      | 3:C:83:THR:HG23   | 2.14                     | 0.47              |
| 9:K:307:SER:HA    | 9:K:310:MET:SD    | 2.55                     | 0.47              |
| 9:K:408:LYS:HD2   | 21:W:94:PHE:HD2   | 1.80                     | 0.47              |
| 13:O:156:HIS:ND1  | 13:O:246:THR:O    | 2.47                     | 0.47              |
| 2:b:150:THR:HG22  | 2:b:352:ASN:ND2   | 2.28                     | 0.47              |
| 3:c:126:ILE:O     | 3:c:130:ASN:ND2   | 2.46                     | 0.47              |
| 8:j:201:LEU:HD11  | 26:j:404:HEM:HAA1 | 1.97                     | 0.47              |
| 10:l:126:ARG:HH22 | 10:l:151:LEU:N    | 2.12                     | 0.47              |
| 10:l:175:PRO:HG2  | 26:l:401:HEM:HAA1 | 1.95                     | 0.47              |
| 1:A:105:ILE:HG21  | 1:A:384:VAL:HG12  | 1.96                     | 0.47              |
| 9:K:10:ASN:HB3    | 9:K:524:VAL:HG12  | 1.95                     | 0.47              |
| 13:O:89:LEU:O     | 13:O:93:MET:HG2   | 2.15                     | 0.47              |
| 5:f:63:LEU:HD12   | 5:f:64:PRO:HD2    | 1.97                     | 0.47              |
| 8:j:122:ILE:HD12  | 8:j:299:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:301:LYS:HB2   | 1:A:350:GLN:NE2   | 2.30                     | 0.47              |
| 2:B:255:VAL:HG11  | 2:B:343:VAL:HG11  | 1.96                     | 0.47              |
| 3:C:33:THR:HG23   | 7:H:25:THR:HG21   | 1.96                     | 0.47              |
| 22:C:303:PEF:H432 | 22:C:303:PEF:H371 | 1.96                     | 0.47              |
| 8:J:57:ASN:OD1    | 8:J:177:GLN:NE2   | 2.47                     | 0.47              |
| 8:J:285:ILE:HG13  | 8:J:294:THR:HG21  | 1.96                     | 0.47              |
| 9:K:39:GLU:HG3    | 9:K:48:LEU:HD12   | 1.96                     | 0.47              |
| 13:O:254:ASP:OD1  | 13:O:255:VAL:N    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:a:457:TRP:HD1   | 4:e:14:ASN:HB2    | 1.80                     | 0.47              |
| 10:l:82:PHE:CE2   | 10:l:271:LEU:HD11 | 2.50                     | 0.47              |
| 8:j:339:ILE:HD11  | 8:j:348:TYR:CD1   | 2.49                     | 0.47              |
| 22:j:406:PEF:H111 | 22:j:406:PEF:H142 | 1.70                     | 0.47              |
| 2:B:66:LYS:HG3    | 2:B:67:LEU:HG     | 1.96                     | 0.47              |
| 3:C:183:SER:OG    | 24:C:301:FES:S1   | 2.65                     | 0.47              |
| 29:K:603:HEA:H211 | 29:K:603:HEA:H271 | 1.80                     | 0.47              |
| 14:P:115:MET:SD   | 14:P:175:ILE:HG22 | 2.55                     | 0.47              |
| 21:W:126:LYS:HG3  | 21:W:150:VAL:HG11 | 1.96                     | 0.47              |
| 3:C:96:VAL:HG22   | 3:C:109:VAL:HG11  | 1.96                     | 0.47              |
| 5:F:63:LEU:HD11   | 5:F:103:LEU:HD12  | 1.97                     | 0.47              |
| 9:K:340:TYR:CE1   | 9:K:414:PHE:HB2   | 2.50                     | 0.47              |
| 9:K:440:ILE:HG23  | 14:P:230:ALA:HB1  | 1.96                     | 0.47              |
| 13:O:136:GLU:HB3  | 17:S:74:GLU:HG2   | 1.95                     | 0.47              |
| 8:j:50:MET:HE1    | 8:j:68:ILE:HG21   | 1.96                     | 0.47              |
| 2:B:353:TYR:HB3   | 2:B:365:LEU:HD12  | 1.95                     | 0.46              |
| 3:C:181:HIS:CD2   | 8:j:282:LEU:HD22  | 2.50                     | 0.46              |
| 8:J:60:LEU:O      | 8:J:64:SER:N      | 2.38                     | 0.46              |
| 9:K:129:VAL:HG23  | 9:K:232:TYR:HE2   | 1.80                     | 0.46              |
| 14:P:217:PHE:HD2  | 14:P:236:ILE:HD11 | 1.80                     | 0.46              |
| 21:W:79:GLU:O     | 21:W:84:ARG:NH1   | 2.47                     | 0.46              |
| 1:a:353:ARG:HA    | 1:a:356:ILE:HG22  | 1.97                     | 0.46              |
| 6:g:82:ARG:HH12   | 6:g:139:ALA:HB2   | 1.80                     | 0.46              |
| 6:g:107:ILE:C     | 6:g:111:GLN:HE22  | 2.23                     | 0.46              |
| 1:A:158:ASN:O     | 1:A:162:GLU:HG2   | 2.15                     | 0.46              |
| 1:A:447:ARG:NH2   | 8:J:18:ILE:O      | 2.49                     | 0.46              |
| 2:B:225:LEU:HA    | 2:B:352:ASN:HD21  | 1.79                     | 0.46              |
| 5:F:95:LYS:HB2    | 5:F:98:GLU:HG2    | 1.96                     | 0.46              |
| 6:G:145:LYS:O     | 6:G:147:LYS:NZ    | 2.35                     | 0.46              |
| 8:J:80:TYR:HB3    | 8:J:244:VAL:HG23  | 1.97                     | 0.46              |
| 9:K:2:VAL:HG22    | 9:K:6:LEU:HG      | 1.97                     | 0.46              |
| 9:K:397:SER:OG    | 9:K:398:PRO:HD3   | 2.15                     | 0.46              |
| 13:O:106:PHE:HA   | 13:O:109:TYR:CZ   | 2.50                     | 0.46              |
| 18:T:66:LEU:HD23  | 18:T:66:LEU:H     | 1.80                     | 0.46              |
| 7:h:30:SER:O      | 7:h:32:TYR:N      | 2.48                     | 0.46              |
| 27:j:405:UQ6:H272 | 27:j:405:UQ6:H311 | 1.69                     | 0.46              |
| 3:C:159:CYS:HB2   | 3:C:164:CYS:O     | 2.16                     | 0.46              |
| 4:E:26:PHE:O      | 4:E:29:GLN:HG2    | 2.14                     | 0.46              |
| 9:K:521:PRO:O     | 11:M:33:GLY:HA3   | 2.15                     | 0.46              |
| 3:c:162:LEU:HG    | 3:c:181:HIS:HE1   | 1.79                     | 0.46              |
| 25:c:302:PCF:H461 | 25:c:302:PCF:H282 | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:j:327:PHE:HA    | 8:j:330:VAL:HG12  | 1.96                     | 0.46              |
| 6:G:121:GLU:HB3   | 7:H:86:ARG:HH11   | 1.81                     | 0.46              |
| 8:J:58:ILE:HD12   | 8:J:58:ILE:H      | 1.80                     | 0.46              |
| 2:b:270:LEU:HG    | 2:b:304:ILE:HD11  | 1.98                     | 0.46              |
| 3:c:85:THR:OG1    | 3:c:86:ALA:N      | 2.47                     | 0.46              |
| 7:h:76:TYR:HD2    | 8:j:347:PRO:HG3   | 1.81                     | 0.46              |
| 8:j:129:PHE:HE2   | 8:j:147:ILE:HB    | 1.80                     | 0.46              |
| 1:A:431:ILE:HG21  | 1:A:452:MET:HE1   | 1.97                     | 0.46              |
| 7:H:62:PRO:HB2    | 8:J:331:PHE:CD2   | 2.50                     | 0.46              |
| 8:J:36:LEU:HG     | 8:J:92:VAL:HG13   | 1.96                     | 0.46              |
| 9:K:374:VAL:HA    | 9:K:377:PHE:CD1   | 2.50                     | 0.46              |
| 9:K:386:ILE:HG21  | 29:K:602:HEA:H262 | 1.96                     | 0.46              |
| 1:a:344:ILE:HG21  | 1:a:448:ILE:HG13  | 1.98                     | 0.46              |
| 3:C:158:ILE:HG13  | 3:C:163:GLY:HA2   | 1.97                     | 0.46              |
| 9:K:368:HIS:NE2   | 14:P:196:LYS:O    | 2.44                     | 0.46              |
| 9:K:409:LEU:HD13  | 9:K:471:ILE:HG12  | 1.96                     | 0.46              |
| 10:l:262:GLU:OE1  | 10:l:266:ARG:HB3  | 2.16                     | 0.46              |
| 1:A:121:ASN:O     | 1:A:125:ILE:HG12  | 2.16                     | 0.46              |
| 9:K:408:LYS:HA    | 21:W:95:ILE:HD11  | 1.97                     | 0.46              |
| 10:L:76:TRP:H     | 10:L:79:ASN:HD21  | 1.64                     | 0.46              |
| 12:N:31:TYR:HB3   | 12:N:32:PRO:HD3   | 1.98                     | 0.46              |
| 1:A:356:ILE:HD12  | 1:A:457:TRP:NE1   | 2.30                     | 0.46              |
| 27:J:405:UQ6:H172 | 27:J:405:UQ6:H151 | 1.60                     | 0.46              |
| 9:K:442:ASP:OD1   | 9:K:442:ASP:N     | 2.46                     | 0.46              |
| 13:O:140:LEU:O    | 13:O:144:ILE:HG12 | 2.16                     | 0.46              |
| 2:b:104:ALA:O     | 2:b:108:VAL:HG23  | 2.15                     | 0.46              |
| 10:l:264:ASP:OD1  | 10:l:264:ASP:N    | 2.49                     | 0.46              |
| 2:B:33:VAL:HG23   | 2:B:187:VAL:HG22  | 1.97                     | 0.46              |
| 2:B:255:VAL:HA    | 2:B:321:THR:HG21  | 1.98                     | 0.46              |
| 10:L:284:SER:HA   | 10:L:287:VAL:HG12 | 1.98                     | 0.46              |
| 8:j:273:TRP:HA    | 8:j:276:LEU:HD23  | 1.98                     | 0.46              |
| 10:l:122:ASN:O    | 10:l:126:ARG:HG2  | 2.15                     | 0.46              |
| 2:B:270:LEU:HD12  | 2:B:300:ASN:HB3   | 1.98                     | 0.46              |
| 3:C:79:ILE:O      | 3:C:83:THR:N      | 2.49                     | 0.46              |
| 3:C:119:ARG:HE    | 3:C:187:ILE:HD11  | 1.81                     | 0.46              |
| 5:F:51:GLU:HG3    | 5:F:71:ARG:HH21   | 1.81                     | 0.46              |
| 10:L:105:HIS:CE1  | 26:L:401:HEM:NA   | 2.82                     | 0.46              |
| 1:a:341:ASP:OD1   | 1:a:342:ASP:N     | 2.48                     | 0.46              |
| 6:g:94:LEU:HD12   | 6:g:98:TYR:CE2    | 2.51                     | 0.46              |
| 8:j:257:TYR:HB3   | 10:l:179:LEU:HD23 | 1.97                     | 0.46              |
| 10:l:97:TYR:CZ    | 10:l:107:LEU:HD12 | 2.51                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:164:CYS:HB2  | 8:j:142:TRP:CD1   | 2.51                     | 0.45              |
| 3:C:169:GLU:N    | 3:C:175:GLY:O     | 2.49                     | 0.45              |
| 3:C:186:ASP:OD1  | 3:C:190:ARG:N     | 2.49                     | 0.45              |
| 7:H:39:GLY:HA2   | 22:H:101:PEF:H31  | 1.98                     | 0.45              |
| 9:K:413:GLN:O    | 9:K:417:ILE:HD12  | 2.16                     | 0.45              |
| 17:S:85:LYS:O    | 17:S:123:ARG:NH1  | 2.49                     | 0.45              |
| 1:a:183:GLU:HA   | 1:a:186:GLU:HG3   | 1.98                     | 0.45              |
| 1:a:300:ILE:HG12 | 1:a:301:LYS:H     | 1.81                     | 0.45              |
| 8:j:182:LEU:O    | 8:j:186:VAL:HG12  | 2.16                     | 0.45              |
| 10:l:91:ARG:NH2  | 10:l:119:SER:O    | 2.49                     | 0.45              |
| 1:A:431:ILE:O    | 1:A:445:TYR:OH    | 2.32                     | 0.45              |
| 2:B:54:PHE:CE2   | 2:B:114:PHE:HA    | 2.42                     | 0.45              |
| 2:B:117:HIS:HB3  | 5:f:62:ARG:HD3    | 1.97                     | 0.45              |
| 3:C:143:ASP:OD1  | 3:C:146:ARG:NH2   | 2.49                     | 0.45              |
| 5:F:3:GLN:NE2    | 5:F:7:SER:OG      | 2.50                     | 0.45              |
| 13:O:18:MET:O    | 13:O:20:SER:N     | 2.49                     | 0.45              |
| 1:a:224:GLU:OE1  | 1:a:226:LYS:NZ    | 2.49                     | 0.45              |
| 2:b:60:ASN:ND2   | 2:b:112:THR:O     | 2.46                     | 0.45              |
| 5:f:34:ASN:HA    | 5:f:39:LYS:HD3    | 1.97                     | 0.45              |
| 8:j:191:ALA:HA   | 8:j:194:VAL:HG12  | 1.99                     | 0.45              |
| 9:K:380:VAL:HB   | 29:K:603:HEA:CBC  | 2.47                     | 0.45              |
| 13:O:133:GLN:H   | 17:S:81:ARG:HH22  | 1.64                     | 0.45              |
| 14:P:45:PHE:O    | 14:P:49:VAL:HG13  | 2.16                     | 0.45              |
| 16:R:24:LEU:HD21 | 20:V:42:GLN:HG2   | 1.99                     | 0.45              |
| 18:T:63:GLU:HB2  | 18:T:68:ARG:HB3   | 1.98                     | 0.45              |
| 21:W:37:ARG:HG3  | 21:W:40:ASN:HB2   | 1.98                     | 0.45              |
| 21:W:79:GLU:H    | 21:W:83:ARG:HD2   | 1.82                     | 0.45              |
| 4:e:9:THR:O      | 4:e:13:ARG:NH1    | 2.46                     | 0.45              |
| 2:B:233:PHE:HB3  | 2:B:357:GLY:HA2   | 1.99                     | 0.45              |
| 3:C:83:THR:HG22  | 8:j:164:TRP:CD1   | 2.52                     | 0.45              |
| 14:P:146:TYR:H   | 14:P:164:ASP:HB2  | 1.82                     | 0.45              |
| 14:P:193:LEU:HB3 | 14:P:195:ILE:HG12 | 1.99                     | 0.45              |
| 21:W:83:ARG:HB2  | 21:W:83:ARG:HH11  | 1.81                     | 0.45              |
| 2:B:267:LEU:HD22 | 2:B:304:ILE:HG12  | 1.98                     | 0.45              |
| 3:C:155:MET:SD   | 3:C:200:LEU:HB2   | 2.57                     | 0.45              |
| 9:K:493:LYS:NZ   | 9:K:510:LYS:H     | 2.14                     | 0.45              |
| 10:L:136:ASP:HB3 | 10:L:147:ARG:HB3  | 1.98                     | 0.45              |
| 14:P:124:TRP:HE1 | 14:P:226:GLY:HA3  | 1.80                     | 0.45              |
| 15:Q:55:ARG:O    | 15:Q:58:LYS:HG3   | 2.16                     | 0.45              |
| 1:a:311:LEU:O    | 1:a:334:THR:OG1   | 2.26                     | 0.45              |
| 8:j:35:LEU:HD13  | 8:j:233:VAL:HA    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:18:VAL:O      | 4:E:21:ILE:HG22   | 2.17                     | 0.45              |
| 9:K:262:TYR:HB3   | 9:K:338:MET:HE1   | 1.99                     | 0.45              |
| 9:K:500:SER:HB2   | 9:K:503:ILE:HG12  | 1.98                     | 0.45              |
| 10:L:276:ILE:HG23 | 10:L:277:LEU:HD22 | 1.99                     | 0.45              |
| 14:P:41:ASP:HA    | 14:P:44:MET:HG2   | 1.98                     | 0.45              |
| 18:T:134:CYS:HB3  | 18:T:138:GLY:H    | 1.81                     | 0.45              |
| 5:f:5:PHE:HE2     | 8:j:312:VAL:HG21  | 1.82                     | 0.45              |
| 8:j:30:TRP:NE1    | 26:j:404:HEM:O1D  | 2.50                     | 0.45              |
| 8:j:121:PHE:O     | 8:j:125:ILE:HG12  | 2.17                     | 0.45              |
| 10:L:86:ASP:OD1   | 10:L:86:ASP:N     | 2.50                     | 0.45              |
| 7:h:62:PRO:HB2    | 8:j:331:PHE:CD2   | 2.52                     | 0.45              |
| 8:j:257:TYR:HB2   | 10:l:183:ALA:HB2  | 1.98                     | 0.45              |
| 8:J:305:LEU:HD22  | 8:J:363:PHE:HE2   | 1.82                     | 0.45              |
| 27:J:405:UQ6:H322 | 27:J:405:UQ6:H301 | 1.77                     | 0.45              |
| 9:K:374:VAL:HG23  | 9:K:377:PHE:CZ    | 2.52                     | 0.45              |
| 1:a:202:LEU:HG    | 1:a:231:GLN:HB3   | 1.98                     | 0.45              |
| 5:f:62:ARG:NH1    | 5:f:109:GLU:OE2   | 2.50                     | 0.45              |
| 8:j:35:LEU:HD11   | 8:j:236:PHE:CD1   | 2.52                     | 0.45              |
| 1:A:425:ARG:HA    | 1:A:425:ARG:HD2   | 1.85                     | 0.45              |
| 8:J:38:LEU:O      | 8:J:42:ILE:HG12   | 2.17                     | 0.45              |
| 10:L:218:PHE:HD2  | 10:L:223:ILE:HD11 | 1.82                     | 0.45              |
| 14:P:77:HIS:ND1   | 14:P:79:GLN:HG3   | 2.32                     | 0.45              |
| 1:A:57:SER:OG     | 1:A:205:ASN:ND2   | 2.50                     | 0.45              |
| 8:J:116:VAL:O     | 8:J:120:ILE:HG13  | 2.17                     | 0.45              |
| 8:J:352:GLY:O     | 8:J:356:THR:HG23  | 2.17                     | 0.45              |
| 9:K:52:SER:OG     | 14:P:227:THR:O    | 2.30                     | 0.45              |
| 9:K:54:LEU:O      | 9:K:58:LEU:HD12   | 2.16                     | 0.45              |
| 21:W:128:TRP:HZ3  | 21:W:131:LYS:HZ1  | 1.64                     | 0.45              |
| 1:a:443:LEU:HD13  | 1:a:447:ARG:HD2   | 1.99                     | 0.45              |
| 2:b:132:ALA:O     | 2:b:136:GLN:HG2   | 2.17                     | 0.45              |
| 3:c:111:TRP:CZ2   | 3:c:215:GLY:HA2   | 2.52                     | 0.45              |
| 3:c:154:ILE:HD13  | 3:c:212:VAL:HG11  | 1.98                     | 0.45              |
| 8:j:40:LEU:HD12   | 8:j:89:PHE:CZ     | 2.51                     | 0.45              |
| 8:j:107:ARG:HA    | 8:j:107:ARG:HD3   | 1.70                     | 0.45              |
| 1:A:61:ASN:HD21   | 1:A:235:LYS:HD2   | 1.82                     | 0.44              |
| 8:J:316:ASN:HD21  | 8:J:322:SER:HB3   | 1.83                     | 0.44              |
| 2:b:152:ARG:O     | 2:b:154:GLY:N     | 2.40                     | 0.44              |
| 8:j:23:PRO:HG2    | 8:j:26:ILE:HD11   | 1.98                     | 0.44              |
| 10:l:175:PRO:HD2  | 26:l:401:HEM:HAA1 | 2.00                     | 0.44              |
| 2:B:33:VAL:HG11   | 2:B:105:LEU:HD21  | 1.98                     | 0.44              |
| 9:K:32:MET:HE1    | 9:K:58:LEU:O      | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:112:TRP:NE1  | 10:L:155:ILE:HG13 | 2.27                     | 0.44              |
| 11:M:56:PHE:HA    | 11:M:59:ILE:HG12  | 1.98                     | 0.44              |
| 13:O:219:LEU:O    | 13:O:222:MET:HG3  | 2.17                     | 0.44              |
| 18:T:106:TYR:O    | 18:T:107:ARG:NE   | 2.50                     | 0.44              |
| 8:j:145:THR:HA    | 8:j:148:THR:HG22  | 1.99                     | 0.44              |
| 1:A:416:LYS:HD2   | 1:A:416:LYS:HA    | 1.78                     | 0.44              |
| 23:H:102:PGT:H202 | 23:H:102:PGT:H172 | 1.87                     | 0.44              |
| 9:K:380:VAL:HG23  | 9:K:381:LEU:HD22  | 2.00                     | 0.44              |
| 16:R:12:ARG:HG2   | 16:R:16:MET:HE3   | 2.00                     | 0.44              |
| 3:C:62:ALA:HA     | 3:C:65:LEU:HD12   | 1.98                     | 0.44              |
| 3:C:143:ASP:N     | 3:C:190:ARG:HH21  | 2.16                     | 0.44              |
| 8:J:30:TRP:HD1    | 26:J:404:HEM:CBA  | 2.30                     | 0.44              |
| 9:K:333:ARG:O     | 9:K:338:MET:HG3   | 2.16                     | 0.44              |
| 10:L:104:CYS:SG   | 26:L:401:HEM:HMC3 | 2.57                     | 0.44              |
| 13:O:253:LEU:HG   | 13:O:257:TRP:CD1  | 2.52                     | 0.44              |
| 14:P:90:ALA:O     | 14:P:93:LEU:HG    | 2.18                     | 0.44              |
| 18:T:124:LEU:HG   | 18:T:141:TYR:HE2  | 1.82                     | 0.44              |
| 21:W:91:ASP:O     | 21:W:95:ILE:HG12  | 2.18                     | 0.44              |
| 8:j:123:LEU:HD22  | 8:j:190:ILE:CD1   | 2.47                     | 0.44              |
| 10:l:95:GLN:HE22  | 10:l:234:VAL:HG13 | 1.82                     | 0.44              |
| 8:J:278:PHE:O     | 8:J:281:ILE:HG22  | 2.17                     | 0.44              |
| 9:K:108:MET:HE1   | 13:O:34:ALA:HB2   | 2.00                     | 0.44              |
| 9:K:134:SER:O     | 9:K:134:SER:OG    | 2.30                     | 0.44              |
| 9:K:339:LEU:HD12  | 9:K:340:TYR:N     | 2.32                     | 0.44              |
| 10:L:121:THR:HG23 | 10:L:122:ASN:N    | 2.33                     | 0.44              |
| 18:T:79:ASP:OD1   | 18:T:79:ASP:N     | 2.50                     | 0.44              |
| 4:e:41:GLU:HG2    | 4:e:50:LYS:NZ     | 2.32                     | 0.44              |
| 10:l:236:TYR:CD2  | 10:l:241:PRO:HG3  | 2.52                     | 0.44              |
| 5:F:88:LEU:HB3    | 5:F:92:GLU:HG2    | 1.99                     | 0.44              |
| 2:b:65:LEU:HD11   | 2:b:66:LYS:HE3    | 2.00                     | 0.44              |
| 23:j:408:PGT:H412 | 23:j:408:PGT:H161 | 2.00                     | 0.44              |
| 10:l:121:THR:OG1  | 10:l:122:ASN:N    | 2.47                     | 0.44              |
| 10:l:281:TYR:O    | 10:l:285:ILE:HG12 | 2.18                     | 0.44              |
| 2:B:70:GLU:O      | 2:B:74:LEU:N      | 2.49                     | 0.44              |
| 3:C:108:VAL:HB    | 8:j:263:LEU:HD13  | 2.00                     | 0.44              |
| 8:J:97:MET:HE1    | 8:J:121:PHE:CG    | 2.53                     | 0.44              |
| 13:O:33:LEU:HB2   | 13:O:58:LEU:HD13  | 1.99                     | 0.44              |
| 13:O:115:SER:O    | 13:O:115:SER:OG   | 2.30                     | 0.44              |
| 1:a:282:ALA:HB2   | 1:a:328:TRP:HE1   | 1.83                     | 0.44              |
| 3:c:180:CYS:HB2   | 3:c:181:HIS:CD2   | 2.53                     | 0.44              |
| 2:B:226:GLY:N     | 2:B:352:ASN:OD1   | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:42:GLY:HA2    | 5:F:94:ILE:HG12   | 1.99                     | 0.44              |
| 8:J:95:MET:HE2    | 8:J:95:MET:HB3    | 1.88                     | 0.44              |
| 8:J:132:TYR:CZ    | 8:J:140:SER:HA    | 2.53                     | 0.44              |
| 2:B:79:LYS:HE3    | 2:B:79:LYS:HB3    | 1.76                     | 0.44              |
| 9:K:17:LEU:HD21   | 9:K:103:PHE:CZ    | 2.52                     | 0.44              |
| 10:L:173:LEU:O    | 26:L:401:HEM:HAD1 | 2.18                     | 0.44              |
| 1:a:66:ASN:HD21   | 1:a:192:ASP:CG    | 2.26                     | 0.44              |
| 2:B:152:ARG:O     | 2:B:154:GLY:N     | 2.43                     | 0.43              |
| 7:H:84:ALA:HB1    | 7:H:88:GLU:HB3    | 1.99                     | 0.43              |
| 8:J:369:VAL:O     | 8:J:373:ILE:HG12  | 2.18                     | 0.43              |
| 12:N:17:LYS:HD2   | 12:N:17:LYS:HA    | 1.84                     | 0.43              |
| 15:Q:88:ILE:HD13  | 15:Q:111:LEU:HD21 | 1.99                     | 0.43              |
| 18:T:96:ASP:OD1   | 18:T:96:ASP:N     | 2.50                     | 0.43              |
| 1:a:320:LEU:HD12  | 1:a:327:LEU:HD23  | 2.00                     | 0.43              |
| 9:K:323:TRP:CE3   | 9:K:345:LEU:HD11  | 2.53                     | 0.43              |
| 1:a:238:LEU:H     | 1:a:238:LEU:HD23  | 1.83                     | 0.43              |
| 4:e:48:LEU:CD2    | 4:e:49:TRP:H      | 2.25                     | 0.43              |
| 10:l:105:HIS:HE1  | 26:l:401:HEM:C4D  | 2.32                     | 0.43              |
| 10:l:213:ASN:OD1  | 10:l:226:ALA:HA   | 2.18                     | 0.43              |
| 2:B:315:SER:C     | 2:B:317:ALA:H     | 2.26                     | 0.43              |
| 3:C:35:ARG:HH11   | 3:C:35:ARG:HG2    | 1.83                     | 0.43              |
| 9:K:59:VAL:HG13   | 29:K:602:HEA:HBA1 | 1.99                     | 0.43              |
| 13:O:85:LYS:HA    | 13:O:85:LYS:HD3   | 1.78                     | 0.43              |
| 14:P:167:MET:HB2  | 14:P:236:ILE:HG22 | 2.00                     | 0.43              |
| 17:S:95:ASP:OD1   | 17:S:95:ASP:N     | 2.50                     | 0.43              |
| 1:a:297:LEU:HD13  | 2:b:65:LEU:HD22   | 2.00                     | 0.43              |
| 2:b:19:VAL:HG23   | 2:b:198:LYS:NZ    | 2.33                     | 0.43              |
| 4:e:42:ASN:O      | 4:e:45:LYS:NZ     | 2.48                     | 0.43              |
| 10:l:130:GLU:HA   | 10:l:148:PRO:CB   | 2.48                     | 0.43              |
| 1:A:214:ILE:HD12  | 1:A:218:ASP:HB2   | 1.99                     | 0.43              |
| 2:B:239:ALA:HB3   | 2:B:301:ILE:HG21  | 2.01                     | 0.43              |
| 22:J:407:PEF:H142 | 22:J:407:PEF:H111 | 1.73                     | 0.43              |
| 9:K:347:LEU:HB3   | 9:K:383:MET:HE3   | 2.01                     | 0.43              |
| 9:K:358:LEU:HD11  | 9:K:373:VAL:HG12  | 2.00                     | 0.43              |
| 9:K:450:TRP:HA    | 9:K:453:VAL:HG22  | 1.99                     | 0.43              |
| 12:N:46:LEU:HD23  | 12:N:46:LEU:H     | 1.83                     | 0.43              |
| 13:O:37:THR:O     | 13:O:40:THR:OG1   | 2.27                     | 0.43              |
| 16:R:38:MET:HA    | 16:R:41:ILE:HG22  | 2.00                     | 0.43              |
| 1:a:447:ARG:HH12  | 8:j:222:HIS:HB3   | 1.83                     | 0.43              |
| 2:b:83:ASP:CG     | 2:b:84:ARG:H      | 2.25                     | 0.43              |
| 14:P:126:TRP:HB3  | 14:P:128:TYR:HE1  | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:U:53:LYS:HA    | 19:U:56:ASN:HB3   | 2.00                     | 0.43              |
| 20:V:57:VAL:O     | 20:V:61:SER:OG    | 2.31                     | 0.43              |
| 22:c:303:PEF:H412 | 8:j:237:MET:HG3   | 2.00                     | 0.43              |
| 4:e:49:TRP:HZ2    | 10:l:121:THR:HA   | 1.84                     | 0.43              |
| 1:A:391:GLY:HA2   | 1:A:394:VAL:HG12  | 2.00                     | 0.43              |
| 9:K:53:GLN:O      | 9:K:57:VAL:HG23   | 2.19                     | 0.43              |
| 9:K:240:GLY:O     | 9:K:244:VAL:N     | 2.47                     | 0.43              |
| 13:O:143:ILE:HD12 | 13:O:146:LEU:HD12 | 2.01                     | 0.43              |
| 15:Q:132:ARG:O    | 15:Q:136:GLY:N    | 2.52                     | 0.43              |
| 16:R:39:ASP:HA    | 16:R:42:ASN:ND2   | 2.33                     | 0.43              |
| 18:T:68:ARG:HA    | 18:T:71:LEU:HG    | 2.00                     | 0.43              |
| 22:V:101:PEF:H152 | 22:V:101:PEF:H121 | 1.80                     | 0.43              |
| 2:b:66:LYS:H      | 2:b:66:LYS:HD2    | 1.83                     | 0.43              |
| 10:l:146:LYS:HB2  | 10:l:146:LYS:HE3  | 1.83                     | 0.43              |
| 4:E:52:VAL:O      | 4:E:56:ILE:HG12   | 2.18                     | 0.43              |
| 9:K:243:GLU:HA    | 9:K:246:ILE:HD12  | 1.99                     | 0.43              |
| 14:P:56:TRP:CD1   | 16:R:21:GLY:HA2   | 2.54                     | 0.43              |
| 14:P:193:LEU:HD23 | 14:P:195:ILE:HD13 | 2.00                     | 0.43              |
| 1:a:125:ILE:HG13  | 1:a:126:GLN:N     | 2.33                     | 0.43              |
| 2:b:195:ALA:HB1   | 2:b:199:ARG:NH2   | 2.34                     | 0.43              |
| 6:g:76:ASP:N      | 6:g:76:ASP:OD1    | 2.52                     | 0.43              |
| 7:h:88:GLU:O      | 7:h:92:VAL:HG23   | 2.18                     | 0.43              |
| 8:j:3:PHE:HA      | 8:j:6:SER:HB3     | 2.01                     | 0.43              |
| 1:A:29:VAL:HG21   | 1:A:400:LYS:HE3   | 2.00                     | 0.43              |
| 2:B:45:ASP:OD1    | 2:B:45:ASP:N      | 2.52                     | 0.43              |
| 5:F:88:LEU:HG     | 5:F:89:PRO:HD2    | 2.00                     | 0.43              |
| 6:G:94:LEU:HA     | 6:G:97:HIS:HE1    | 1.84                     | 0.43              |
| 9:K:112:CYS:HB2   | 9:K:146:LEU:HD22  | 2.01                     | 0.43              |
| 9:K:344:PHE:CE1   | 9:K:384:GLY:HA2   | 2.53                     | 0.43              |
| 13:O:4:LEU:HD23   | 13:O:8:ARG:HD3    | 2.00                     | 0.43              |
| 18:T:82:ASP:OD1   | 18:T:82:ASP:N     | 2.50                     | 0.43              |
| 18:T:93:THR:OG1   | 18:T:94:MET:N     | 2.50                     | 0.43              |
| 1:a:447:ARG:HH22  | 8:j:222:HIS:HB3   | 1.84                     | 0.43              |
| 1:a:455:MET:SD    | 1:a:455:MET:N     | 2.91                     | 0.43              |
| 4:e:32:PHE:O      | 4:e:36:ILE:HG12   | 2.19                     | 0.43              |
| 6:g:87:ASN:ND2    | 6:g:90:GLU:OE1    | 2.39                     | 0.43              |
| 7:h:58:TYR:CE2    | 8:j:323:LYS:HD2   | 2.54                     | 0.43              |
| 8:j:132:TYR:O     | 8:j:135:VAL:HG22  | 2.19                     | 0.43              |
| 8:j:201:LEU:O     | 8:j:205:GLY:N     | 2.33                     | 0.43              |
| 2:B:146:LEU:HD21  | 2:B:242:GLY:HA3   | 2.00                     | 0.43              |
| 3:C:117:PHE:CE2   | 3:C:157:GLY:HA2   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:7:SER:O       | 5:F:11:ILE:HG13   | 2.19                     | 0.43              |
| 7:H:63:ALA:HB2    | 8:J:331:PHE:CZ    | 2.54                     | 0.43              |
| 9:K:248:ILE:HG13  | 29:K:603:HEA:HBC2 | 1.99                     | 0.43              |
| 9:K:342:ILE:HD12  | 14:P:58:LEU:HD11  | 2.01                     | 0.43              |
| 14:P:46:TYR:O     | 14:P:49:VAL:HG22  | 2.18                     | 0.43              |
| 15:Q:125:LEU:O    | 15:Q:128:LEU:HG   | 2.19                     | 0.43              |
| 18:T:122:MET:HE2  | 18:T:122:MET:HB2  | 1.97                     | 0.43              |
| 4:e:40:TYR:CD1    | 10:l:268:ARG:HB3  | 2.54                     | 0.43              |
| 8:j:34:SER:OG     | 27:j:405:UQ6:O5   | 2.27                     | 0.43              |
| 8:j:88:PHE:HB3    | 8:j:236:PHE:CZ    | 2.50                     | 0.43              |
| 10:l:97:TYR:OH    | 10:l:107:LEU:HB2  | 2.19                     | 0.43              |
| 10:l:235:GLU:N    | 10:l:241:PRO:HG2  | 2.32                     | 0.43              |
| 1:A:252:ARG:HB3   | 1:A:252:ARG:NH1   | 2.33                     | 0.43              |
| 8:J:362:TYR:HA    | 8:J:366:ILE:HG22  | 2.00                     | 0.43              |
| 2:b:247:LYS:HE2   | 2:b:281:ASP:HA    | 2.01                     | 0.43              |
| 3:c:106:ASN:OD1   | 3:c:119:ARG:NH1   | 2.44                     | 0.43              |
| 5:f:13:ASP:O      | 5:f:17:LYS:HD3    | 2.18                     | 0.43              |
| 8:j:82:HIS:HE1    | 26:j:403:HEM:NC   | 2.17                     | 0.43              |
| 2:B:60:ASN:N      | 2:B:112:THR:HB    | 2.33                     | 0.42              |
| 7:H:12:TRP:H      | 7:H:15:HIS:CD2    | 2.37                     | 0.42              |
| 8:J:187:PRO:HA    | 8:J:190:ILE:HB    | 2.01                     | 0.42              |
| 8:J:329:PHE:HE1   | 8:J:359:TYR:CD1   | 2.36                     | 0.42              |
| 14:P:77:HIS:HD1   | 14:P:79:GLN:HG3   | 1.83                     | 0.42              |
| 8:j:297:ALA:O     | 8:j:301:VAL:HG13  | 2.18                     | 0.42              |
| 1:A:280:LEU:O     | 1:A:284:ILE:HG13  | 2.19                     | 0.42              |
| 2:B:302:LYS:HZ2   | 2:B:363:PRO:HG3   | 1.84                     | 0.42              |
| 3:C:161:HIS:CE1   | 3:C:181:HIS:CG    | 3.07                     | 0.42              |
| 1:a:357:SER:HA    | 1:a:419:LYS:HE2   | 2.01                     | 0.42              |
| 1:a:407:PHE:HA    | 1:a:410:ILE:HG22  | 2.01                     | 0.42              |
| 2:b:181:THR:O     | 2:b:185:LEU:HG    | 2.19                     | 0.42              |
| 2:b:281:ASP:OD1   | 2:b:281:ASP:N     | 2.52                     | 0.42              |
| 22:c:303:PEF:H401 | 8:j:42:ILE:HG21   | 2.00                     | 0.42              |
| 8:j:22:GLN:HB2    | 8:j:225:PHE:CE2   | 2.54                     | 0.42              |
| 2:B:44:LYS:HD2    | 2:B:167:VAL:HG12  | 2.01                     | 0.42              |
| 4:E:49:TRP:CE3    | 4:E:52:VAL:HG21   | 2.54                     | 0.42              |
| 8:J:1:MET:HA      | 8:J:5:LYS:HG3     | 2.01                     | 0.42              |
| 15:Q:102:PRO:HG3  | 21:W:72:VAL:HG13  | 2.01                     | 0.42              |
| 1:a:67:ASN:HB3    | 1:a:180:GLY:HA2   | 2.02                     | 0.42              |
| 1:a:138:GLU:O     | 1:a:142:LYS:HG2   | 2.19                     | 0.42              |
| 2:b:255:VAL:HG11  | 2:b:343:VAL:HG11  | 2.01                     | 0.42              |
| 2:b:353:TYR:HE1   | 2:b:355:ALA:HB2   | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:e:52:VAL:HG13   | 10:l:88:ALA:HA    | 2.00                     | 0.42              |
| 1:A:141:LYS:NZ    | 1:A:186:GLU:HA    | 2.34                     | 0.42              |
| 1:A:356:ILE:HD12  | 1:A:457:TRP:CD1   | 2.54                     | 0.42              |
| 8:J:102:TYR:OH    | 22:J:401:PEF:O2P  | 2.34                     | 0.42              |
| 8:J:132:TYR:O     | 8:J:140:SER:HB2   | 2.19                     | 0.42              |
| 10:L:150:LYS:HG2  | 10:L:153:ASP:HB2  | 2.02                     | 0.42              |
| 14:P:31:PRO:HA    | 14:P:34:GLU:HG2   | 2.01                     | 0.42              |
| 1:a:447:ARG:NH2   | 8:j:220:PRO:HB2   | 2.32                     | 0.42              |
| 10:l:263:HIS:O    | 10:l:266:ARG:HG2  | 2.20                     | 0.42              |
| 1:A:395:LEU:HD23  | 1:A:395:LEU:HA    | 1.88                     | 0.42              |
| 6:G:125:GLU:HG2   | 6:G:126:GLU:N     | 2.34                     | 0.42              |
| 8:J:42:ILE:O      | 8:J:46:THR:HG22   | 2.19                     | 0.42              |
| 8:J:235:LEU:HD12  | 10:L:281:TYR:CZ   | 2.55                     | 0.42              |
| 14:P:163:THR:HG22 | 14:P:164:ASP:N    | 2.33                     | 0.42              |
| 21:W:97:LYS:HE2   | 23:W:201:PGT:H122 | 2.00                     | 0.42              |
| 2:b:181:THR:HB    | 2:b:212:GLY:H     | 1.84                     | 0.42              |
| 3:c:126:ILE:HD11  | 3:c:151:GLN:HA    | 2.02                     | 0.42              |
| 4:e:48:LEU:CD2    | 4:e:50:LYS:HZ3    | 2.24                     | 0.42              |
| 7:h:57:LEU:HD23   | 7:h:57:LEU:H      | 1.85                     | 0.42              |
| 7:h:58:TYR:HB3    | 8:j:327:PHE:CE2   | 2.54                     | 0.42              |
| 1:A:76:ILE:HG23   | 1:A:131:LEU:HD21  | 2.00                     | 0.42              |
| 10:L:177:LEU:HD23 | 10:L:180:ILE:HG13 | 2.02                     | 0.42              |
| 13:O:64:LEU:O     | 13:O:67:ARG:HG3   | 2.18                     | 0.42              |
| 13:O:157:HIS:HA   | 13:O:160:ILE:HG22 | 2.01                     | 0.42              |
| 14:P:177:PHE:CE1  | 14:P:195:ILE:HD13 | 2.54                     | 0.42              |
| 1:a:113:THR:HG21  | 1:a:214:ILE:HG21  | 2.01                     | 0.42              |
| 2:b:54:PHE:CE2    | 2:b:114:PHE:HA    | 2.55                     | 0.42              |
| 2:b:324:LYS:HA    | 2:b:324:LYS:HD2   | 1.89                     | 0.42              |
| 8:j:294:THR:HG23  | 8:j:295:MET:CE    | 2.49                     | 0.42              |
| 1:A:67:ASN:CG     | 1:A:176:LEU:HD12  | 2.44                     | 0.42              |
| 22:A:501:PEF:H341 | 22:A:501:PEF:H372 | 1.87                     | 0.42              |
| 22:H:101:PEF:H382 | 23:W:201:PGT:H221 | 2.00                     | 0.42              |
| 8:J:67:HIS:ND1    | 8:J:71:ASP:HB3    | 2.34                     | 0.42              |
| 8:J:219:ILE:HG21  | 10:L:295:ILE:HD11 | 2.02                     | 0.42              |
| 3:c:74:THR:HG21   | 22:c:303:PEF:H181 | 2.01                     | 0.42              |
| 4:e:51:ASP:O      | 4:e:55:ARG:HB3    | 2.20                     | 0.42              |
| 8:j:60:LEU:O      | 8:j:64:SER:HB2    | 2.19                     | 0.42              |
| 8:J:4:ARG:HD2     | 8:J:18:ILE:HG21   | 2.02                     | 0.42              |
| 8:J:43:GLN:OE1    | 8:J:82:HIS:ND1    | 2.53                     | 0.42              |
| 1:a:379:GLU:HG3   | 2:b:26:THR:HG23   | 2.01                     | 0.42              |
| 3:c:72:LYS:HE3    | 3:c:72:LYS:HB3    | 1.86                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:f:5:PHE:CE2     | 8:j:312:VAL:HG21  | 2.54                     | 0.42              |
| 8:j:291:GLY:O     | 8:j:295:MET:HG2   | 2.18                     | 0.42              |
| 1:A:125:ILE:HG22  | 1:A:229:SER:HA    | 2.01                     | 0.42              |
| 6:G:78:LEU:O      | 6:G:82:ARG:HG2    | 2.20                     | 0.42              |
| 9:K:71:VAL:HG11   | 9:K:247:LEU:HD13  | 2.02                     | 0.42              |
| 10:L:80:GLY:O     | 10:L:267:LYS:NZ   | 2.53                     | 0.42              |
| 12:N:44:PRO:O     | 12:N:48:ILE:HG13  | 2.20                     | 0.42              |
| 13:O:243:TYR:O    | 13:O:247:ILE:HG12 | 2.20                     | 0.42              |
| 20:V:45:ALA:HA    | 22:V:102:PEF:H241 | 2.01                     | 0.42              |
| 22:j:406:PEF:H312 | 22:j:406:PEF:H342 | 1.72                     | 0.42              |
| 10:l:284:SER:HA   | 10:l:287:VAL:HG12 | 2.02                     | 0.42              |
| 2:B:99:PRO:HA     | 2:B:102:VAL:HG12  | 2.02                     | 0.42              |
| 7:H:34:GLN:NE2    | 10:L:297:THR:HG21 | 2.31                     | 0.42              |
| 9:K:188:SER:OG    | 9:K:249:ILE:HG22  | 2.20                     | 0.42              |
| 14:P:53:LEU:HD11  | 14:P:57:MET:HE2   | 2.01                     | 0.42              |
| 17:S:28:VAL:O     | 17:S:31:GLN:HG3   | 2.20                     | 0.42              |
| 2:b:115:LYS:HA    | 2:b:115:LYS:HD3   | 1.64                     | 0.42              |
| 8:j:66:GLU:O      | 8:j:70:ARG:HG2    | 2.20                     | 0.42              |
| 10:l:225:MET:HE2  | 10:l:227:ARG:NH2  | 2.34                     | 0.42              |
| 1:A:256:LEU:HD12  | 1:A:437:GLY:HA2   | 2.02                     | 0.41              |
| 1:A:354:LEU:HD12  | 1:A:358:VAL:HG11  | 2.02                     | 0.41              |
| 1:A:375:GLY:O     | 1:A:379:GLU:CB    | 2.67                     | 0.41              |
| 9:K:184:LEU:HD23  | 9:K:184:LEU:HA    | 1.95                     | 0.41              |
| 9:K:334:LEU:O     | 21:W:86:VAL:HG21  | 2.20                     | 0.41              |
| 10:L:180:ILE:HA   | 10:L:183:ALA:HB3  | 2.02                     | 0.41              |
| 10:L:182:LYS:HG3  | 10:L:182:LYS:O    | 2.20                     | 0.41              |
| 13:O:133:GLN:H    | 17:S:81:ARG:HH12  | 1.68                     | 0.41              |
| 14:P:21:TYR:HD2   | 20:V:57:VAL:HG13  | 1.84                     | 0.41              |
| 14:P:189:ALA:HA   | 14:P:196:LYS:HG3  | 2.02                     | 0.41              |
| 17:S:96:TYR:CE2   | 17:S:98:PHE:HB2   | 2.55                     | 0.41              |
| 1:a:349:LYS:HD3   | 1:a:349:LYS:HA    | 1.71                     | 0.41              |
| 1:a:457:TRP:CD1   | 4:e:14:ASN:HB2    | 2.55                     | 0.41              |
| 10:l:298:ARG:HE   | 10:l:300:PHE:HZ   | 1.67                     | 0.41              |
| 2:B:37:GLY:HA2    | 2:B:41:TYR:CD2    | 2.55                     | 0.41              |
| 2:B:236:ASP:OD2   | 2:B:290:ARG:NH2   | 2.53                     | 0.41              |
| 9:K:347:LEU:HA    | 9:K:350:MET:HE2   | 2.02                     | 0.41              |
| 10:L:281:TYR:CE1  | 10:L:285:ILE:HD11 | 2.54                     | 0.41              |
| 13:O:21:PRO:O     | 13:O:24:ILE:HG22  | 2.20                     | 0.41              |
| 14:P:113:PRO:HD2  | 19:U:13:GLY:O     | 2.20                     | 0.41              |
| 6:g:99:GLU:HG3    | 6:g:127:PHE:CZ    | 2.55                     | 0.41              |
| 8:j:118:VAL:N     | 26:j:404:HEM:HBC2 | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 8:j:247:SER:OG   | 8:j:250:THR:OG1  | 2.18                     | 0.41              |
| 3:C:192:ARG:HE   | 3:C:192:ARG:HB3  | 1.67                     | 0.41              |
| 9:K:40:LEU:HD11  | 9:K:55:PHE:HE1   | 1.85                     | 0.41              |
| 9:K:525:HIS:CE1  | 11:M:29:HIS:HB2  | 2.56                     | 0.41              |
| 13:O:263:VAL:C   | 13:O:265:TYR:H   | 2.28                     | 0.41              |
| 17:S:65:LEU:O    | 17:S:69:ASN:ND2  | 2.53                     | 0.41              |
| 17:S:73:VAL:O    | 17:S:77:HIS:ND1  | 2.40                     | 0.41              |
| 1:a:77:PHE:CE2   | 1:a:104:TYR:HB3  | 2.56                     | 0.41              |
| 1:a:250:ARG:NH2  | 1:a:444:ASP:HA   | 2.35                     | 0.41              |
| 2:b:119:LEU:O    | 2:b:124:LEU:HD23 | 2.21                     | 0.41              |
| 2:b:138:PRO:HG3  | 2:b:233:PHE:HE2  | 1.85                     | 0.41              |
| 5:f:52:GLU:HG2   | 8:j:109:PRO:HG2  | 2.02                     | 0.41              |
| 10:l:63:THR:O    | 10:l:66:GLU:HG3  | 2.20                     | 0.41              |
| 10:l:101:CYS:HB3 | 26:l:401:HEM:C3B | 2.55                     | 0.41              |
| 10:l:260:GLU:N   | 10:l:260:GLU:OE1 | 2.53                     | 0.41              |
| 10:l:260:GLU:O   | 10:l:260:GLU:HG2 | 2.19                     | 0.41              |
| 1:A:67:ASN:HD21  | 1:A:176:LEU:HB2  | 1.85                     | 0.41              |
| 2:B:353:TYR:CE2  | 2:B:355:ALA:HB2  | 2.55                     | 0.41              |
| 9:K:37:ARG:NH2   | 9:K:451:ASN:OD1  | 2.54                     | 0.41              |
| 9:K:297:LEU:HD12 | 9:K:301:THR:HB   | 2.01                     | 0.41              |
| 9:K:391:ALA:O    | 9:K:395:TYR:HB3  | 2.20                     | 0.41              |
| 9:K:413:GLN:NE2  | 9:K:467:LEU:HB3  | 2.35                     | 0.41              |
| 10:L:225:MET:SD  | 26:L:401:HEM:C4D | 3.13                     | 0.41              |
| 13:O:3:HIS:HA    | 13:O:6:ARG:HG2   | 2.02                     | 0.41              |
| 14:P:56:TRP:HD1  | 16:R:21:GLY:HA2  | 1.85                     | 0.41              |
| 17:S:66:THR:HA   | 17:S:69:ASN:ND2  | 2.34                     | 0.41              |
| 1:a:126:GLN:HA   | 1:a:127:GLN:HA   | 1.75                     | 0.41              |
| 1:a:134:SER:O    | 1:a:137:PHE:N    | 2.52                     | 0.41              |
| 1:a:183:GLU:HG2  | 1:a:184:SER:N    | 2.36                     | 0.41              |
| 1:a:279:LYS:HG3  | 1:a:370:LEU:HD11 | 2.02                     | 0.41              |
| 3:c:159:CYS:O    | 3:c:163:GLY:N    | 2.54                     | 0.41              |
| 2:B:97:ASP:O     | 2:B:101:TYR:HD1  | 2.02                     | 0.41              |
| 2:B:164:VAL:HG21 | 2:b:232:ARG:HB3  | 2.03                     | 0.41              |
| 8:J:23:PRO:HG2   | 8:J:26:ILE:HD11  | 2.03                     | 0.41              |
| 8:J:331:PHE:HA   | 8:J:334:VAL:HG22 | 2.01                     | 0.41              |
| 9:K:37:ARG:O     | 9:K:41:ALA:N     | 2.54                     | 0.41              |
| 9:K:297:LEU:HD23 | 9:K:297:LEU:H    | 1.85                     | 0.41              |
| 13:O:75:TYR:CD2  | 13:O:76:LEU:HD12 | 2.56                     | 0.41              |
| 15:Q:106:ARG:NH2 | 21:W:77:TYR:HA   | 2.35                     | 0.41              |
| 1:a:298:GLN:O    | 1:a:303:LEU:HD23 | 2.20                     | 0.41              |
| 8:j:189:ILE:O    | 8:j:193:MET:HE2  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:j:311:SER:OG    | 8:j:319:LYS:NZ    | 2.51                     | 0.41              |
| 2:B:116:PRO:HB3   | 2:B:169:LEU:HD22  | 2.02                     | 0.41              |
| 13:O:80:THR:H     | 13:O:83:VAL:HG12  | 1.85                     | 0.41              |
| 14:P:206:GLN:HG2  | 19:U:21:GLN:O     | 2.20                     | 0.41              |
| 17:S:14:PRO:HA    | 17:S:15:PRO:HD3   | 1.86                     | 0.41              |
| 1:a:112:SER:HB2   | 1:a:115:LYS:HD2   | 2.03                     | 0.41              |
| 7:h:61:ILE:HB     | 7:h:62:PRO:HD3    | 2.01                     | 0.41              |
| 22:A:501:PEF:H321 | 22:A:501:PEF:H352 | 1.80                     | 0.41              |
| 2:B:143:GLU:HG3   | 2:B:288:PHE:HZ    | 1.85                     | 0.41              |
| 3:C:101:ILE:HG12  | 3:C:107:VAL:HG21  | 2.03                     | 0.41              |
| 6:G:76:ASP:OD1    | 6:G:76:ASP:N      | 2.54                     | 0.41              |
| 10:L:150:LYS:HG3  | 10:L:152:SER:H    | 1.84                     | 0.41              |
| 12:N:4:LYS:HA     | 12:N:4:LYS:HD3    | 1.93                     | 0.41              |
| 13:O:95:VAL:O     | 13:O:99:VAL:HG23  | 2.20                     | 0.41              |
| 21:W:52:LYS:HD2   | 21:W:52:LYS:HA    | 1.76                     | 0.41              |
| 23:W:201:PGT:H352 | 23:W:201:PGT:H321 | 1.84                     | 0.41              |
| 5:f:32:PHE:HD1    | 8:j:320:VAL:HG21  | 1.85                     | 0.41              |
| 8:j:362:TYR:HA    | 8:j:366:ILE:HB    | 2.02                     | 0.41              |
| 6:G:77:GLN:HE22   | 6:G:145:LYS:HA    | 1.85                     | 0.41              |
| 8:J:58:ILE:HG23   | 8:J:136:TYR:CE2   | 2.56                     | 0.41              |
| 8:J:153:ALA:HB2   | 8:J:288:LYS:HD3   | 2.03                     | 0.41              |
| 9:K:56:ASN:OD1    | 9:K:124:GLY:HA3   | 2.21                     | 0.41              |
| 9:K:347:LEU:HB3   | 9:K:383:MET:HG2   | 2.02                     | 0.41              |
| 7:h:51:ARG:HA     | 7:h:51:ARG:HD3    | 1.86                     | 0.41              |
| 8:j:30:TRP:CH2    | 8:j:209:PRO:HG3   | 2.56                     | 0.41              |
| 22:j:406:PEF:H161 | 22:j:406:PEF:H131 | 1.86                     | 0.41              |
| 10:l:218:PHE:CD1  | 10:l:219:PRO:HD2  | 2.56                     | 0.41              |
| 26:l:401:HEM:HHA  | 26:l:401:HEM:HBA1 | 2.02                     | 0.41              |
| 1:A:126:GLN:HA    | 1:A:127:GLN:HA    | 1.55                     | 0.41              |
| 2:B:74:LEU:HD22   | 2:B:101:TYR:CE1   | 2.56                     | 0.41              |
| 3:C:119:ARG:HH21  | 3:C:125:GLU:CD    | 2.29                     | 0.41              |
| 4:E:17:PHE:CE2    | 4:E:21:ILE:HD12   | 2.56                     | 0.41              |
| 5:F:10:ARG:HA     | 5:F:13:ASP:OD2    | 2.21                     | 0.41              |
| 5:F:32:PHE:HA     | 5:F:35:LEU:HG     | 2.03                     | 0.41              |
| 8:J:175:THR:O     | 8:J:178:ARG:HG2   | 2.21                     | 0.41              |
| 8:J:276:LEU:HD12  | 8:J:340:GLY:C     | 2.46                     | 0.41              |
| 8:J:329:PHE:HE1   | 8:J:359:TYR:HD1   | 1.68                     | 0.41              |
| 9:K:26:GLY:HA3    | 9:K:70:LEU:HD13   | 2.03                     | 0.41              |
| 9:K:323:TRP:HE3   | 9:K:345:LEU:HD11  | 1.85                     | 0.41              |
| 9:K:379:TYR:OH    | 9:K:428:MET:HB2   | 2.21                     | 0.41              |
| 9:K:444:PRO:HD3   | 14:P:160:LEU:HD23 | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:K:517:LEU:HD13  | 18:T:123:TRP:CZ2  | 2.54                     | 0.41              |
| 10:L:189:ASP:OD1  | 10:L:189:ASP:N    | 2.53                     | 0.41              |
| 12:N:43:THR:HB    | 12:N:47:TYR:CE2   | 2.56                     | 0.41              |
| 13:O:92:LEU:HA    | 13:O:95:VAL:HG22  | 2.01                     | 0.41              |
| 16:R:56:LYS:HD3   | 16:R:56:LYS:HA    | 1.83                     | 0.41              |
| 19:U:15:ASP:N     | 19:U:15:ASP:OD1   | 2.54                     | 0.41              |
| 21:W:47:GLN:HA    | 21:W:50:VAL:HG22  | 2.03                     | 0.41              |
| 2:b:63:SER:OG     | 2:b:64:ALA:N      | 2.52                     | 0.41              |
| 2:b:230:ARG:NH1   | 2:b:359:VAL:HG22  | 2.36                     | 0.41              |
| 2:b:299:SER:O     | 2:b:303:LYS:HG2   | 2.21                     | 0.41              |
| 3:c:80:SER:O      | 3:c:83:THR:HG22   | 2.20                     | 0.41              |
| 3:c:116:VAL:HA    | 3:c:156:LEU:HA    | 2.03                     | 0.41              |
| 6:g:141:ARG:HD3   | 6:g:141:ARG:HA    | 1.97                     | 0.41              |
| 8:j:68:ILE:O      | 8:j:72:VAL:HG12   | 2.20                     | 0.41              |
| 8:j:283:ARG:HH12  | 8:j:344:VAL:HB    | 1.85                     | 0.41              |
| 1:A:252:ARG:HD2   | 1:A:440:GLU:CD    | 2.46                     | 0.41              |
| 3:C:103:LEU:HD13  | 3:C:120:HIS:CE1   | 2.56                     | 0.41              |
| 9:K:113:LEU:HD23  | 9:K:113:LEU:HA    | 1.88                     | 0.41              |
| 9:K:347:LEU:CB    | 9:K:383:MET:HG2   | 2.51                     | 0.41              |
| 9:K:352:GLY:HA3   | 29:K:603:HEA:H14  | 2.03                     | 0.41              |
| 9:K:520:SER:O     | 9:K:521:PRO:C     | 2.65                     | 0.41              |
| 1:a:283:GLN:O     | 1:a:283:GLN:NE2   | 2.54                     | 0.41              |
| 1:a:352:ASN:HA    | 1:a:355:THR:HG22  | 2.02                     | 0.41              |
| 2:b:195:ALA:HB1   | 2:b:199:ARG:HH22  | 1.85                     | 0.41              |
| 3:c:105:LYS:HD2   | 3:c:105:LYS:HA    | 1.85                     | 0.41              |
| 4:e:3:PHE:HB3     | 4:e:7:TYR:HB2     | 2.03                     | 0.41              |
| 1:A:99:ARG:HA     | 1:A:99:ARG:HD3    | 1.84                     | 0.40              |
| 2:B:181:THR:OG1   | 2:B:210:PRO:O     | 2.29                     | 0.40              |
| 3:C:66:LEU:HD22   | 10:L:276:ILE:HD11 | 2.03                     | 0.40              |
| 6:G:85:PHE:CE2    | 6:G:139:ALA:HA    | 2.56                     | 0.40              |
| 6:G:94:LEU:HA     | 6:G:97:HIS:CE1    | 2.55                     | 0.40              |
| 8:J:118:VAL:O     | 8:J:122:ILE:HG13  | 2.21                     | 0.40              |
| 9:K:308:ALA:O     | 9:K:312:ILE:HG12  | 2.21                     | 0.40              |
| 13:O:146:LEU:HD21 | 13:O:261:TYR:HD2  | 1.86                     | 0.40              |
| 13:O:160:ILE:HB   | 13:O:247:ILE:HD11 | 2.03                     | 0.40              |
| 18:T:87:ASP:OD1   | 18:T:87:ASP:N     | 2.54                     | 0.40              |
| 21:W:41:MET:HE2   | 21:W:46:GLN:CG    | 2.50                     | 0.40              |
| 1:A:120:LEU:HD12  | 1:A:120:LEU:HA    | 1.97                     | 0.40              |
| 23:A:502:PGT:O1P  | 23:A:502:PGT:O6   | 2.35                     | 0.40              |
| 2:B:291:ASP:HB2   | 2:B:297:VAL:HG23  | 2.03                     | 0.40              |
| 9:K:273:MET:O     | 9:K:273:MET:HG3   | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:101:PHE:O    | 14:P:104:LEU:HG   | 2.21                     | 0.40              |
| 21:W:139:LYS:HG2  | 21:W:140:ASN:N    | 2.35                     | 0.40              |
| 3:c:146:ARG:NH2   | 3:c:190:ARG:HG2   | 2.37                     | 0.40              |
| 7:h:74:ASN:O      | 7:h:77:ASN:HB2    | 2.21                     | 0.40              |
| 22:j:401:PEF:H191 | 22:j:401:PEF:H372 | 2.03                     | 0.40              |
| 27:j:405:UQ6:H251 | 27:j:405:UQ6:H271 | 1.67                     | 0.40              |
| 10:l:110:VAL:O    | 10:l:155:ILE:HG12 | 2.22                     | 0.40              |
| 1:A:230:LEU:H     | 1:A:230:LEU:HD23  | 1.85                     | 0.40              |
| 3:C:137:LEU:HD22  | 3:C:190:ARG:HD2   | 2.03                     | 0.40              |
| 9:K:443:TYR:C     | 14:P:159:ARG:HH12 | 2.29                     | 0.40              |
| 21:W:78:GLY:O     | 21:W:79:GLU:HG2   | 2.21                     | 0.40              |
| 1:a:141:LYS:HE2   | 1:a:186:GLU:HA    | 2.03                     | 0.40              |
| 5:f:15:ILE:HG13   | 5:f:16:LEU:HD22   | 2.03                     | 0.40              |
| 8:j:367:VAL:HG23  | 8:j:368:PRO:HD3   | 2.03                     | 0.40              |
| 2:B:257:ALA:O     | 2:B:261:THR:HG22  | 2.22                     | 0.40              |
| 7:H:60:LEU:H      | 7:H:60:LEU:HD23   | 1.86                     | 0.40              |
| 9:K:514:ILE:HD11  | 18:T:125:LYS:HD3  | 2.02                     | 0.40              |
| 21:W:114:ARG:HG3  | 25:W:202:PCF:H122 | 2.04                     | 0.40              |
| 8:j:276:LEU:N     | 8:j:277:PRO:HD2   | 2.37                     | 0.40              |
| 10:l:157:GLY:HA2  | 10:l:158:PRO:HD3  | 1.92                     | 0.40              |
| 3:C:178:CYS:CB    | 24:C:301:FES:S1   | 3.10                     | 0.40              |
| 4:E:39:TRP:HZ3    | 10:L:271:LEU:HD21 | 1.85                     | 0.40              |
| 8:J:193:MET:HE2   | 8:J:193:MET:HB2   | 1.94                     | 0.40              |
| 9:K:34:LEU:HB2    | 9:K:462:THR:HG21  | 2.03                     | 0.40              |
| 9:K:359:ALA:HB2   | 29:K:603:HEA:CMB  | 2.52                     | 0.40              |
| 9:K:424:ILE:HG13  | 9:K:457:GLY:HA3   | 2.04                     | 0.40              |
| 13:O:229:ARG:NH1  | 13:O:232:ASN:OD1  | 2.55                     | 0.40              |
| 14:P:81:ILE:HG22  | 14:P:85:TRP:CE3   | 2.56                     | 0.40              |
| 3:c:110:LYS:HB2   | 3:c:110:LYS:HE2   | 1.88                     | 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     | 429/457 (94%)   | 394 (92%)  | 35 (8%)  | 0        | 100         | 100 |
| 1   | a     | 429/457 (94%)   | 400 (93%)  | 29 (7%)  | 0        | 100         | 100 |
| 2   | B     | 350/368 (95%)   | 330 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 2   | b     | 350/368 (95%)   | 329 (94%)  | 21 (6%)  | 0        | 100         | 100 |
| 3   | C     | 183/215 (85%)   | 173 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 3   | c     | 183/215 (85%)   | 173 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 4   | E     | 55/66 (83%)     | 54 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 4   | e     | 55/66 (83%)     | 51 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 5   | F     | 124/127 (98%)   | 119 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 5   | f     | 124/127 (98%)   | 117 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 6   | G     | 72/147 (49%)    | 65 (90%)   | 7 (10%)  | 0        | 100         | 100 |
| 6   | g     | 72/147 (49%)    | 63 (88%)   | 9 (12%)  | 0        | 100         | 100 |
| 7   | H     | 91/94 (97%)     | 82 (90%)   | 9 (10%)  | 0        | 100         | 100 |
| 7   | h     | 91/94 (97%)     | 78 (86%)   | 13 (14%) | 0        | 100         | 100 |
| 8   | J     | 383/385 (100%)  | 365 (95%)  | 18 (5%)  | 0        | 100         | 100 |
| 8   | j     | 383/385 (100%)  | 371 (97%)  | 12 (3%)  | 0        | 100         | 100 |
| 9   | K     | 532/534 (100%)  | 509 (96%)  | 23 (4%)  | 0        | 100         | 100 |
| 10  | L     | 246/309 (80%)   | 219 (89%)  | 27 (11%) | 0        | 100         | 100 |
| 10  | l     | 246/309 (80%)   | 211 (86%)  | 35 (14%) | 0        | 100         | 100 |
| 11  | M     | 45/78 (58%)     | 43 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 12  | N     | 57/60 (95%)     | 53 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 13  | O     | 267/269 (99%)   | 249 (93%)  | 18 (7%)  | 0        | 100         | 100 |
| 14  | P     | 234/251 (93%)   | 220 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 15  | Q     | 100/148 (68%)   | 97 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 16  | R     | 53/59 (90%)     | 49 (92%)   | 4 (8%)   | 0        | 100         | 100 |
| 17  | S     | 111/129 (86%)   | 102 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 18  | T     | 119/155 (77%)   | 112 (94%)  | 6 (5%)   | 1 (1%)   | 16          | 45  |
| 19  | U     | 75/83 (90%)     | 71 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 20  | V     | 38/66 (58%)     | 34 (90%)   | 4 (10%)  | 0        | 100         | 100 |
| 21  | W     | 131/153 (86%)   | 117 (89%)  | 14 (11%) | 0        | 100         | 100 |
| All | All   | 5628/6321 (89%) | 5250 (93%) | 377 (7%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | T     | 145 | 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     | 370/393 (94%)  | 370 (100%) | 0        | 100         | 100 |
| 1   | a     | 370/393 (94%)  | 370 (100%) | 0        | 100         | 100 |
| 2   | B     | 301/313 (96%)  | 301 (100%) | 0        | 100         | 100 |
| 2   | b     | 301/313 (96%)  | 301 (100%) | 0        | 100         | 100 |
| 3   | C     | 151/179 (84%)  | 151 (100%) | 0        | 100         | 100 |
| 3   | c     | 151/179 (84%)  | 151 (100%) | 0        | 100         | 100 |
| 4   | E     | 47/54 (87%)    | 47 (100%)  | 0        | 100         | 100 |
| 4   | e     | 47/54 (87%)    | 47 (100%)  | 0        | 100         | 100 |
| 5   | F     | 110/111 (99%)  | 110 (100%) | 0        | 100         | 100 |
| 5   | f     | 110/111 (99%)  | 110 (100%) | 0        | 100         | 100 |
| 6   | G     | 67/131 (51%)   | 67 (100%)  | 0        | 100         | 100 |
| 6   | g     | 67/131 (51%)   | 67 (100%)  | 0        | 100         | 100 |
| 7   | H     | 77/78 (99%)    | 77 (100%)  | 0        | 100         | 100 |
| 7   | h     | 77/78 (99%)    | 77 (100%)  | 0        | 100         | 100 |
| 8   | J     | 338/338 (100%) | 338 (100%) | 0        | 100         | 100 |
| 8   | j     | 338/338 (100%) | 338 (100%) | 0        | 100         | 100 |
| 9   | K     | 447/447 (100%) | 447 (100%) | 0        | 100         | 100 |
| 10  | L     | 206/251 (82%)  | 206 (100%) | 0        | 100         | 100 |
| 10  | l     | 206/251 (82%)  | 206 (100%) | 0        | 100         | 100 |
| 11  | M     | 39/67 (58%)    | 39 (100%)  | 0        | 100         | 100 |
| 12  | N     | 50/51 (98%)    | 50 (100%)  | 0        | 100         | 100 |
| 13  | O     | 228/228 (100%) | 228 (100%) | 0        | 100         | 100 |
| 14  | P     | 209/224 (93%)  | 209 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 15  | Q     | 91/131 (70%)    | 91 (100%)   | 0        | 100         | 100 |
| 16  | R     | 46/50 (92%)     | 46 (100%)   | 0        | 100         | 100 |
| 17  | S     | 99/113 (88%)    | 99 (100%)   | 0        | 100         | 100 |
| 18  | T     | 102/135 (76%)   | 102 (100%)  | 0        | 100         | 100 |
| 19  | U     | 69/74 (93%)     | 69 (100%)   | 0        | 100         | 100 |
| 20  | V     | 33/53 (62%)     | 33 (100%)   | 0        | 100         | 100 |
| 21  | W     | 110/127 (87%)   | 110 (100%)  | 0        | 100         | 100 |
| All | All   | 4857/5396 (90%) | 4857 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | ASN  |
| 1   | A     | 283 | GLN  |
| 1   | A     | 385 | ASN  |
| 2   | B     | 52  | ASN  |
| 2   | B     | 328 | GLN  |
| 2   | B     | 361 | ASN  |
| 3   | C     | 120 | HIS  |
| 3   | C     | 184 | HIS  |
| 5   | F     | 30  | ASN  |
| 5   | F     | 86  | HIS  |
| 6   | G     | 77  | GLN  |
| 7   | H     | 34  | GLN  |
| 7   | H     | 43  | ASN  |
| 8   | J     | 138 | GLN  |
| 8   | J     | 177 | GLN  |
| 8   | J     | 253 | HIS  |
| 9   | K     | 3   | GLN  |
| 10  | L     | 78  | HIS  |
| 10  | L     | 185 | HIS  |
| 10  | L     | 303 | ASN  |
| 12  | N     | 23  | HIS  |
| 14  | P     | 205 | ASN  |
| 15  | Q     | 117 | ASN  |
| 17  | S     | 16  | ASN  |
| 17  | S     | 100 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | S     | 122 | ASN  |
| 18  | T     | 41  | ASN  |
| 19  | U     | 23  | GLN  |
| 21  | W     | 142 | ASN  |
| 1   | a     | 227 | ASN  |
| 1   | a     | 336 | ASN  |
| 1   | a     | 385 | ASN  |
| 2   | b     | 258 | ASN  |
| 3   | c     | 112 | GLN  |
| 5   | f     | 3   | GLN  |
| 5   | f     | 57  | GLN  |
| 8   | j     | 149 | ASN  |
| 8   | j     | 197 | HIS  |
| 10  | l     | 105 | HIS  |
| 10  | l     | 141 | GLN  |
| 10  | l     | 169 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 1 is monoatomic and 2 are modelled with single atom - leaving 38 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 |
| 23  | PGT  | C     | 302 | -    | 50,50,50     | 0.49 | 0        | 53,56,56    | 0.46 | 0        |
| 22  | PEF  | J     | 406 | -    | 30,30,46     | 0.50 | 0        | 33,35,51    | 1.35 | 4 (12%)  |
| 27  | UQ6  | j     | 405 | -    | 43,43,43     | 0.43 | 0        | 54,55,55    | 1.65 | 14 (25%) |
| 26  | HEM  | l     | 401 | 10   | 50,50,50     | 1.54 | 7 (14%)  | 67,82,82    | 1.11 | 5 (7%)   |
| 29  | HEA  | K     | 602 | 9    | 67,67,67     | 1.26 | 7 (10%)  | 81,103,103  | 1.54 | 14 (17%) |
| 22  | PEF  | J     | 407 | -    | 28,28,46     | 0.51 | 0        | 31,33,51    | 1.30 | 4 (12%)  |
| 25  | PCF  | E     | 101 | -    | 46,46,49     | 0.64 | 0        | 52,54,57    | 0.55 | 0        |
| 27  | UQ6  | J     | 405 | -    | 43,43,43     | 0.42 | 0        | 54,55,55    | 1.65 | 14 (25%) |
| 24  | FES  | c     | 301 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 23  | PGT  | j     | 408 | -    | 48,48,50     | 0.50 | 0        | 51,54,56    | 0.46 | 0        |
| 23  | PGT  | W     | 201 | -    | 50,50,50     | 0.49 | 0        | 53,56,56    | 0.45 | 0        |
| 22  | PEF  | J     | 402 | -    | 30,30,46     | 0.50 | 0        | 33,35,51    | 1.33 | 4 (12%)  |
| 22  | PEF  | V     | 101 | -    | 32,32,46     | 0.49 | 0        | 35,37,51    | 1.31 | 4 (11%)  |
| 22  | PEF  | A     | 501 | -    | 39,39,46     | 0.47 | 0        | 42,44,51    | 1.26 | 4 (9%)   |
| 26  | HEM  | j     | 404 | 8    | 50,50,50     | 1.58 | 7 (14%)  | 67,82,82    | 1.15 | 6 (8%)   |
| 22  | PEF  | C     | 303 | -    | 42,42,46     | 0.46 | 0        | 45,47,51    | 1.24 | 4 (8%)   |
| 22  | PEF  | H     | 101 | -    | 35,35,46     | 0.49 | 0        | 38,40,51    | 1.28 | 4 (10%)  |
| 26  | HEM  | J     | 403 | 8    | 50,50,50     | 1.60 | 7 (14%)  | 67,82,82    | 1.12 | 5 (7%)   |
| 25  | PCF  | W     | 203 | -    | 49,49,49     | 0.63 | 0        | 55,57,57    | 0.54 | 0        |
| 23  | PGT  | L     | 402 | -    | 50,50,50     | 0.48 | 0        | 53,56,56    | 0.48 | 0        |
| 22  | PEF  | j     | 406 | -    | 30,30,46     | 0.50 | 0        | 33,35,51    | 1.31 | 4 (12%)  |
| 22  | PEF  | J     | 401 | -    | 44,44,46     | 0.45 | 0        | 47,49,51    | 1.23 | 4 (8%)   |
| 22  | PEF  | j     | 407 | -    | 28,28,46     | 0.51 | 0        | 31,33,51    | 1.35 | 4 (12%)  |
| 22  | PEF  | V     | 102 | -    | 40,40,46     | 0.47 | 0        | 43,45,51    | 1.27 | 5 (11%)  |
| 22  | PEF  | a     | 501 | -    | 39,39,46     | 0.47 | 0        | 42,44,51    | 1.25 | 4 (9%)   |
| 25  | PCF  | W     | 202 | -    | 35,35,49     | 0.71 | 0        | 41,43,57    | 0.57 | 0        |
| 22  | PEF  | c     | 303 | -    | 42,42,46     | 0.46 | 0        | 45,47,51    | 1.26 | 4 (8%)   |
| 29  | HEA  | K     | 603 | 9    | 67,67,67     | 1.28 | 8 (11%)  | 81,103,103  | 1.58 | 14 (17%) |
| 24  | FES  | C     | 301 | 3    | 0,4,4        | -    | -        | -           |      |          |
| 26  | HEM  | L     | 401 | 10   | 50,50,50     | 1.58 | 7 (14%)  | 67,82,82    | 1.15 | 7 (10%)  |
| 23  | PGT  | A     | 502 | -    | 50,50,50     | 0.49 | 0        | 53,56,56    | 0.46 | 0        |
| 22  | PEF  | j     | 401 | -    | 44,44,46     | 0.45 | 0        | 47,49,51    | 1.21 | 4 (8%)   |
| 23  | PGT  | a     | 502 | -    | 50,50,50     | 0.48 | 0        | 53,56,56    | 0.48 | 0        |
| 22  | PEF  | j     | 402 | -    | 30,30,46     | 0.50 | 0        | 33,35,51    | 1.31 | 4 (12%)  |
| 25  | PCF  | c     | 302 | -    | 46,46,49     | 0.64 | 0        | 52,54,57    | 0.61 | 0        |
| 26  | HEM  | j     | 403 | 8    | 50,50,50     | 1.60 | 7 (14%)  | 67,82,82    | 1.11 | 6 (8%)   |
| 26  | HEM  | J     | 404 | 8    | 50,50,50     | 1.61 | 8 (16%)  | 67,82,82    | 1.14 | 5 (7%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | PGT  | H     | 102 | -    | 48,48,50     | 0.49 | 0        | 51,54,56    | 0.47 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 23  | PGT  | C     | 302 | -    | -       | 12/55/55/55 | -       |
| 22  | PEF  | J     | 406 | -    | -       | 4/34/34/50  | -       |
| 27  | UQ6  | j     | 405 | -    | -       | 11/39/39/39 | 0/1/1/1 |
| 26  | HEM  | l     | 401 | 10   | -       | 10/14/54/54 | -       |
| 29  | HEA  | K     | 602 | 9    | -       | 19/36/76/76 | -       |
| 22  | PEF  | J     | 407 | -    | -       | 8/32/32/50  | -       |
| 25  | PCF  | E     | 101 | -    | -       | 13/50/50/53 | -       |
| 27  | UQ6  | J     | 405 | -    | -       | 10/39/39/39 | 0/1/1/1 |
| 24  | FES  | c     | 301 | 3    | -       | -           | 0/1/1/1 |
| 23  | PGT  | j     | 408 | -    | -       | 18/53/53/55 | -       |
| 23  | PGT  | W     | 201 | -    | -       | 22/55/55/55 | -       |
| 22  | PEF  | J     | 402 | -    | -       | 5/34/34/50  | -       |
| 22  | PEF  | V     | 101 | -    | -       | 5/36/36/50  | -       |
| 22  | PEF  | A     | 501 | -    | -       | 8/43/43/50  | -       |
| 26  | HEM  | j     | 404 | 8    | -       | 7/14/54/54  | -       |
| 22  | PEF  | C     | 303 | -    | -       | 9/46/46/50  | -       |
| 22  | PEF  | H     | 101 | -    | -       | 9/39/39/50  | -       |
| 26  | HEM  | J     | 403 | 8    | -       | 4/14/54/54  | -       |
| 25  | PCF  | W     | 203 | -    | -       | 11/53/53/53 | -       |
| 23  | PGT  | L     | 402 | -    | -       | 20/55/55/55 | -       |
| 22  | PEF  | j     | 406 | -    | -       | 3/34/34/50  | -       |
| 22  | PEF  | J     | 401 | -    | -       | 11/48/48/50 | -       |
| 22  | PEF  | j     | 407 | -    | -       | 6/32/32/50  | -       |
| 22  | PEF  | V     | 102 | -    | -       | 9/44/44/50  | -       |
| 22  | PEF  | a     | 501 | -    | -       | 11/43/43/50 | -       |
| 25  | PCF  | W     | 202 | -    | -       | 8/39/39/53  | -       |
| 22  | PEF  | c     | 303 | -    | -       | 10/46/46/50 | -       |
| 29  | HEA  | K     | 603 | 9    | -       | 18/36/76/76 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 26  | HEM  | L     | 401 | 10   | -       | 6/14/54/54  | -       |
| 24  | FES  | C     | 301 | 3    | -       | -           | 0/1/1/1 |
| 23  | PGT  | A     | 502 | -    | -       | 24/55/55/55 | -       |
| 22  | PEF  | j     | 401 | -    | -       | 9/48/48/50  | -       |
| 23  | PGT  | a     | 502 | -    | -       | 21/55/55/55 | -       |
| 22  | PEF  | j     | 402 | -    | -       | 3/34/34/50  | -       |
| 25  | PCF  | c     | 302 | -    | -       | 14/50/50/53 | -       |
| 26  | HEM  | j     | 403 | 8    | -       | 12/14/54/54 | -       |
| 26  | HEM  | J     | 404 | 8    | -       | 8/14/54/54  | -       |
| 23  | PGT  | H     | 102 | -    | -       | 13/53/53/55 | -       |

All (58) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | l     | 401 | HEM  | FE-ND   | 5.65  | 2.12        | 1.94     |
| 26  | J     | 403 | HEM  | FE-ND   | 5.64  | 2.12        | 1.94     |
| 26  | L     | 401 | HEM  | FE-ND   | 5.60  | 2.12        | 1.94     |
| 26  | j     | 403 | HEM  | FE-ND   | 5.60  | 2.12        | 1.94     |
| 26  | J     | 404 | HEM  | FE-ND   | 5.56  | 2.12        | 1.94     |
| 26  | j     | 404 | HEM  | FE-ND   | 5.46  | 2.11        | 1.94     |
| 29  | K     | 603 | HEA  | CMA-C3A | -4.01 | 1.36        | 1.45     |
| 29  | K     | 602 | HEA  | CMA-C3A | -3.97 | 1.36        | 1.45     |
| 26  | l     | 401 | HEM  | FE-NC   | 3.47  | 2.06        | 1.95     |
| 26  | j     | 403 | HEM  | FE-NC   | 3.36  | 2.06        | 1.95     |
| 26  | j     | 404 | HEM  | FE-NC   | 3.35  | 2.06        | 1.95     |
| 26  | L     | 401 | HEM  | FE-NC   | 3.33  | 2.06        | 1.95     |
| 26  | J     | 404 | HEM  | FE-NC   | 3.32  | 2.06        | 1.95     |
| 26  | J     | 403 | HEM  | FE-NC   | 3.30  | 2.06        | 1.95     |
| 26  | J     | 404 | HEM  | CAB-C3B | 3.01  | 1.55        | 1.47     |
| 29  | K     | 603 | HEA  | CHC-C1C | -2.94 | 1.32        | 1.39     |
| 29  | K     | 602 | HEA  | C4C-NC  | -2.94 | 1.34        | 1.39     |
| 26  | J     | 404 | HEM  | C3C-C2C | -2.91 | 1.31        | 1.37     |
| 29  | K     | 602 | HEA  | CHC-C1C | -2.90 | 1.32        | 1.39     |
| 26  | j     | 403 | HEM  | C3C-C2C | -2.88 | 1.31        | 1.37     |
| 29  | K     | 603 | HEA  | C4C-NC  | -2.88 | 1.34        | 1.39     |
| 26  | J     | 403 | HEM  | C3C-C2C | -2.87 | 1.31        | 1.37     |
| 26  | L     | 401 | HEM  | C3C-C2C | -2.86 | 1.31        | 1.37     |
| 26  | L     | 401 | HEM  | CAB-C3B | 2.83  | 1.54        | 1.47     |
| 26  | l     | 401 | HEM  | CAB-C3B | 2.82  | 1.54        | 1.47     |
| 26  | J     | 403 | HEM  | CAB-C3B | 2.82  | 1.54        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | j     | 404 | HEM  | CAB-C3B | 2.78  | 1.54        | 1.47     |
| 26  | j     | 404 | HEM  | C3C-C2C | -2.78 | 1.31        | 1.37     |
| 26  | j     | 403 | HEM  | CAB-C3B | 2.77  | 1.54        | 1.47     |
| 26  | l     | 401 | HEM  | C3C-C2C | -2.74 | 1.31        | 1.37     |
| 26  | L     | 401 | HEM  | FE-NB   | -2.71 | 1.86        | 1.94     |
| 26  | j     | 404 | HEM  | FE-NB   | -2.69 | 1.86        | 1.94     |
| 26  | j     | 403 | HEM  | FE-NB   | -2.66 | 1.86        | 1.94     |
| 26  | J     | 403 | HEM  | FE-NB   | -2.65 | 1.86        | 1.94     |
| 26  | J     | 404 | HEM  | FE-NB   | -2.64 | 1.86        | 1.94     |
| 26  | j     | 404 | HEM  | C2A-C3A | -2.62 | 1.32        | 1.38     |
| 26  | J     | 403 | HEM  | C2A-C3A | -2.59 | 1.32        | 1.38     |
| 26  | l     | 401 | HEM  | CAC-C3C | 2.59  | 1.54        | 1.47     |
| 26  | j     | 404 | HEM  | CAC-C3C | 2.57  | 1.54        | 1.47     |
| 26  | L     | 401 | HEM  | CAC-C3C | 2.57  | 1.54        | 1.47     |
| 26  | J     | 404 | HEM  | C2A-C3A | -2.54 | 1.32        | 1.38     |
| 26  | l     | 401 | HEM  | C2A-C3A | -2.53 | 1.32        | 1.38     |
| 26  | L     | 401 | HEM  | C2A-C3A | -2.52 | 1.32        | 1.38     |
| 29  | K     | 603 | HEA  | C1D-C2D | 2.51  | 1.49        | 1.44     |
| 26  | J     | 404 | HEM  | CAC-C3C | 2.50  | 1.54        | 1.47     |
| 26  | j     | 403 | HEM  | CAC-C3C | 2.49  | 1.54        | 1.47     |
| 26  | J     | 403 | HEM  | CAC-C3C | 2.47  | 1.54        | 1.47     |
| 29  | K     | 602 | HEA  | C1D-C2D | 2.46  | 1.49        | 1.44     |
| 26  | j     | 403 | HEM  | C2A-C3A | -2.43 | 1.32        | 1.38     |
| 29  | K     | 602 | HEA  | C3C-C2C | -2.40 | 1.33        | 1.41     |
| 29  | K     | 603 | HEA  | C3C-C2C | -2.40 | 1.33        | 1.41     |
| 29  | K     | 602 | HEA  | C1D-ND  | -2.39 | 1.36        | 1.40     |
| 29  | K     | 603 | HEA  | C1D-ND  | -2.36 | 1.36        | 1.40     |
| 29  | K     | 602 | HEA  | FE-NC   | 2.03  | 2.01        | 1.95     |
| 26  | J     | 404 | HEM  | C3D-C2D | -2.02 | 1.32        | 1.36     |
| 29  | K     | 603 | HEA  | FE-NC   | 2.01  | 2.01        | 1.95     |
| 29  | K     | 603 | HEA  | CHA-C1A | -2.01 | 1.34        | 1.38     |
| 26  | l     | 401 | HEM  | CMB-C2B | 2.01  | 1.54        | 1.50     |

All (151) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | K     | 603 | HEA  | CMD-C2D-C1D | 5.83  | 134.14      | 125.03   |
| 29  | K     | 602 | HEA  | CMD-C2D-C1D | 5.68  | 133.91      | 125.03   |
| 27  | J     | 405 | UQ6  | C7-C8-C9    | -5.04 | 120.19      | 127.42   |
| 27  | j     | 405 | UQ6  | C7-C8-C9    | -4.93 | 120.36      | 127.42   |
| 29  | K     | 603 | HEA  | CHB-C4A-NA  | -4.66 | 119.38      | 124.45   |
| 29  | K     | 602 | HEA  | CHB-C4A-NA  | -4.44 | 119.61      | 124.45   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | c     | 303 | PEF  | O2-C10-C11  | 4.11  | 120.38      | 111.48   |
| 22  | J     | 406 | PEF  | O2-C10-C11  | 4.01  | 120.15      | 111.48   |
| 22  | a     | 501 | PEF  | O2-C10-C11  | 3.95  | 120.03      | 111.48   |
| 22  | J     | 401 | PEF  | O2-C10-C11  | 3.94  | 120.01      | 111.48   |
| 22  | j     | 407 | PEF  | O2-C10-C11  | 3.94  | 120.01      | 111.48   |
| 22  | C     | 303 | PEF  | O2-C10-C11  | 3.90  | 119.91      | 111.48   |
| 22  | A     | 501 | PEF  | O2-C10-C11  | 3.89  | 119.91      | 111.48   |
| 22  | j     | 401 | PEF  | O2-C10-C11  | 3.88  | 119.88      | 111.48   |
| 22  | V     | 101 | PEF  | O2-C10-C11  | 3.87  | 119.86      | 111.48   |
| 22  | H     | 101 | PEF  | O2-C10-C11  | 3.87  | 119.86      | 111.48   |
| 22  | J     | 402 | PEF  | O2-C10-C11  | 3.83  | 119.76      | 111.48   |
| 22  | j     | 402 | PEF  | O2-C10-C11  | 3.78  | 119.66      | 111.48   |
| 22  | j     | 406 | PEF  | O2-C10-C11  | 3.69  | 119.46      | 111.48   |
| 22  | J     | 407 | PEF  | O2-C10-C11  | 3.65  | 119.38      | 111.48   |
| 22  | V     | 102 | PEF  | O2-C10-C11  | 3.36  | 118.75      | 111.48   |
| 26  | L     | 401 | HEM  | CAC-C3C-C4C | 3.26  | 132.59      | 124.82   |
| 26  | j     | 403 | HEM  | CAC-C3C-C4C | 3.26  | 132.59      | 124.82   |
| 26  | J     | 404 | HEM  | CAC-C3C-C4C | 3.24  | 132.55      | 124.82   |
| 27  | J     | 405 | UQ6  | C12-C13-C14 | -3.18 | 120.35      | 127.62   |
| 27  | J     | 405 | UQ6  | C22-C23-C24 | -3.14 | 120.43      | 127.62   |
| 29  | K     | 603 | HEA  | C12-C11-C3B | 3.10  | 116.97      | 112.12   |
| 22  | H     | 101 | PEF  | P-O4P-C4    | -3.09 | 106.56      | 121.26   |
| 22  | J     | 406 | PEF  | P-O4P-C4    | -3.08 | 106.62      | 121.26   |
| 26  | l     | 401 | HEM  | CAC-C3C-C4C | 3.07  | 132.14      | 124.82   |
| 22  | j     | 402 | PEF  | P-O4P-C4    | -3.06 | 106.67      | 121.26   |
| 26  | j     | 404 | HEM  | CAC-C3C-C4C | 3.06  | 132.12      | 124.82   |
| 22  | C     | 303 | PEF  | P-O4P-C4    | -3.05 | 106.73      | 121.26   |
| 22  | j     | 406 | PEF  | P-O4P-C4    | -3.04 | 106.77      | 121.26   |
| 22  | c     | 303 | PEF  | P-O4P-C4    | -3.04 | 106.80      | 121.26   |
| 27  | j     | 405 | UQ6  | C17-C18-C19 | -3.02 | 120.71      | 127.62   |
| 27  | j     | 405 | UQ6  | C27-C28-C29 | -3.01 | 120.73      | 127.62   |
| 22  | j     | 407 | PEF  | P-O4P-C4    | -3.01 | 106.93      | 121.26   |
| 22  | J     | 407 | PEF  | P-O4P-C4    | -3.01 | 106.94      | 121.26   |
| 22  | J     | 401 | PEF  | P-O4P-C4    | -3.01 | 106.94      | 121.26   |
| 22  | A     | 501 | PEF  | P-O4P-C4    | -3.00 | 106.98      | 121.26   |
| 27  | J     | 405 | UQ6  | C27-C28-C29 | -2.99 | 120.79      | 127.62   |
| 27  | j     | 405 | UQ6  | C12-C13-C14 | -2.98 | 120.80      | 127.62   |
| 22  | V     | 101 | PEF  | P-O4P-C4    | -2.98 | 107.06      | 121.26   |
| 22  | J     | 402 | PEF  | P-O4P-C4    | -2.98 | 107.08      | 121.26   |
| 27  | j     | 405 | UQ6  | C22-C23-C24 | -2.98 | 120.81      | 127.62   |
| 29  | K     | 603 | HEA  | C2A-C1A-NA  | 2.97  | 113.19      | 110.32   |
| 22  | V     | 102 | PEF  | P-O4P-C4    | -2.97 | 107.13      | 121.26   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | K     | 602 | HEA  | C2A-C1A-NA  | 2.96  | 113.18      | 110.32   |
| 22  | a     | 501 | PEF  | P-O4P-C4    | -2.94 | 107.26      | 121.26   |
| 29  | K     | 603 | HEA  | CHB-C4A-C3A | 2.93  | 130.14      | 125.21   |
| 27  | J     | 405 | UQ6  | C17-C18-C19 | -2.92 | 120.94      | 127.62   |
| 22  | V     | 102 | PEF  | C2-O2-C10   | 2.89  | 124.71      | 117.80   |
| 22  | j     | 401 | PEF  | P-O4P-C4    | -2.88 | 107.56      | 121.26   |
| 27  | j     | 405 | UQ6  | C25-C24-C26 | 2.84  | 120.17      | 115.23   |
| 27  | j     | 405 | UQ6  | C3M-O3-C3   | -2.84 | 107.03      | 114.74   |
| 29  | K     | 602 | HEA  | O1D-CGD-CBD | -2.82 | 114.14      | 123.09   |
| 27  | J     | 405 | UQ6  | C30-C29-C31 | 2.81  | 120.11      | 115.23   |
| 29  | K     | 603 | HEA  | CHD-C1D-ND  | -2.80 | 120.90      | 124.37   |
| 26  | j     | 404 | HEM  | CMB-C2B-C1B | -2.79 | 120.68      | 125.03   |
| 27  | J     | 405 | UQ6  | C15-C14-C16 | 2.77  | 120.03      | 115.23   |
| 26  | J     | 403 | HEM  | CAC-C3C-C4C | 2.77  | 131.43      | 124.82   |
| 27  | j     | 405 | UQ6  | C15-C14-C16 | 2.76  | 120.02      | 115.23   |
| 22  | c     | 303 | PEF  | O3-C30-C31  | 2.76  | 120.24      | 111.83   |
| 27  | J     | 405 | UQ6  | C3M-O3-C3   | -2.75 | 107.28      | 114.74   |
| 22  | J     | 402 | PEF  | O3-C30-C31  | 2.74  | 120.18      | 111.83   |
| 26  | J     | 403 | HEM  | CMB-C2B-C1B | -2.72 | 120.78      | 125.03   |
| 22  | J     | 406 | PEF  | O3-C30-C31  | 2.72  | 120.14      | 111.83   |
| 29  | K     | 603 | HEA  | O1D-CGD-CBD | -2.72 | 114.46      | 123.09   |
| 22  | C     | 303 | PEF  | O3-C30-C31  | 2.72  | 120.12      | 111.83   |
| 22  | A     | 501 | PEF  | O3-C30-C31  | 2.71  | 120.11      | 111.83   |
| 27  | j     | 405 | UQ6  | C4M-O4-C4   | -2.69 | 107.43      | 114.74   |
| 29  | K     | 602 | HEA  | CHD-C1D-ND  | -2.69 | 121.04      | 124.37   |
| 22  | j     | 402 | PEF  | O3-C30-C31  | 2.68  | 120.01      | 111.83   |
| 22  | H     | 101 | PEF  | P-O3P-C1    | -2.68 | 106.00      | 121.35   |
| 22  | a     | 501 | PEF  | O3-C30-C31  | 2.68  | 120.00      | 111.83   |
| 26  | j     | 403 | HEM  | CAC-C3C-C2C | -2.68 | 119.73      | 128.43   |
| 26  | J     | 404 | HEM  | CMB-C2B-C1B | -2.67 | 120.85      | 125.03   |
| 26  | l     | 401 | HEM  | CMB-C2B-C1B | -2.67 | 120.86      | 125.03   |
| 27  | j     | 405 | UQ6  | C30-C29-C31 | 2.67  | 119.86      | 115.23   |
| 22  | V     | 101 | PEF  | O3-C30-C31  | 2.67  | 119.97      | 111.83   |
| 22  | j     | 406 | PEF  | O3-C30-C31  | 2.66  | 119.94      | 111.83   |
| 29  | K     | 602 | HEA  | CHB-C4A-C3A | 2.66  | 129.69      | 125.21   |
| 22  | J     | 407 | PEF  | O3-C30-C31  | 2.64  | 119.89      | 111.83   |
| 22  | J     | 401 | PEF  | O3-C30-C31  | 2.63  | 119.86      | 111.83   |
| 22  | J     | 401 | PEF  | P-O3P-C1    | -2.63 | 106.30      | 121.35   |
| 22  | H     | 101 | PEF  | O3-C30-C31  | 2.62  | 119.82      | 111.83   |
| 27  | J     | 405 | UQ6  | C4M-O4-C4   | -2.62 | 107.64      | 114.74   |
| 22  | V     | 101 | PEF  | P-O3P-C1    | -2.62 | 106.36      | 121.35   |
| 27  | J     | 405 | UQ6  | C20-C19-C21 | 2.61  | 119.76      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 22  | V     | 102 | PEF  | P-O3P-C1    | -2.61 | 106.42      | 121.35   |
| 22  | j     | 401 | PEF  | O3-C30-C31  | 2.61  | 119.78      | 111.83   |
| 27  | j     | 405 | UQ6  | C20-C19-C21 | 2.61  | 119.75      | 115.23   |
| 22  | j     | 407 | PEF  | O3-C30-C31  | 2.60  | 119.77      | 111.83   |
| 26  | L     | 401 | HEM  | CAC-C3C-C2C | -2.57 | 120.06      | 128.43   |
| 22  | A     | 501 | PEF  | P-O3P-C1    | -2.57 | 106.61      | 121.35   |
| 22  | j     | 407 | PEF  | P-O3P-C1    | -2.57 | 106.62      | 121.35   |
| 22  | V     | 102 | PEF  | O3-C30-C31  | 2.57  | 119.67      | 111.83   |
| 22  | j     | 406 | PEF  | P-O3P-C1    | -2.57 | 106.64      | 121.35   |
| 27  | J     | 405 | UQ6  | C25-C24-C26 | 2.56  | 119.67      | 115.23   |
| 22  | j     | 401 | PEF  | P-O3P-C1    | -2.54 | 106.79      | 121.35   |
| 26  | J     | 404 | HEM  | CAC-C3C-C2C | -2.54 | 120.18      | 128.43   |
| 26  | l     | 401 | HEM  | CAC-C3C-C2C | -2.53 | 120.19      | 128.43   |
| 22  | C     | 303 | PEF  | P-O3P-C1    | -2.53 | 106.84      | 121.35   |
| 22  | J     | 402 | PEF  | P-O3P-C1    | -2.52 | 106.89      | 121.35   |
| 22  | J     | 406 | PEF  | P-O3P-C1    | -2.51 | 106.97      | 121.35   |
| 27  | J     | 405 | UQ6  | C10-C9-C11  | 2.51  | 119.58      | 115.23   |
| 27  | j     | 405 | UQ6  | C10-C9-C11  | 2.50  | 119.57      | 115.23   |
| 22  | j     | 402 | PEF  | P-O3P-C1    | -2.50 | 107.01      | 121.35   |
| 29  | K     | 603 | HEA  | CMB-C2B-C3B | -2.47 | 125.50      | 130.28   |
| 26  | L     | 401 | HEM  | CMC-C2C-C3C | -2.47 | 122.46      | 128.43   |
| 26  | j     | 404 | HEM  | CAC-C3C-C2C | -2.46 | 120.42      | 128.43   |
| 22  | a     | 501 | PEF  | P-O3P-C1    | -2.45 | 107.33      | 121.35   |
| 26  | J     | 403 | HEM  | CMC-C2C-C3C | -2.43 | 122.54      | 128.43   |
| 26  | j     | 404 | HEM  | CMC-C2C-C3C | -2.40 | 122.63      | 128.43   |
| 22  | J     | 407 | PEF  | P-O3P-C1    | -2.39 | 107.66      | 121.35   |
| 26  | j     | 403 | HEM  | CMB-C2B-C1B | -2.38 | 121.31      | 125.03   |
| 29  | K     | 602 | HEA  | C1D-C2D-C3D | -2.36 | 104.50      | 106.98   |
| 22  | c     | 303 | PEF  | P-O3P-C1    | -2.35 | 107.90      | 121.35   |
| 26  | j     | 403 | HEM  | CMC-C2C-C3C | -2.33 | 122.80      | 128.43   |
| 26  | J     | 403 | HEM  | CAC-C3C-C2C | -2.32 | 120.88      | 128.43   |
| 26  | l     | 401 | HEM  | CMC-C2C-C3C | -2.30 | 122.85      | 128.43   |
| 26  | J     | 403 | HEM  | CMC-C2C-C1C | 2.29  | 128.76      | 124.73   |
| 29  | K     | 602 | HEA  | C3D-C4D-ND  | 2.26  | 112.53      | 110.35   |
| 27  | j     | 405 | UQ6  | C36-C34-C35 | 2.26  | 119.78      | 114.59   |
| 29  | K     | 602 | HEA  | CMB-C2B-C3B | -2.23 | 125.96      | 130.28   |
| 27  | J     | 405 | UQ6  | C36-C34-C35 | 2.23  | 119.72      | 114.59   |
| 29  | K     | 602 | HEA  | C3C-C4C-NC  | 2.23  | 111.67      | 109.80   |
| 26  | L     | 401 | HEM  | CMB-C2B-C1B | -2.22 | 121.56      | 125.03   |
| 29  | K     | 602 | HEA  | C26-C15-C14 | -2.22 | 117.93      | 123.63   |
| 26  | L     | 401 | HEM  | C3C-C2C-C1C | 2.20  | 109.13      | 107.05   |
| 26  | J     | 404 | HEM  | CMC-C2C-C3C | -2.18 | 123.16      | 128.43   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | K     | 603 | HEA  | C1D-C2D-C3D | -2.16 | 104.70      | 106.98   |
| 29  | K     | 602 | HEA  | C3B-C4B-NB  | 2.16  | 112.32      | 109.84   |
| 29  | K     | 603 | HEA  | C3D-C4D-ND  | 2.15  | 112.43      | 110.35   |
| 29  | K     | 602 | HEA  | C12-C11-C3B | 2.14  | 115.46      | 112.12   |
| 26  | j     | 403 | HEM  | CMC-C2C-C1C | 2.13  | 128.48      | 124.73   |
| 26  | j     | 403 | HEM  | CAA-CBA-CGA | -2.13 | 108.03      | 113.67   |
| 27  | J     | 405 | UQ6  | C32-C33-C34 | -2.11 | 120.61      | 127.64   |
| 26  | j     | 404 | HEM  | CMC-C2C-C1C | 2.10  | 128.43      | 124.73   |
| 27  | j     | 405 | UQ6  | C32-C33-C34 | -2.10 | 120.64      | 127.64   |
| 26  | L     | 401 | HEM  | CMC-C2C-C1C | 2.09  | 128.41      | 124.73   |
| 29  | K     | 603 | HEA  | C3B-C4B-NB  | 2.08  | 112.23      | 109.84   |
| 29  | K     | 603 | HEA  | OMA-CMA-C3A | -2.07 | 120.94      | 125.62   |
| 29  | K     | 603 | HEA  | CHA-C1A-NA  | -2.05 | 122.22      | 124.45   |
| 29  | K     | 603 | HEA  | C4B-C3B-C2B | -2.05 | 104.00      | 107.44   |
| 26  | l     | 401 | HEM  | CMC-C2C-C1C | 2.04  | 128.33      | 124.73   |
| 26  | J     | 404 | HEM  | C3C-C2C-C1C | 2.03  | 108.97      | 107.05   |
| 29  | K     | 602 | HEA  | C4B-C3B-C2B | -2.03 | 104.03      | 107.44   |
| 26  | j     | 404 | HEM  | C3C-C2C-C1C | 2.01  | 108.94      | 107.05   |
| 26  | L     | 401 | HEM  | C1B-NB-C4B  | 2.00  | 107.58      | 105.21   |

There are no chirality outliers.

All (391) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 22  | A     | 501 | PEF  | C31-C30-O3-C3 |
| 22  | J     | 402 | PEF  | C31-C30-O3-C3 |
| 22  | J     | 402 | PEF  | O5-C30-O3-C3  |
| 22  | j     | 401 | PEF  | C4-O4P-P-O1P  |
| 22  | j     | 401 | PEF  | C4-O4P-P-O3P  |
| 23  | A     | 502 | PGT  | C32-C31-O2-C2 |
| 23  | A     | 502 | PGT  | C1-O3P-P-O2P  |
| 23  | A     | 502 | PGT  | C1-O3P-P-O4P  |
| 23  | C     | 302 | PGT  | C1-O3P-P-O2P  |
| 23  | C     | 302 | PGT  | C1-O3P-P-O4P  |
| 23  | H     | 102 | PGT  | O4P-C4-C5-C6  |
| 23  | L     | 402 | PGT  | C4-C5-C6-O6   |
| 23  | W     | 201 | PGT  | C4-O4P-P-O3P  |
| 23  | W     | 201 | PGT  | O4P-C4-C5-O5  |
| 23  | a     | 502 | PGT  | C1-O3P-P-O1P  |
| 23  | a     | 502 | PGT  | C1-O3P-P-O4P  |
| 23  | a     | 502 | PGT  | C4-O4P-P-O3P  |
| 23  | a     | 502 | PGT  | O4P-C4-C5-C6  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | a     | 502 | PGT  | O11-C11-O3-C3   |
| 23  | j     | 408 | PGT  | O31-C31-O2-C2   |
| 23  | j     | 408 | PGT  | C1-O3P-P-O2P    |
| 23  | j     | 408 | PGT  | C1-O3P-P-O4P    |
| 23  | j     | 408 | PGT  | C4-O4P-P-O3P    |
| 23  | j     | 408 | PGT  | C4-O4P-P-O1P    |
| 23  | j     | 408 | PGT  | O4P-C4-C5-O5    |
| 23  | j     | 408 | PGT  | C4-C5-C6-O6     |
| 25  | E     | 101 | PCF  | C1-O11-P-O12    |
| 25  | W     | 203 | PCF  | O21-C2-C3-O31   |
| 26  | J     | 403 | HEM  | C3D-CAD-CBD-CGD |
| 26  | L     | 401 | HEM  | C2C-C3C-CAC-CBC |
| 26  | L     | 401 | HEM  | C4C-C3C-CAC-CBC |
| 26  | j     | 403 | HEM  | C2B-C3B-CAB-CBB |
| 26  | j     | 404 | HEM  | C2C-C3C-CAC-CBC |
| 26  | j     | 404 | HEM  | C4C-C3C-CAC-CBC |
| 26  | l     | 401 | HEM  | C2A-CAA-CBA-CGA |
| 26  | l     | 401 | HEM  | C2B-C3B-CAB-CBB |
| 26  | l     | 401 | HEM  | C2C-C3C-CAC-CBC |
| 27  | J     | 405 | UQ6  | C30-C29-C31-C32 |
| 27  | j     | 405 | UQ6  | C23-C24-C26-C27 |
| 27  | j     | 405 | UQ6  | C25-C24-C26-C27 |
| 29  | K     | 602 | HEA  | C4C-C3C-CAC-CBC |
| 29  | K     | 602 | HEA  | C17-C18-C19-C20 |
| 29  | K     | 602 | HEA  | C17-C18-C19-C27 |
| 29  | K     | 602 | HEA  | C21-C22-C23-C24 |
| 29  | K     | 603 | HEA  | C13-C14-C15-C26 |
| 29  | K     | 603 | HEA  | C17-C18-C19-C27 |
| 22  | A     | 501 | PEF  | O5-C30-O3-C3    |
| 29  | K     | 602 | HEA  | C21-C22-C23-C25 |
| 23  | L     | 402 | PGT  | O11-C11-O3-C3   |
| 25  | W     | 202 | PCF  | O32-C31-O31-C3  |
| 23  | A     | 502 | PGT  | O31-C31-O2-C2   |
| 22  | H     | 101 | PEF  | C31-C30-O3-C3   |
| 23  | L     | 402 | PGT  | C12-C11-O3-C3   |
| 23  | a     | 502 | PGT  | C12-C11-O3-C3   |
| 25  | W     | 202 | PCF  | C32-C31-O31-C3  |
| 23  | j     | 408 | PGT  | C32-C31-O2-C2   |
| 27  | J     | 405 | UQ6  | C15-C14-C16-C17 |
| 29  | K     | 602 | HEA  | C26-C15-C16-C17 |
| 27  | J     | 405 | UQ6  | C13-C14-C16-C17 |
| 27  | J     | 405 | UQ6  | C28-C29-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | K     | 602 | HEA  | C18-C19-C20-C21 |
| 29  | K     | 603 | HEA  | C18-C19-C20-C21 |
| 29  | K     | 603 | HEA  | C3A-C2A-CAA-CBA |
| 29  | K     | 602 | HEA  | C13-C14-C15-C26 |
| 22  | H     | 101 | PEF  | O5-C30-O3-C3    |
| 23  | W     | 201 | PGT  | O11-C11-O3-C3   |
| 29  | K     | 603 | HEA  | C21-C22-C23-C25 |
| 23  | H     | 102 | PGT  | O4P-C4-C5-O5    |
| 23  | L     | 402 | PGT  | O4P-C4-C5-O5    |
| 23  | a     | 502 | PGT  | O4P-C4-C5-O5    |
| 23  | W     | 201 | PGT  | C12-C11-O3-C3   |
| 27  | j     | 405 | UQ6  | C15-C14-C16-C17 |
| 29  | K     | 602 | HEA  | C14-C15-C16-C17 |
| 27  | J     | 405 | UQ6  | C9-C11-C12-C13  |
| 27  | J     | 405 | UQ6  | C24-C26-C27-C28 |
| 27  | j     | 405 | UQ6  | C9-C11-C12-C13  |
| 27  | j     | 405 | UQ6  | C19-C21-C22-C23 |
| 27  | j     | 405 | UQ6  | C29-C31-C32-C33 |
| 26  | j     | 403 | HEM  | C1A-C2A-CAA-CBA |
| 25  | E     | 101 | PCF  | C2-C1-O11-P     |
| 26  | j     | 403 | HEM  | C2A-CAA-CBA-CGA |
| 29  | K     | 602 | HEA  | C2A-CAA-CBA-CGA |
| 23  | L     | 402 | PGT  | C32-C31-O2-C2   |
| 23  | a     | 502 | PGT  | C32-C31-O2-C2   |
| 29  | K     | 603 | HEA  | C1A-C2A-CAA-CBA |
| 23  | L     | 402 | PGT  | O4P-C4-C5-C6    |
| 23  | W     | 201 | PGT  | O4P-C4-C5-C6    |
| 23  | H     | 102 | PGT  | C12-C11-O3-C3   |
| 25  | E     | 101 | PCF  | C11-C12-N-C15   |
| 27  | j     | 405 | UQ6  | C13-C14-C16-C17 |
| 25  | c     | 302 | PCF  | C22-C23-C24-C25 |
| 23  | j     | 408 | PGT  | C11-C12-C13-C14 |
| 22  | A     | 501 | PEF  | O3P-C1-C2-O2    |
| 25  | E     | 101 | PCF  | O21-C2-C3-O31   |
| 23  | L     | 402 | PGT  | O5-C5-C6-O6     |
| 23  | L     | 402 | PGT  | O31-C31-O2-C2   |
| 27  | J     | 405 | UQ6  | C19-C21-C22-C23 |
| 27  | j     | 405 | UQ6  | C14-C16-C17-C18 |
| 25  | E     | 101 | PCF  | C11-C12-N-C13   |
| 22  | j     | 407 | PEF  | C10-C11-C12-C13 |
| 23  | W     | 201 | PGT  | C31-C32-C33-C34 |
| 23  | H     | 102 | PGT  | O11-C11-O3-C3   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | A     | 502 | PGT  | C2-C1-O3P-P     |
| 22  | J     | 401 | PEF  | C10-C11-C12-C13 |
| 22  | V     | 101 | PEF  | C30-C31-C32-C33 |
| 22  | a     | 501 | PEF  | C30-C31-C32-C33 |
| 26  | j     | 403 | HEM  | C3A-C2A-CAA-CBA |
| 23  | A     | 502 | PGT  | O4P-C4-C5-O5    |
| 23  | a     | 502 | PGT  | O31-C31-O2-C2   |
| 26  | J     | 404 | HEM  | C4D-C3D-CAD-CBD |
| 22  | c     | 303 | PEF  | C10-C11-C12-C13 |
| 23  | A     | 502 | PGT  | O4P-C4-C5-C6    |
| 25  | c     | 302 | PCF  | C11-C12-N-C15   |
| 23  | W     | 201 | PGT  | C11-C12-C13-C14 |
| 29  | K     | 603 | HEA  | C27-C19-C20-C21 |
| 23  | j     | 408 | PGT  | C5-C4-O4P-P     |
| 26  | J     | 404 | HEM  | C2D-C3D-CAD-CBD |
| 26  | l     | 401 | HEM  | C3D-CAD-CBD-CGD |
| 23  | A     | 502 | PGT  | C4-C5-C6-O6     |
| 23  | W     | 201 | PGT  | C32-C31-O2-C2   |
| 25  | c     | 302 | PCF  | C11-C12-N-C13   |
| 25  | c     | 302 | PCF  | C11-C12-N-C14   |
| 23  | C     | 302 | PGT  | C15-C16-C17-C18 |
| 23  | W     | 201 | PGT  | C43-C44-C45-C46 |
| 23  | a     | 502 | PGT  | C18-C19-C20-C21 |
| 25  | W     | 203 | PCF  | C22-C23-C24-C25 |
| 25  | E     | 101 | PCF  | C25-C26-C27-C28 |
| 23  | j     | 408 | PGT  | O5-C5-C6-O6     |
| 23  | a     | 502 | PGT  | C35-C36-C37-C38 |
| 25  | W     | 202 | PCF  | C24-C25-C26-C27 |
| 25  | c     | 302 | PCF  | C32-C33-C34-C35 |
| 22  | C     | 303 | PEF  | C34-C35-C36-C37 |
| 23  | A     | 502 | PGT  | C13-C14-C15-C16 |
| 22  | j     | 406 | PEF  | C12-C13-C14-C15 |
| 23  | A     | 502 | PGT  | C36-C37-C38-C39 |
| 23  | A     | 502 | PGT  | C35-C36-C37-C38 |
| 22  | c     | 303 | PEF  | C38-C39-C40-C41 |
| 25  | E     | 101 | PCF  | C11-C12-N-C14   |
| 29  | K     | 602 | HEA  | C2C-C3C-CAC-CBC |
| 23  | C     | 302 | PGT  | C32-C31-O2-C2   |
| 22  | c     | 303 | PEF  | C39-C40-C41-C42 |
| 29  | K     | 603 | HEA  | C3D-CAD-CBD-CGD |
| 22  | V     | 102 | PEF  | C15-C16-C17-C18 |
| 23  | H     | 102 | PGT  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | c     | 303 | PEF  | C35-C36-C37-C38 |
| 23  | W     | 201 | PGT  | O31-C31-O2-C2   |
| 22  | C     | 303 | PEF  | C14-C15-C16-C17 |
| 22  | J     | 401 | PEF  | C15-C16-C17-C18 |
| 22  | C     | 303 | PEF  | C39-C40-C41-C42 |
| 23  | H     | 102 | PGT  | C38-C39-C40-C41 |
| 26  | J     | 404 | HEM  | C2C-C3C-CAC-CBC |
| 26  | L     | 401 | HEM  | C2B-C3B-CAB-CBB |
| 26  | j     | 404 | HEM  | C2B-C3B-CAB-CBB |
| 26  | j     | 403 | HEM  | C4B-C3B-CAB-CBB |
| 26  | l     | 401 | HEM  | C4B-C3B-CAB-CBB |
| 22  | j     | 406 | PEF  | O2-C2-C3-O3     |
| 26  | j     | 403 | HEM  | C4D-C3D-CAD-CBD |
| 22  | A     | 501 | PEF  | O3P-C1-C2-C3    |
| 22  | H     | 101 | PEF  | O3P-C1-C2-C3    |
| 22  | J     | 402 | PEF  | O3P-C1-C2-C3    |
| 23  | C     | 302 | PGT  | O3P-C1-C2-C3    |
| 23  | C     | 302 | PGT  | O31-C31-O2-C2   |
| 22  | a     | 501 | PEF  | C15-C16-C17-C18 |
| 22  | J     | 407 | PEF  | C14-C15-C16-C17 |
| 23  | j     | 408 | PGT  | C35-C36-C37-C38 |
| 22  | A     | 501 | PEF  | C1-C2-C3-O3     |
| 22  | j     | 407 | PEF  | C1-C2-C3-O3     |
| 25  | E     | 101 | PCF  | C1-C2-C3-O31    |
| 25  | W     | 203 | PCF  | C1-C2-C3-O31    |
| 22  | C     | 303 | PEF  | C36-C37-C38-C39 |
| 23  | C     | 302 | PGT  | O4P-C4-C5-O5    |
| 22  | C     | 303 | PEF  | C10-C11-C12-C13 |
| 23  | H     | 102 | PGT  | C31-C32-C33-C34 |
| 23  | L     | 402 | PGT  | C3-C2-O2-C31    |
| 22  | a     | 501 | PEF  | C16-C17-C18-C19 |
| 23  | j     | 408 | PGT  | C33-C34-C35-C36 |
| 29  | K     | 602 | HEA  | C2A-C3A-CMA-OMA |
| 27  | j     | 405 | UQ6  | C18-C19-C21-C22 |
| 22  | A     | 501 | PEF  | O2-C2-C3-O3     |
| 22  | C     | 303 | PEF  | O2-C2-C3-O3     |
| 22  | V     | 101 | PEF  | O2-C2-C3-O3     |
| 22  | j     | 407 | PEF  | O2-C2-C3-O3     |
| 23  | L     | 402 | PGT  | C36-C37-C38-C39 |
| 22  | H     | 101 | PEF  | C37-C38-C39-C40 |
| 29  | K     | 603 | HEA  | C21-C22-C23-C24 |
| 22  | A     | 501 | PEF  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | j     | 405 | UQ6  | C20-C19-C21-C22 |
| 23  | H     | 102 | PGT  | O5-C5-C6-O6     |
| 26  | j     | 403 | HEM  | C2D-C3D-CAD-CBD |
| 23  | W     | 201 | PGT  | C23-C24-C25-C26 |
| 22  | a     | 501 | PEF  | C33-C34-C35-C36 |
| 22  | C     | 303 | PEF  | O3P-C1-C2-C3    |
| 23  | L     | 402 | PGT  | O3P-C1-C2-C3    |
| 23  | H     | 102 | PGT  | C13-C14-C15-C16 |
| 23  | L     | 402 | PGT  | C11-C12-C13-C14 |
| 22  | C     | 303 | PEF  | C1-C2-C3-O3     |
| 22  | j     | 406 | PEF  | C1-C2-C3-O3     |
| 23  | A     | 502 | PGT  | C1-C2-C3-O3     |
| 22  | j     | 401 | PEF  | C37-C38-C39-C40 |
| 29  | K     | 602 | HEA  | C27-C19-C20-C21 |
| 22  | J     | 407 | PEF  | O3P-C1-C2-O2    |
| 22  | V     | 102 | PEF  | O3P-C1-C2-O2    |
| 23  | L     | 402 | PGT  | O3P-C1-C2-O2    |
| 26  | J     | 403 | HEM  | C2A-CAA-CBA-CGA |
| 26  | j     | 403 | HEM  | C3D-CAD-CBD-CGD |
| 22  | J     | 406 | PEF  | O2-C2-C3-O3     |
| 23  | A     | 502 | PGT  | O2-C2-C3-O3     |
| 22  | c     | 303 | PEF  | C37-C38-C39-C40 |
| 22  | j     | 401 | PEF  | C14-C15-C16-C17 |
| 23  | A     | 502 | PGT  | C34-C35-C36-C37 |
| 27  | J     | 405 | UQ6  | C14-C16-C17-C18 |
| 22  | j     | 407 | PEF  | C30-C31-C32-C33 |
| 23  | j     | 408 | PGT  | O4P-C4-C5-C6    |
| 22  | J     | 407 | PEF  | O3P-C1-C2-C3    |
| 22  | a     | 501 | PEF  | O3P-C1-C2-C3    |
| 23  | A     | 502 | PGT  | O3P-C1-C2-C3    |
| 23  | H     | 102 | PGT  | O3P-C1-C2-C3    |
| 22  | A     | 501 | PEF  | C30-C31-C32-C33 |
| 22  | V     | 102 | PEF  | C1-C2-O2-C10    |
| 23  | a     | 502 | PGT  | C3-C2-O2-C31    |
| 22  | j     | 401 | PEF  | C33-C34-C35-C36 |
| 22  | C     | 303 | PEF  | O3P-C1-C2-O2    |
| 22  | H     | 101 | PEF  | O3P-C1-C2-O2    |
| 23  | A     | 502 | PGT  | O3P-C1-C2-O2    |
| 23  | H     | 102 | PGT  | O3P-C1-C2-O2    |
| 22  | a     | 501 | PEF  | C35-C36-C37-C38 |
| 22  | V     | 102 | PEF  | C1-C2-C3-O3     |
| 23  | W     | 201 | PGT  | C1-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | a     | 501 | PEF  | C10-C11-C12-C13 |
| 26  | J     | 403 | HEM  | C4C-C3C-CAC-CBC |
| 26  | j     | 403 | HEM  | C4C-C3C-CAC-CBC |
| 26  | j     | 404 | HEM  | C4B-C3B-CAB-CBB |
| 26  | l     | 401 | HEM  | C4C-C3C-CAC-CBC |
| 25  | W     | 203 | PCF  | C32-C31-O31-C3  |
| 23  | L     | 402 | PGT  | C14-C15-C16-C17 |
| 22  | j     | 402 | PEF  | O2-C2-C3-O3     |
| 23  | W     | 201 | PGT  | O2-C2-C3-O3     |
| 25  | W     | 202 | PCF  | O21-C2-C3-O31   |
| 22  | J     | 401 | PEF  | C31-C32-C33-C34 |
| 23  | a     | 502 | PGT  | C2-C1-O3P-P     |
| 25  | E     | 101 | PCF  | O13-C11-C12-N   |
| 25  | W     | 202 | PCF  | O13-C11-C12-N   |
| 25  | W     | 203 | PCF  | O13-C11-C12-N   |
| 25  | c     | 302 | PCF  | O13-C11-C12-N   |
| 23  | A     | 502 | PGT  | O5-C5-C6-O6     |
| 22  | J     | 401 | PEF  | O3P-C1-C2-C3    |
| 22  | j     | 401 | PEF  | O3P-C1-C2-C3    |
| 22  | j     | 407 | PEF  | O3P-C1-C2-C3    |
| 25  | c     | 302 | PCF  | C34-C35-C36-C37 |
| 25  | c     | 302 | PCF  | C21-C22-C23-C24 |
| 23  | A     | 502 | PGT  | C5-C4-O4P-P     |
| 22  | J     | 401 | PEF  | O3P-C1-C2-O2    |
| 22  | J     | 402 | PEF  | O3P-C1-C2-O2    |
| 22  | a     | 501 | PEF  | O3P-C1-C2-O2    |
| 22  | j     | 401 | PEF  | O3P-C1-C2-O2    |
| 22  | j     | 407 | PEF  | O3P-C1-C2-O2    |
| 23  | C     | 302 | PGT  | O3P-C1-C2-O2    |
| 25  | W     | 203 | PCF  | O32-C31-O31-C3  |
| 25  | W     | 202 | PCF  | C22-C23-C24-C25 |
| 29  | K     | 602 | HEA  | C4A-C3A-CMA-OMA |
| 22  | V     | 102 | PEF  | O2-C2-C3-O3     |
| 22  | J     | 406 | PEF  | C1-C2-C3-O3     |
| 22  | V     | 101 | PEF  | C1-C2-C3-O3     |
| 25  | W     | 202 | PCF  | C1-C2-C3-O31    |
| 23  | A     | 502 | PGT  | C37-C38-C39-C40 |
| 23  | a     | 502 | PGT  | C12-C13-C14-C15 |
| 22  | a     | 501 | PEF  | C37-C38-C39-C40 |
| 23  | A     | 502 | PGT  | C32-C33-C34-C35 |
| 22  | H     | 101 | PEF  | C31-C32-C33-C34 |
| 29  | K     | 602 | HEA  | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 22  | H     | 101 | PEF  | C1-O3P-P-O1P    |
| 22  | J     | 401 | PEF  | C4-O4P-P-O1P    |
| 22  | J     | 402 | PEF  | C4-O4P-P-O1P    |
| 22  | c     | 303 | PEF  | C1-O3P-P-O4P    |
| 23  | W     | 201 | PGT  | C1-O3P-P-O1P    |
| 23  | W     | 201 | PGT  | C4-O4P-P-O1P    |
| 23  | a     | 502 | PGT  | C1-O3P-P-O2P    |
| 23  | a     | 502 | PGT  | C4-O4P-P-O1P    |
| 23  | j     | 408 | PGT  | C4-O4P-P-O2P    |
| 25  | E     | 101 | PCF  | C11-O13-P-O12   |
| 23  | A     | 502 | PGT  | C17-C18-C19-C20 |
| 25  | W     | 203 | PCF  | C25-C26-C27-C28 |
| 22  | V     | 102 | PEF  | C11-C10-O2-C2   |
| 25  | W     | 203 | PCF  | C2-C1-O11-P     |
| 25  | W     | 202 | PCF  | C21-C22-C23-C24 |
| 23  | a     | 502 | PGT  | C15-C16-C17-C18 |
| 22  | V     | 102 | PEF  | C31-C32-C33-C34 |
| 22  | V     | 101 | PEF  | O3P-C1-C2-C3    |
| 22  | V     | 102 | PEF  | O4-C10-O2-C2    |
| 23  | W     | 201 | PGT  | C5-C4-O4P-P     |
| 25  | c     | 302 | PCF  | C2-C1-O11-P     |
| 23  | L     | 402 | PGT  | O2-C2-C3-O3     |
| 23  | A     | 502 | PGT  | C43-C44-C45-C46 |
| 22  | j     | 401 | PEF  | C10-C11-C12-C13 |
| 23  | a     | 502 | PGT  | C44-C45-C46-C47 |
| 23  | j     | 408 | PGT  | C12-C11-O3-C3   |
| 26  | J     | 404 | HEM  | C4C-C3C-CAC-CBC |
| 26  | L     | 401 | HEM  | C4B-C3B-CAB-CBB |
| 23  | C     | 302 | PGT  | C18-C19-C20-C21 |
| 25  | c     | 302 | PCF  | C39-C40-C41-C42 |
| 22  | c     | 303 | PEF  | C16-C17-C18-C19 |
| 23  | j     | 408 | PGT  | O11-C11-O3-C3   |
| 23  | W     | 201 | PGT  | C22-C23-C24-C25 |
| 22  | J     | 407 | PEF  | C11-C12-C13-C14 |
| 22  | c     | 303 | PEF  | C2-C1-O3P-P     |
| 29  | K     | 603 | HEA  | CAD-CBD-CGD-O1D |
| 23  | a     | 502 | PGT  | C37-C38-C39-C40 |
| 26  | j     | 404 | HEM  | CAA-CBA-CGA-O1A |
| 29  | K     | 603 | HEA  | CAA-CBA-CGA-O1A |
| 23  | A     | 502 | PGT  | C12-C13-C14-C15 |
| 23  | A     | 502 | PGT  | C42-C43-C44-C45 |
| 26  | J     | 404 | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | H     | 102 | PGT  | C17-C18-C19-C20 |
| 26  | j     | 403 | HEM  | CAD-CBD-CGD-O1D |
| 29  | K     | 603 | HEA  | CAD-CBD-CGD-O2D |
| 25  | c     | 302 | PCF  | C3-C2-O21-C21   |
| 29  | K     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 29  | K     | 603 | HEA  | C2C-C3C-CAC-CBC |
| 26  | J     | 404 | HEM  | CAD-CBD-CGD-O2D |
| 26  | L     | 401 | HEM  | CAA-CBA-CGA-O2A |
| 22  | j     | 402 | PEF  | C11-C12-C13-C14 |
| 23  | L     | 402 | PGT  | C2-C1-O3P-P     |
| 29  | K     | 602 | HEA  | C3D-CAD-CBD-CGD |
| 29  | K     | 603 | HEA  | C2A-CAA-CBA-CGA |
| 26  | j     | 403 | HEM  | CAA-CBA-CGA-O1A |
| 26  | l     | 401 | HEM  | CAA-CBA-CGA-O2A |
| 23  | W     | 201 | PGT  | C35-C36-C37-C38 |
| 26  | j     | 403 | HEM  | CAD-CBD-CGD-O2D |
| 26  | l     | 401 | HEM  | CAD-CBD-CGD-O2D |
| 27  | J     | 405 | UQ6  | C20-C19-C21-C22 |
| 22  | j     | 401 | PEF  | C13-C14-C15-C16 |
| 22  | J     | 407 | PEF  | C15-C16-C17-C18 |
| 22  | J     | 407 | PEF  | O4-C10-O2-C2    |
| 26  | j     | 404 | HEM  | CAA-CBA-CGA-O2A |
| 22  | J     | 406 | PEF  | C13-C14-C15-C16 |
| 26  | J     | 404 | HEM  | CAD-CBD-CGD-O1D |
| 22  | H     | 101 | PEF  | C36-C37-C38-C39 |
| 29  | K     | 603 | HEA  | CAA-CBA-CGA-O2A |
| 29  | K     | 603 | HEA  | C16-C17-C18-C19 |
| 22  | V     | 101 | PEF  | O3P-C1-C2-O2    |
| 29  | K     | 603 | HEA  | C4C-C3C-CAC-CBC |
| 26  | J     | 404 | HEM  | CAA-CBA-CGA-O2A |
| 29  | K     | 603 | HEA  | C11-C12-C13-C14 |
| 26  | l     | 401 | HEM  | CAD-CBD-CGD-O1D |
| 25  | W     | 203 | PCF  | O11-C1-C2-C3    |
| 23  | L     | 402 | PGT  | O2-C31-C32-C33  |
| 22  | a     | 501 | PEF  | C2-C1-O3P-P     |
| 25  | E     | 101 | PCF  | C32-C33-C34-C35 |
| 22  | c     | 303 | PEF  | C36-C37-C38-C39 |
| 23  | a     | 502 | PGT  | C43-C44-C45-C46 |
| 23  | C     | 302 | PGT  | C38-C39-C40-C41 |
| 23  | W     | 201 | PGT  | C32-C33-C34-C35 |
| 26  | l     | 401 | HEM  | CAA-CBA-CGA-O1A |
| 23  | L     | 402 | PGT  | C16-C17-C18-C19 |

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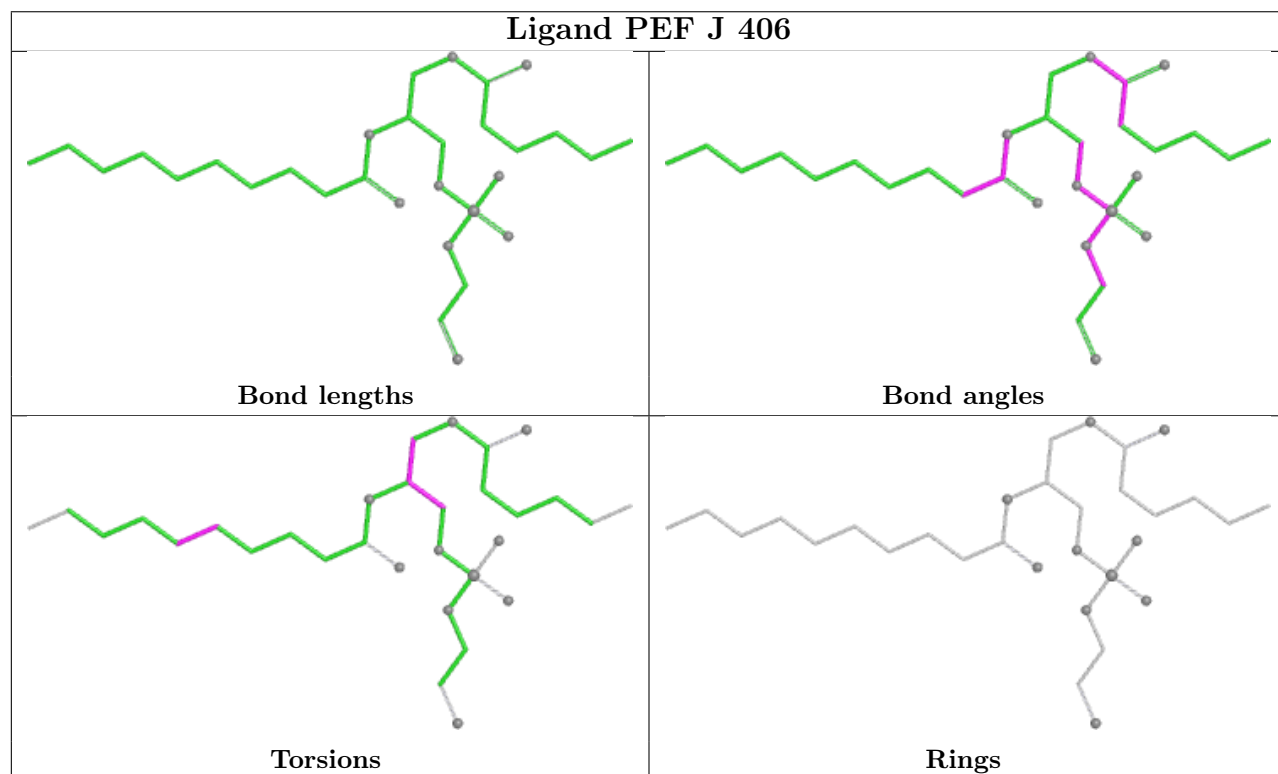
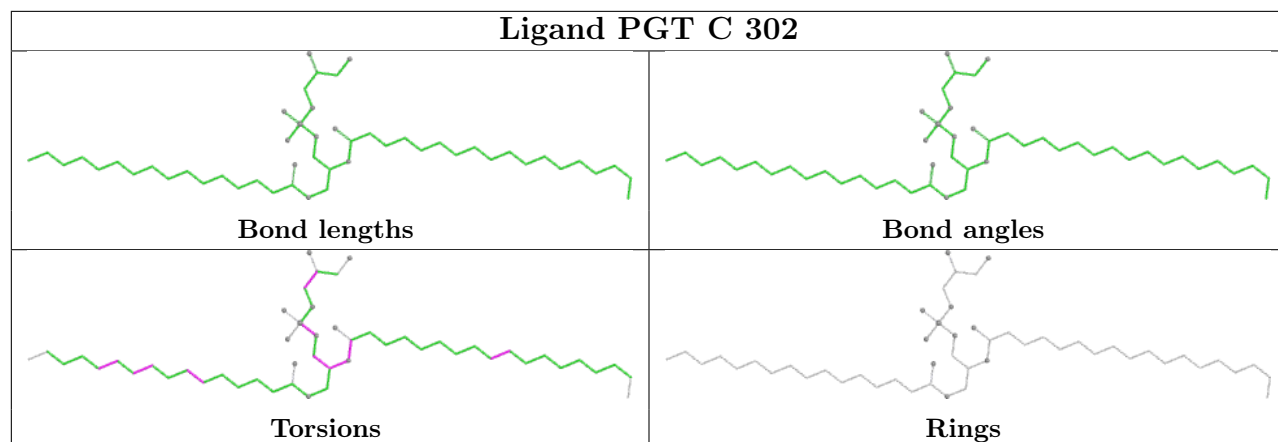
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 23  | L     | 402 | PGT  | C31-C32-C33-C34 |
| 22  | V     | 102 | PEF  | O3P-C1-C2-C3    |
| 29  | K     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 22  | J     | 401 | PEF  | C36-C37-C38-C39 |
| 22  | J     | 407 | PEF  | C11-C10-O2-C2   |
| 26  | L     | 401 | HEM  | CAA-CBA-CGA-O1A |
| 22  | H     | 101 | PEF  | C34-C35-C36-C37 |
| 23  | L     | 402 | PGT  | C13-C14-C15-C16 |
| 23  | j     | 408 | PGT  | O3P-C1-C2-O2    |
| 22  | j     | 402 | PEF  | C1-C2-C3-O3     |
| 23  | W     | 201 | PGT  | C17-C18-C19-C20 |
| 23  | W     | 201 | PGT  | C19-C20-C21-C22 |
| 23  | H     | 102 | PGT  | C16-C17-C18-C19 |
| 22  | J     | 406 | PEF  | O3P-C1-C2-C3    |
| 22  | J     | 401 | PEF  | C33-C34-C35-C36 |
| 23  | C     | 302 | PGT  | C1-C2-O2-C31    |
| 25  | W     | 203 | PCF  | C23-C24-C25-C26 |
| 29  | K     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 26  | J     | 403 | HEM  | C1A-C2A-CAA-CBA |
| 25  | c     | 302 | PCF  | C33-C34-C35-C36 |
| 23  | C     | 302 | PGT  | C20-C21-C22-C23 |
| 22  | J     | 401 | PEF  | C13-C14-C15-C16 |
| 22  | c     | 303 | PEF  | O3P-C1-C2-O2    |
| 25  | E     | 101 | PCF  | C41-C42-C43-C44 |
| 23  | W     | 201 | PGT  | C12-C13-C14-C15 |
| 27  | J     | 405 | UQ6  | C18-C19-C21-C22 |
| 22  | J     | 401 | PEF  | C38-C39-C40-C41 |
| 22  | J     | 407 | PEF  | C10-C11-C12-C13 |
| 25  | E     | 101 | PCF  | C22-C23-C24-C25 |
| 27  | j     | 405 | UQ6  | C6-C7-C8-C9     |
| 22  | J     | 401 | PEF  | C30-C31-C32-C33 |
| 22  | a     | 501 | PEF  | C32-C33-C34-C35 |
| 23  | a     | 502 | PGT  | C41-C42-C43-C44 |
| 25  | W     | 203 | PCF  | C27-C28-C29-C30 |
| 25  | c     | 302 | PCF  | C29-C30-C47-C48 |
| 26  | j     | 404 | HEM  | CAD-CBD-CGD-O2D |
| 25  | c     | 302 | PCF  | C31-C32-C33-C34 |

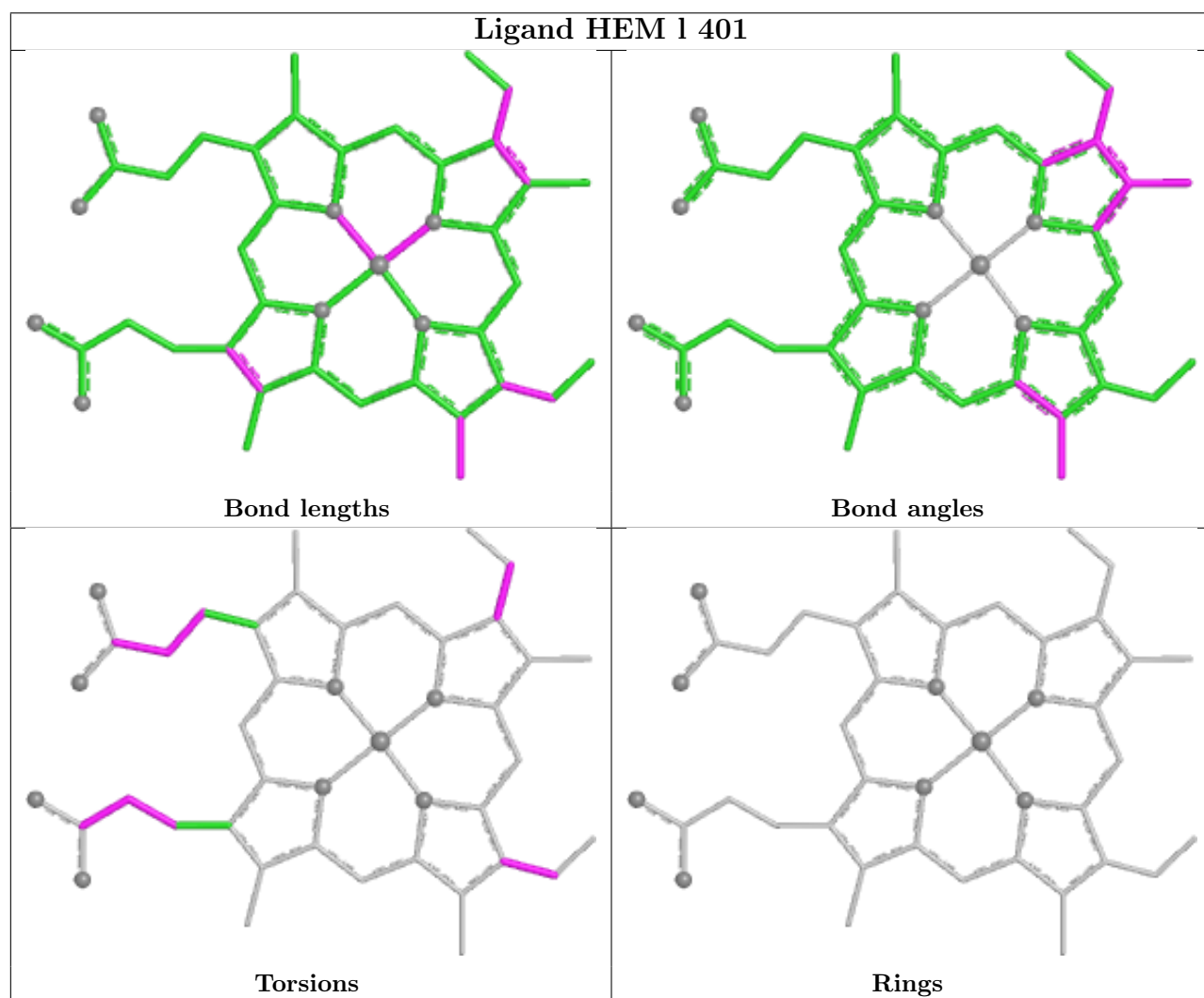
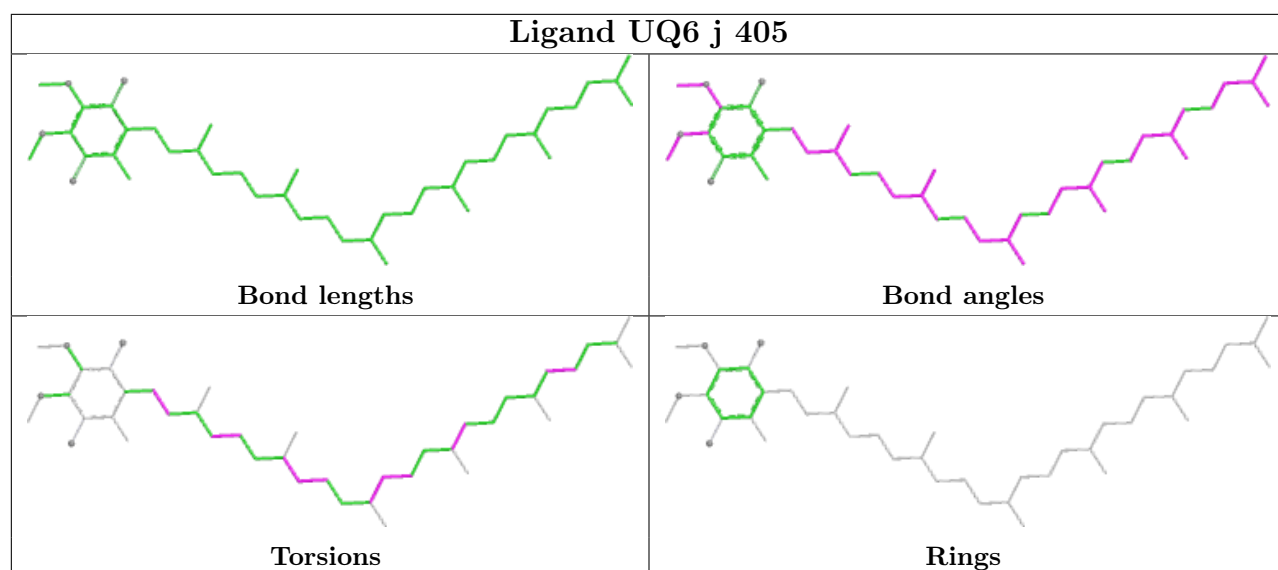
There are no ring outliers.

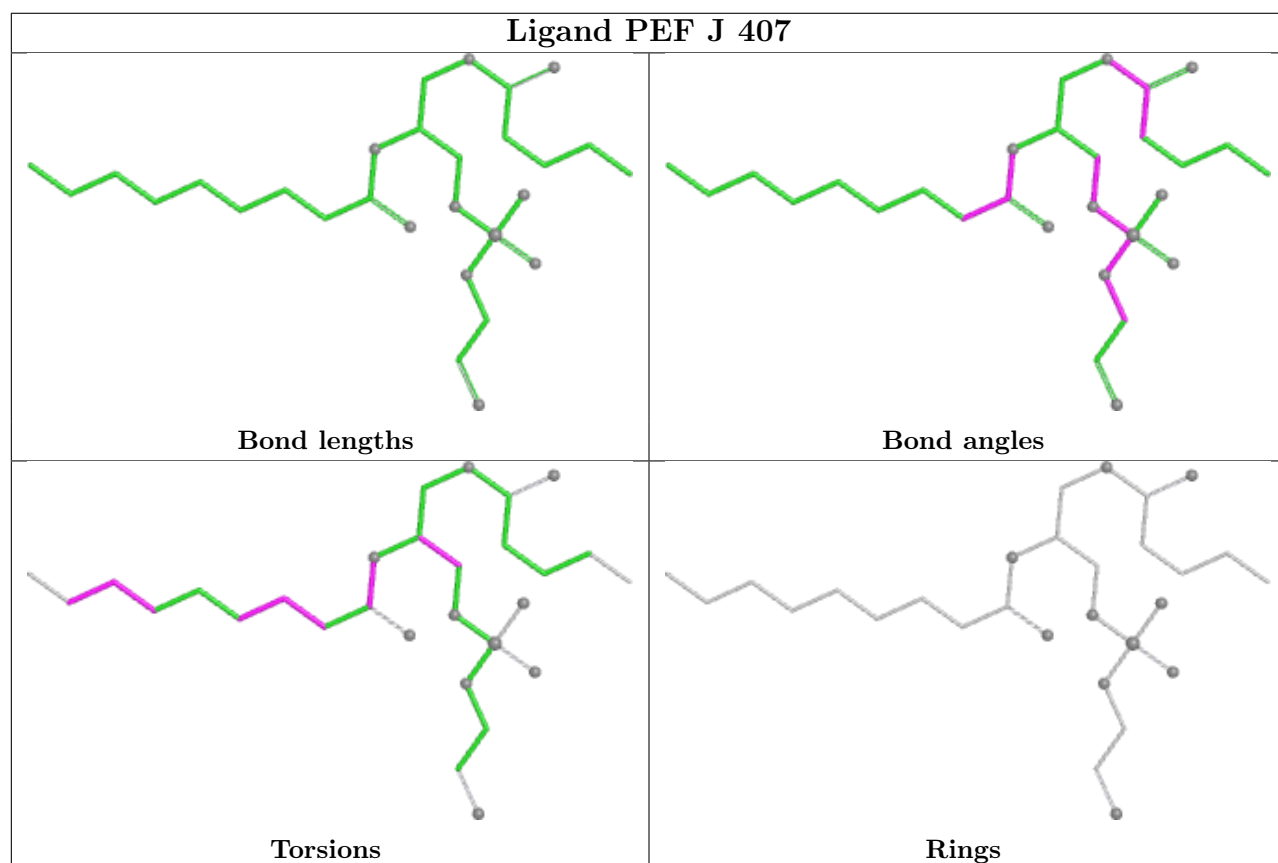
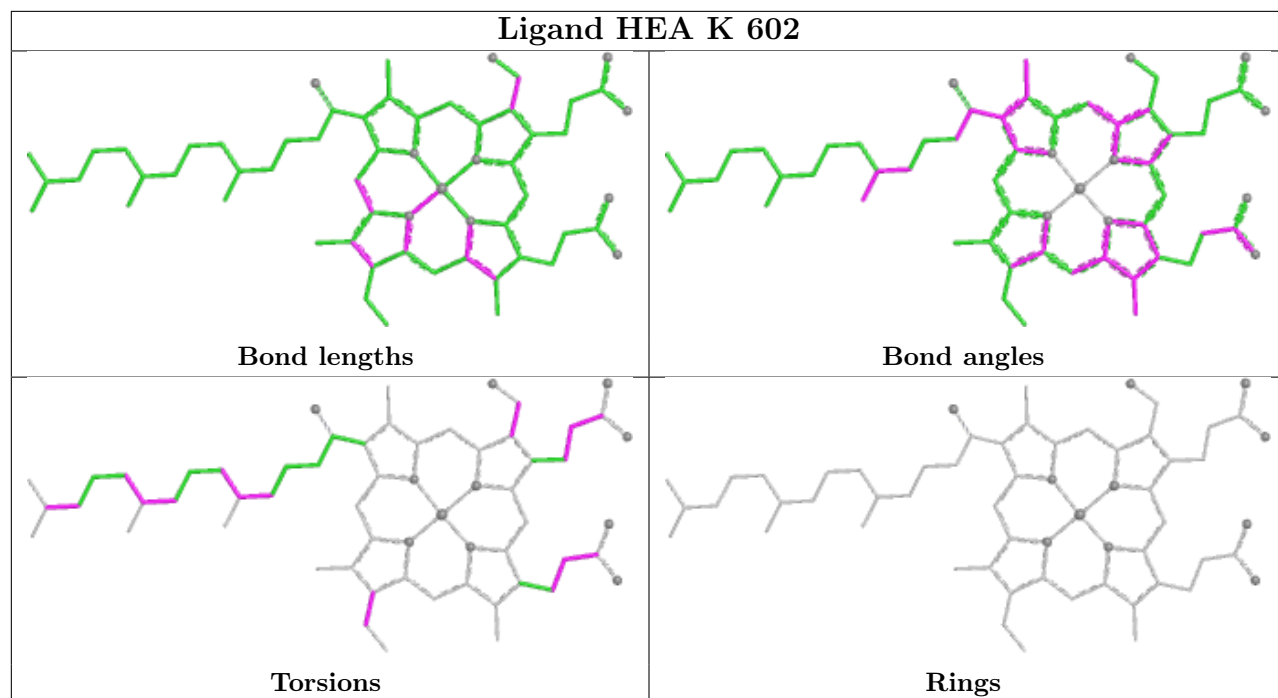
31 monomers are involved in 110 short contacts:

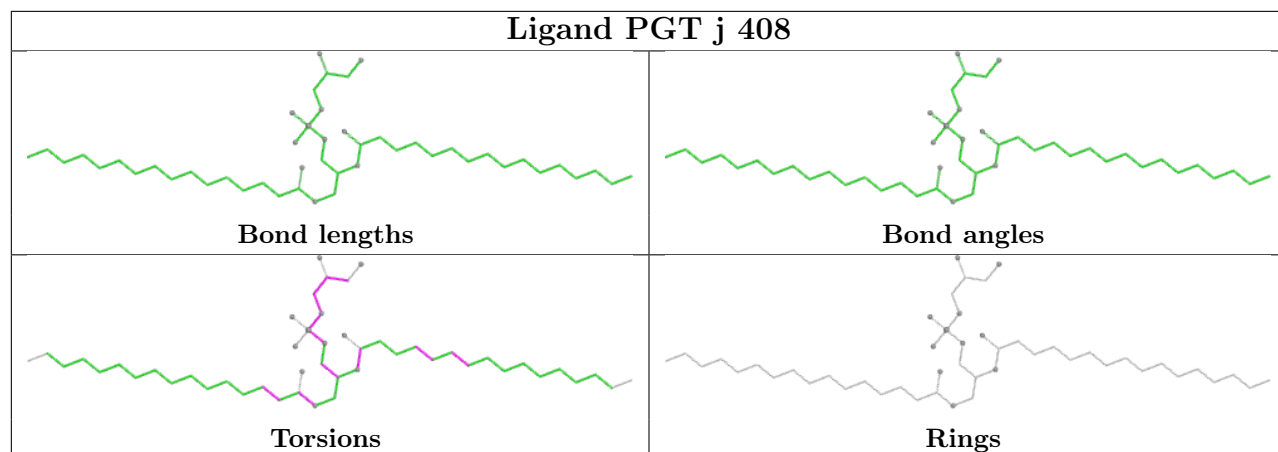
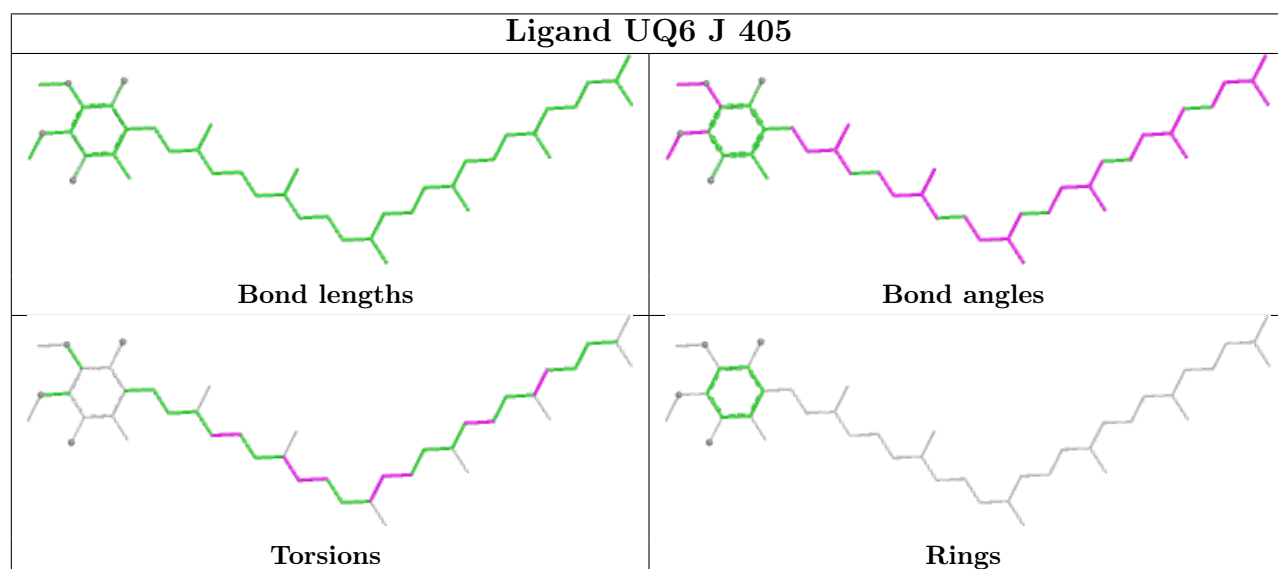
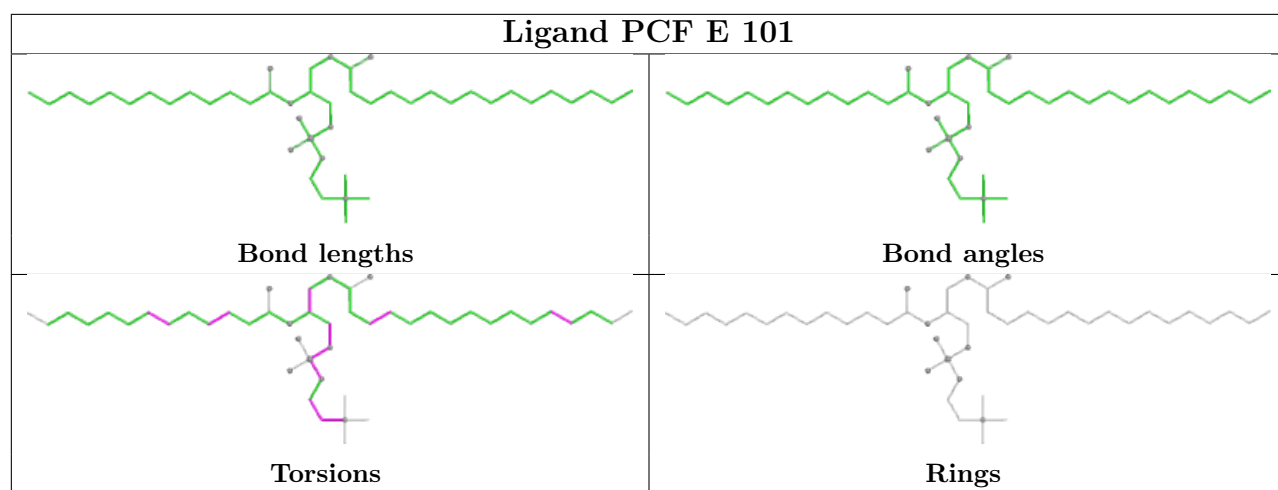
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 23  | C     | 302 | PGT  | 1       | 0            |
| 27  | j     | 405 | UQ6  | 4       | 0            |
| 26  | l     | 401 | HEM  | 13      | 0            |
| 29  | K     | 602 | HEA  | 9       | 0            |
| 22  | J     | 407 | PEF  | 1       | 0            |
| 27  | J     | 405 | UQ6  | 4       | 0            |
| 24  | c     | 301 | FES  | 2       | 0            |
| 23  | j     | 408 | PGT  | 1       | 0            |
| 23  | W     | 201 | PGT  | 3       | 0            |
| 22  | V     | 101 | PEF  | 1       | 0            |
| 22  | A     | 501 | PEF  | 2       | 0            |
| 26  | j     | 404 | HEM  | 7       | 0            |
| 22  | C     | 303 | PEF  | 1       | 0            |
| 22  | H     | 101 | PEF  | 4       | 0            |
| 26  | J     | 403 | HEM  | 3       | 0            |
| 22  | j     | 406 | PEF  | 4       | 0            |
| 22  | J     | 401 | PEF  | 1       | 0            |
| 22  | V     | 102 | PEF  | 1       | 0            |
| 22  | a     | 501 | PEF  | 1       | 0            |
| 25  | W     | 202 | PCF  | 1       | 0            |
| 22  | c     | 303 | PEF  | 5       | 0            |
| 29  | K     | 603 | HEA  | 14      | 0            |
| 24  | C     | 301 | FES  | 2       | 0            |
| 26  | L     | 401 | HEM  | 6       | 0            |
| 23  | A     | 502 | PGT  | 4       | 0            |
| 22  | j     | 401 | PEF  | 2       | 0            |
| 23  | a     | 502 | PGT  | 2       | 0            |
| 25  | c     | 302 | PCF  | 1       | 0            |
| 26  | j     | 403 | HEM  | 5       | 0            |
| 26  | J     | 404 | HEM  | 6       | 0            |
| 23  | H     | 102 | PGT  | 1       | 0            |

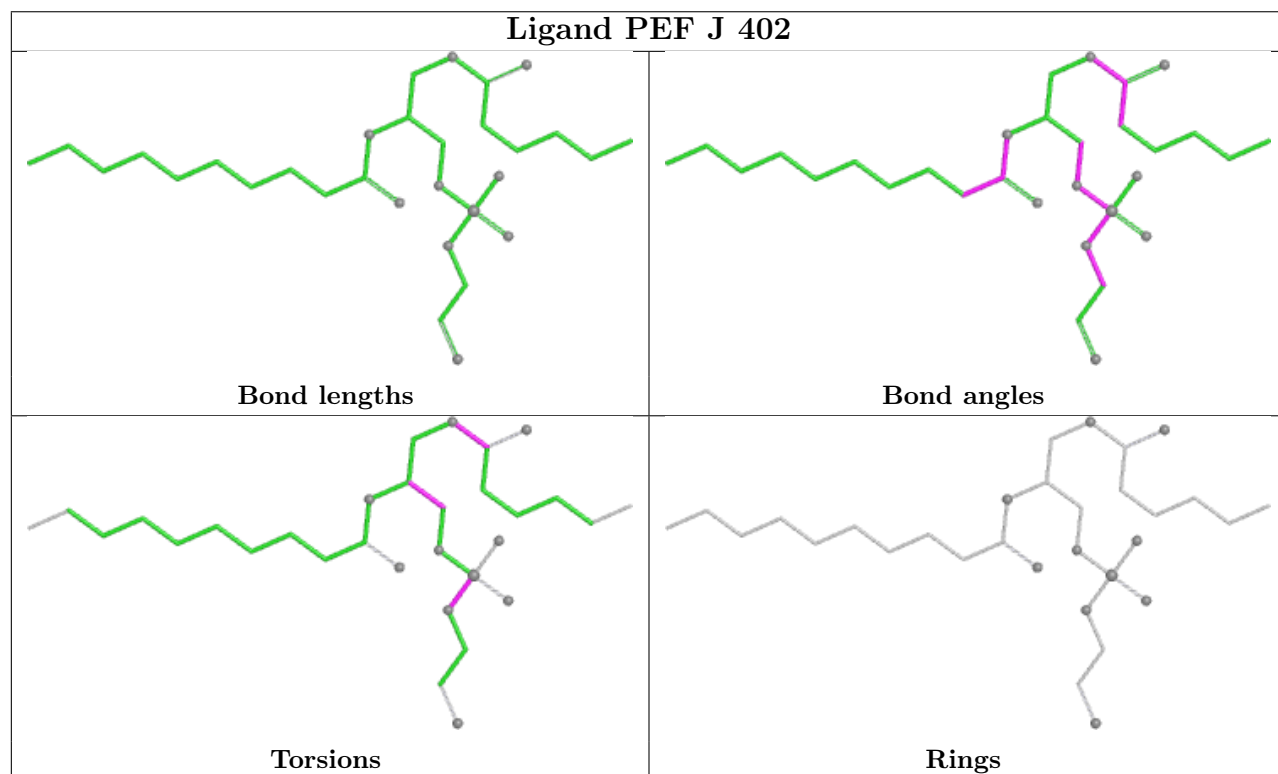
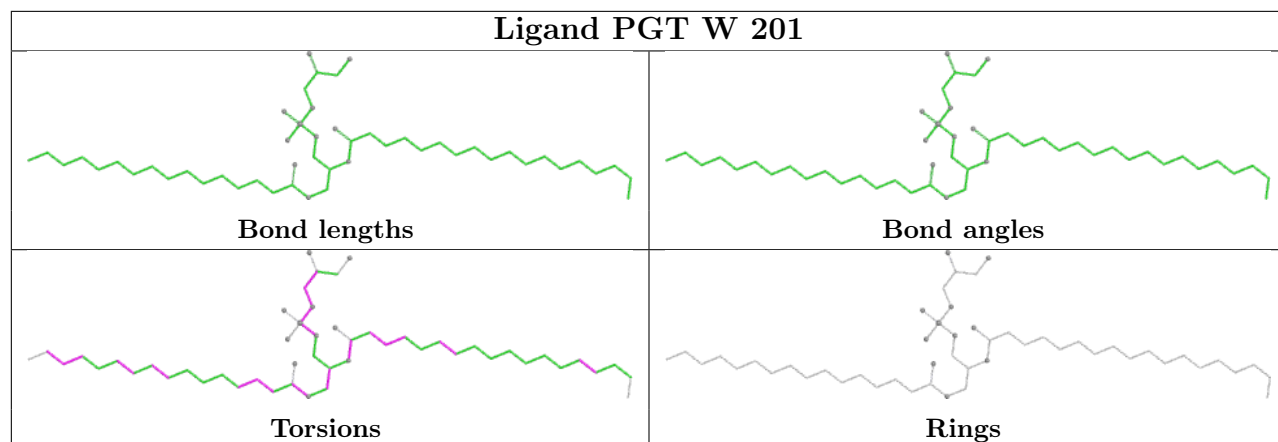
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

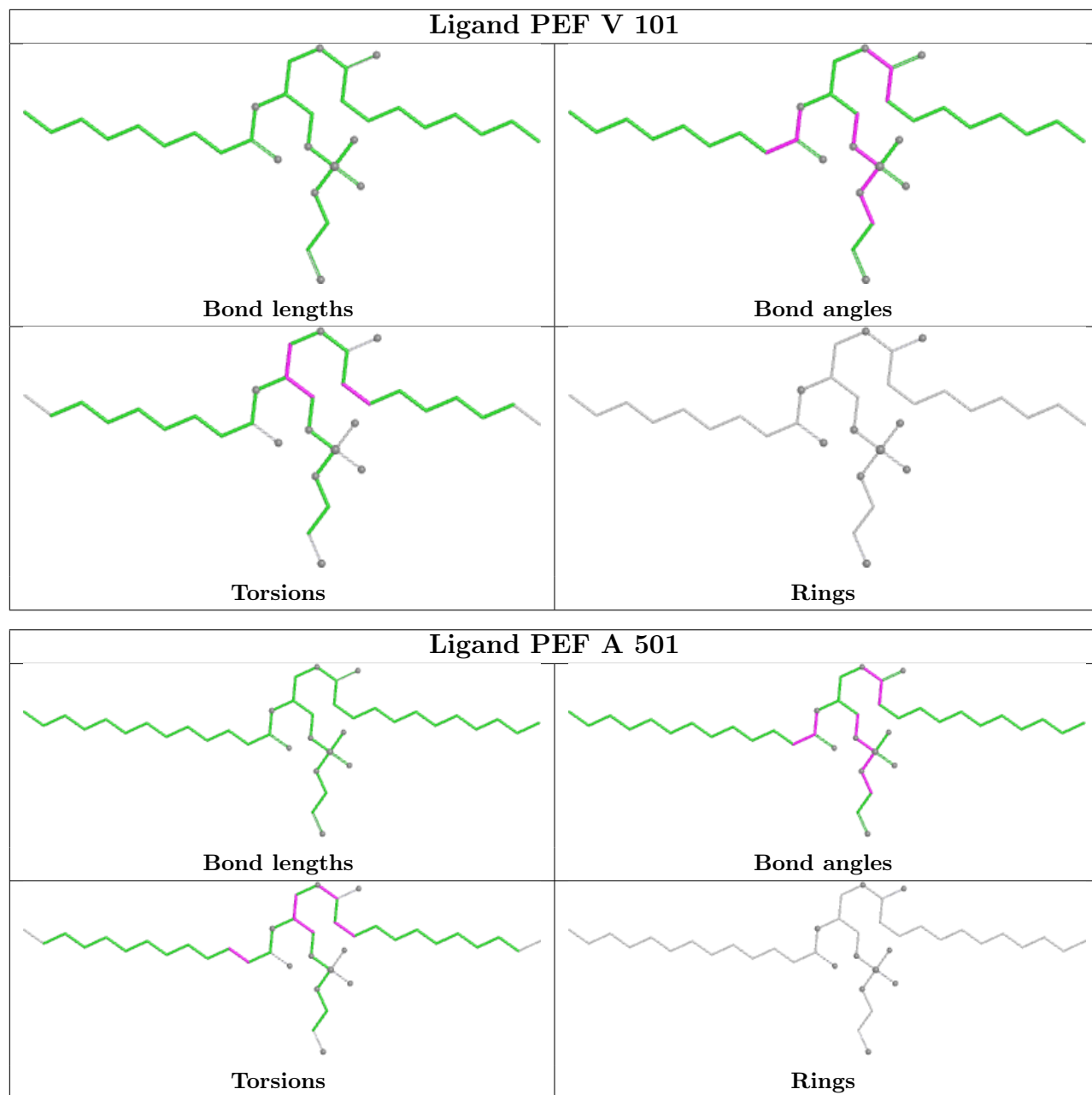




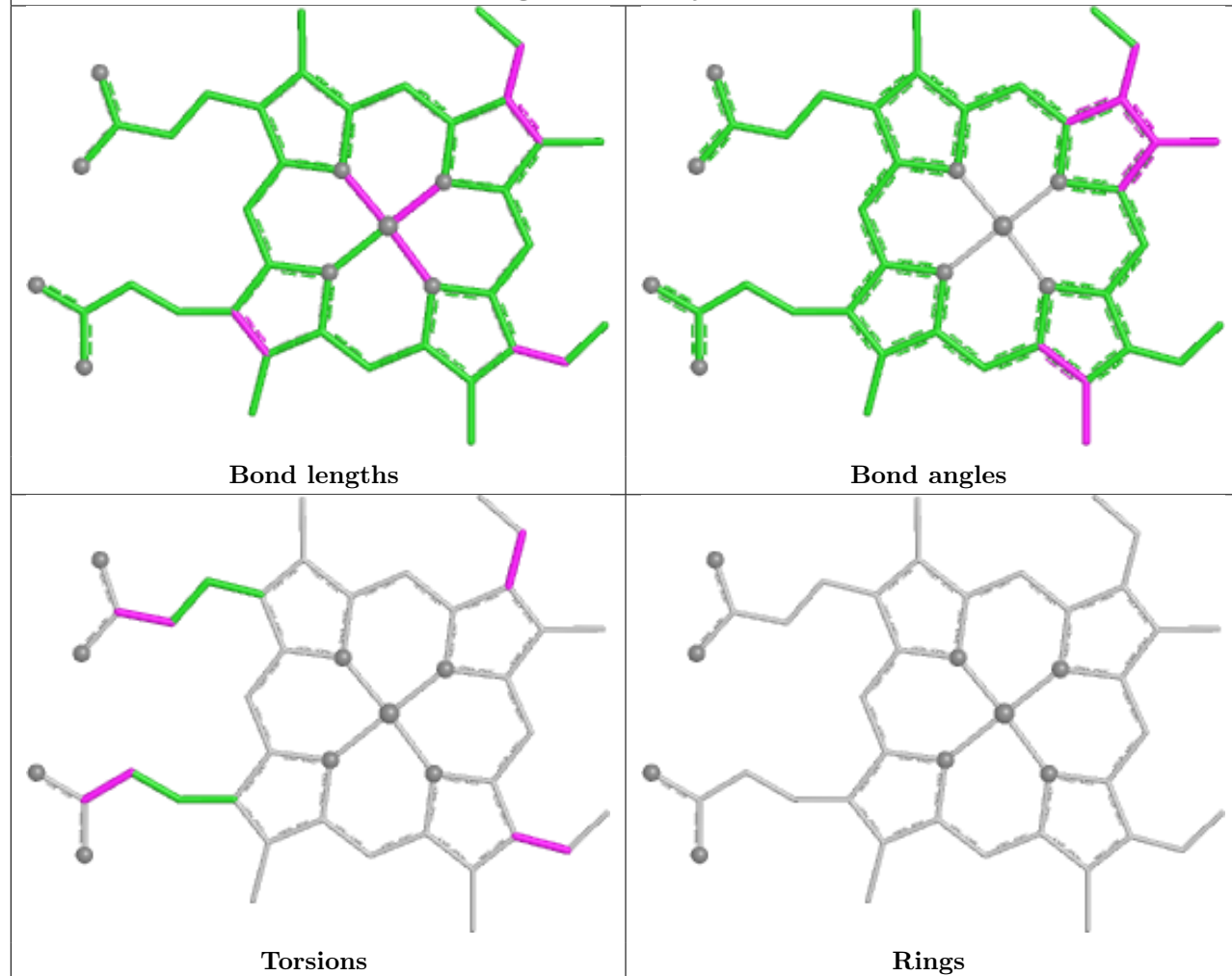




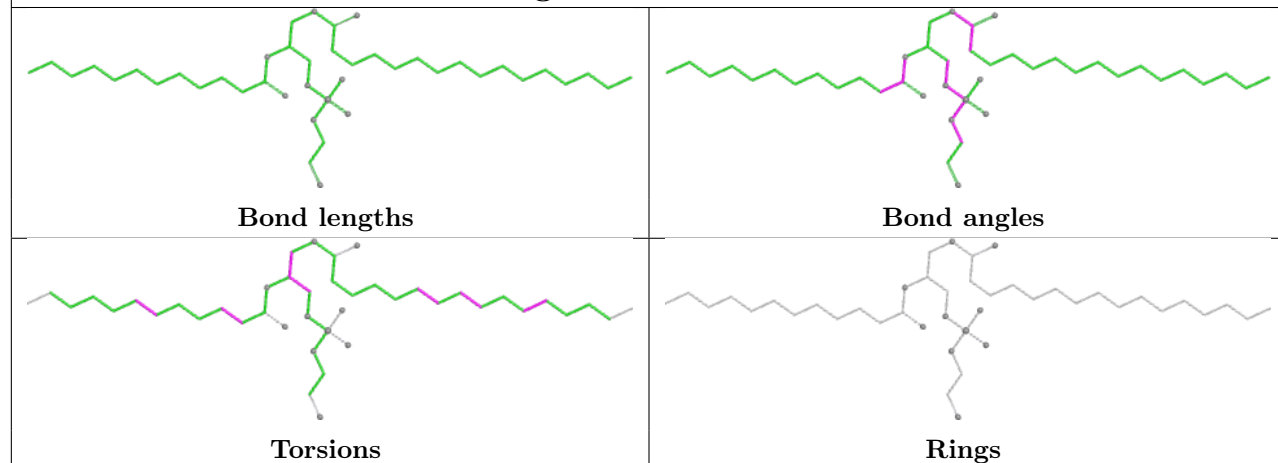




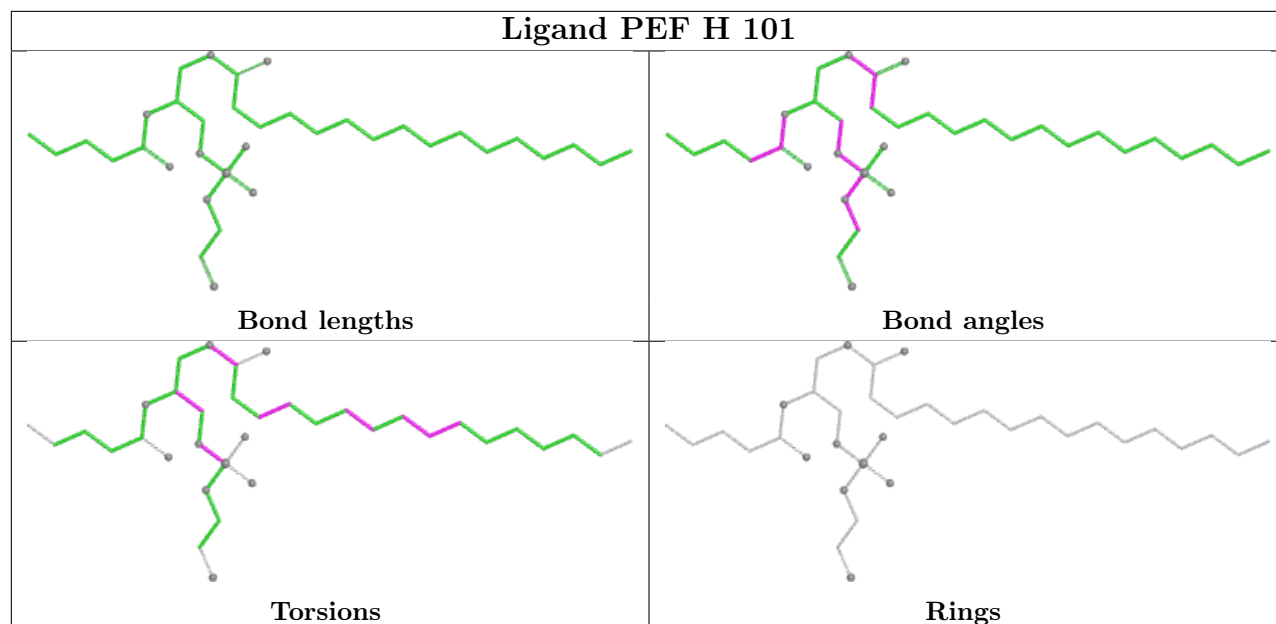
## Ligand HEM j 404



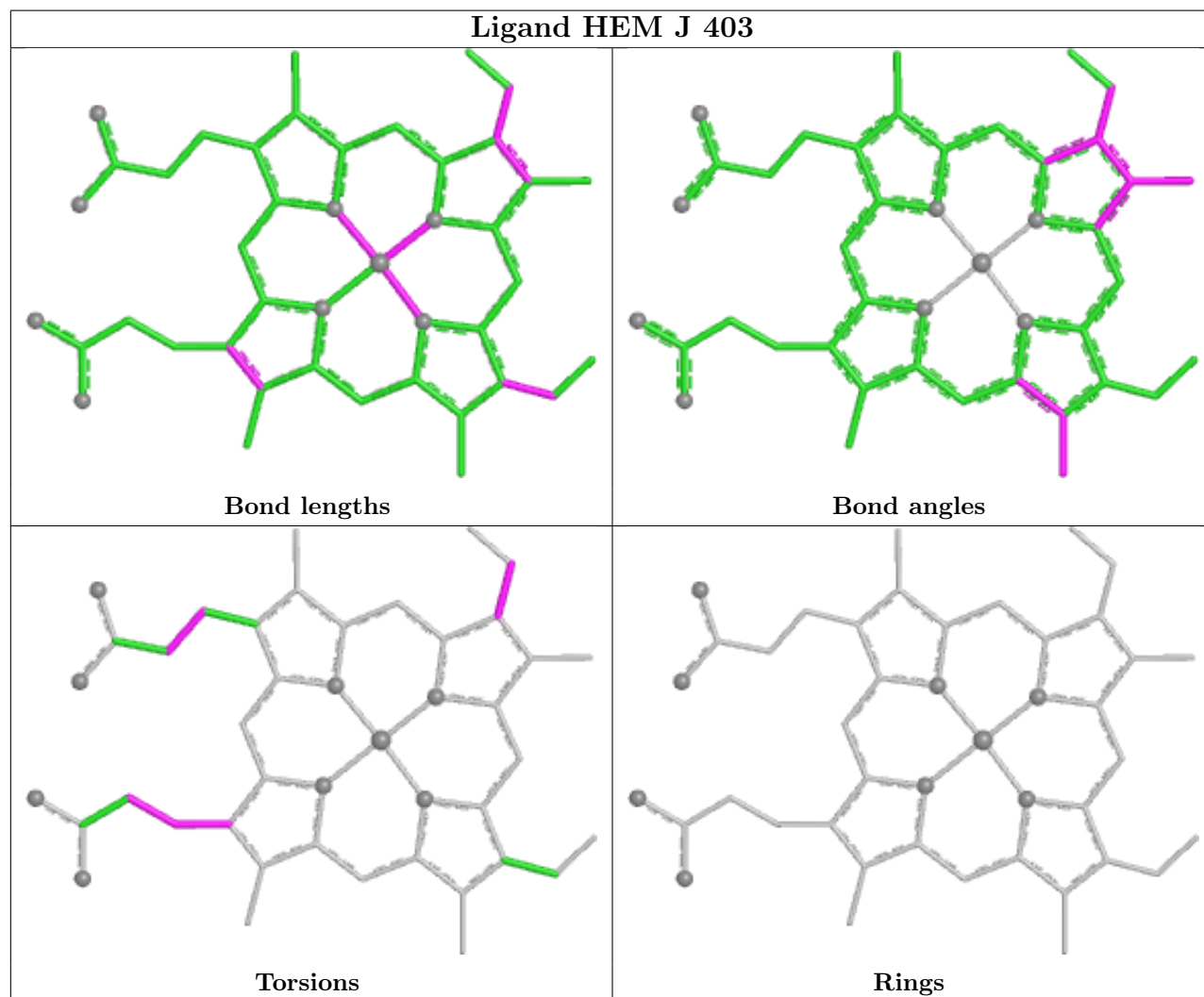
## Ligand PEF C 303

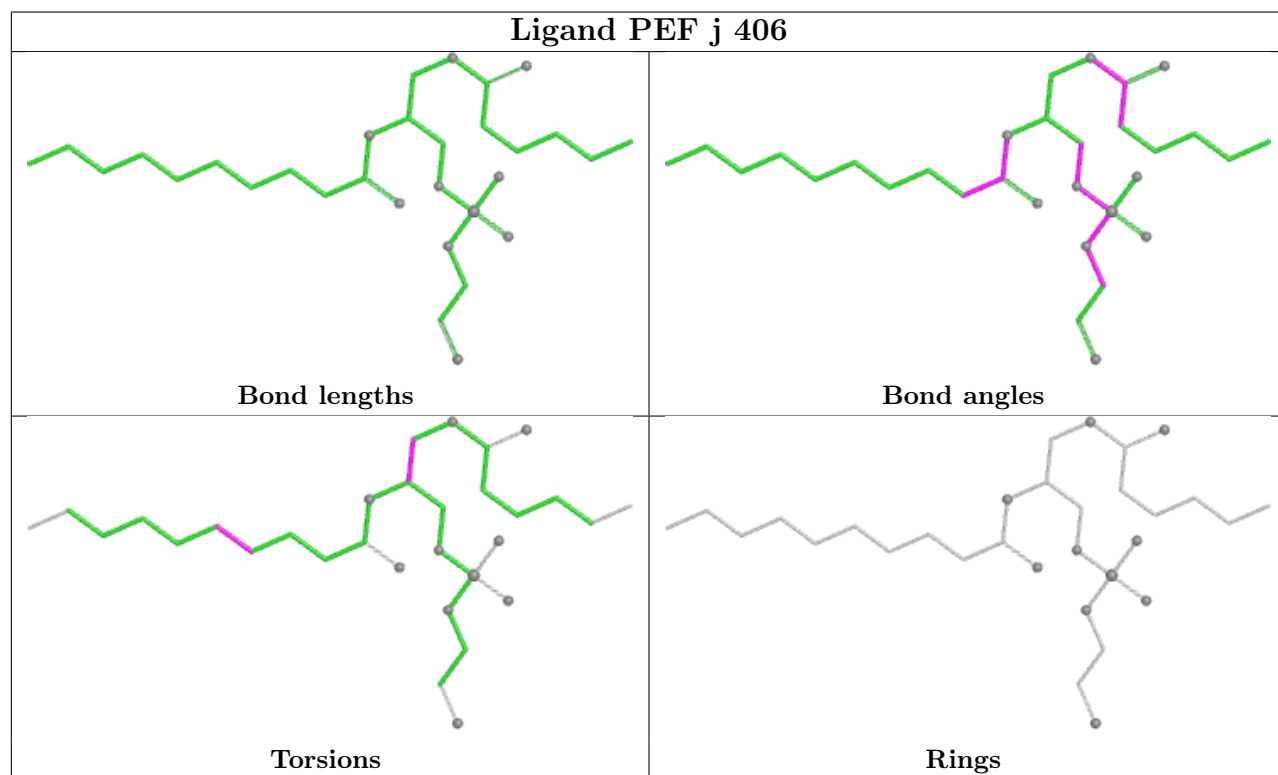
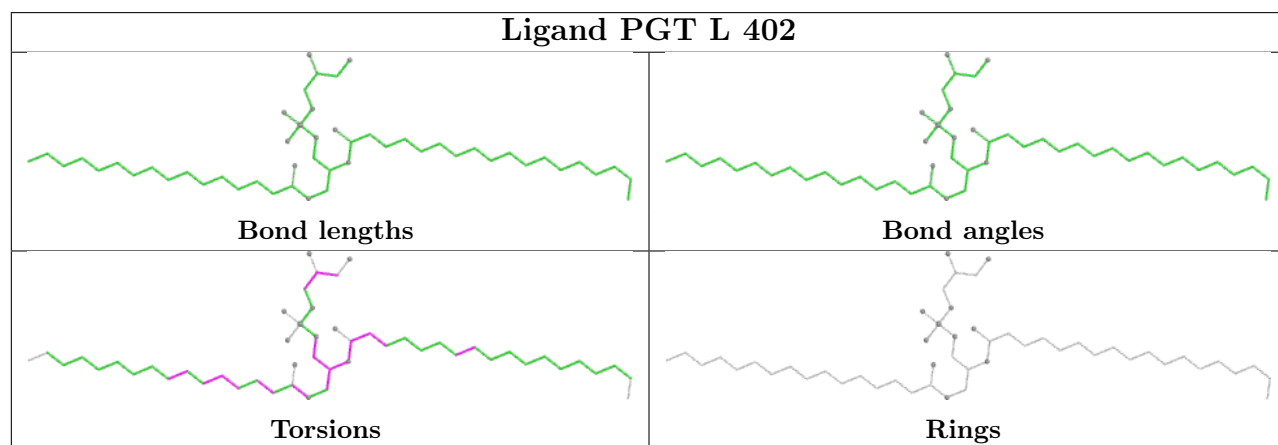
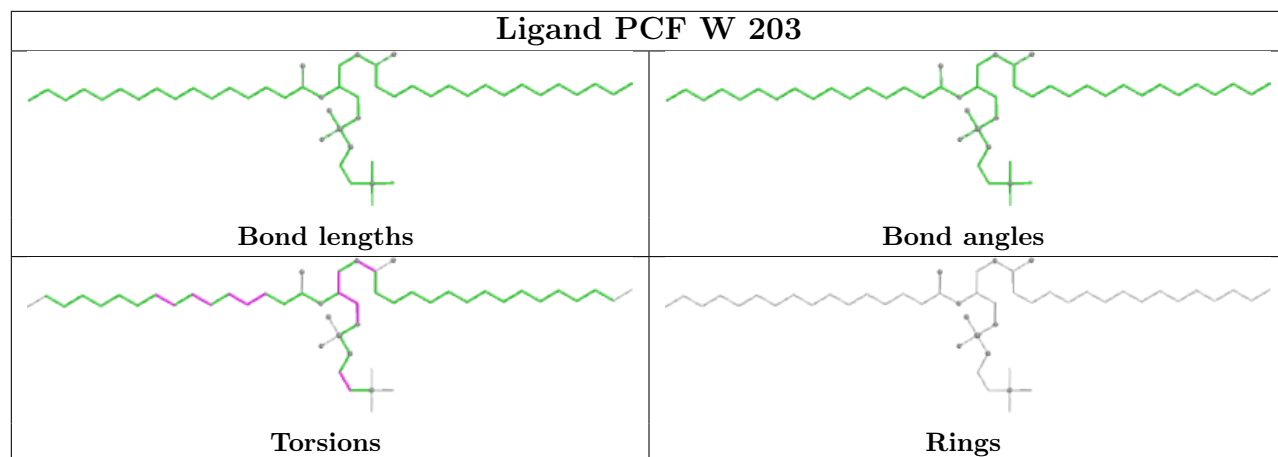


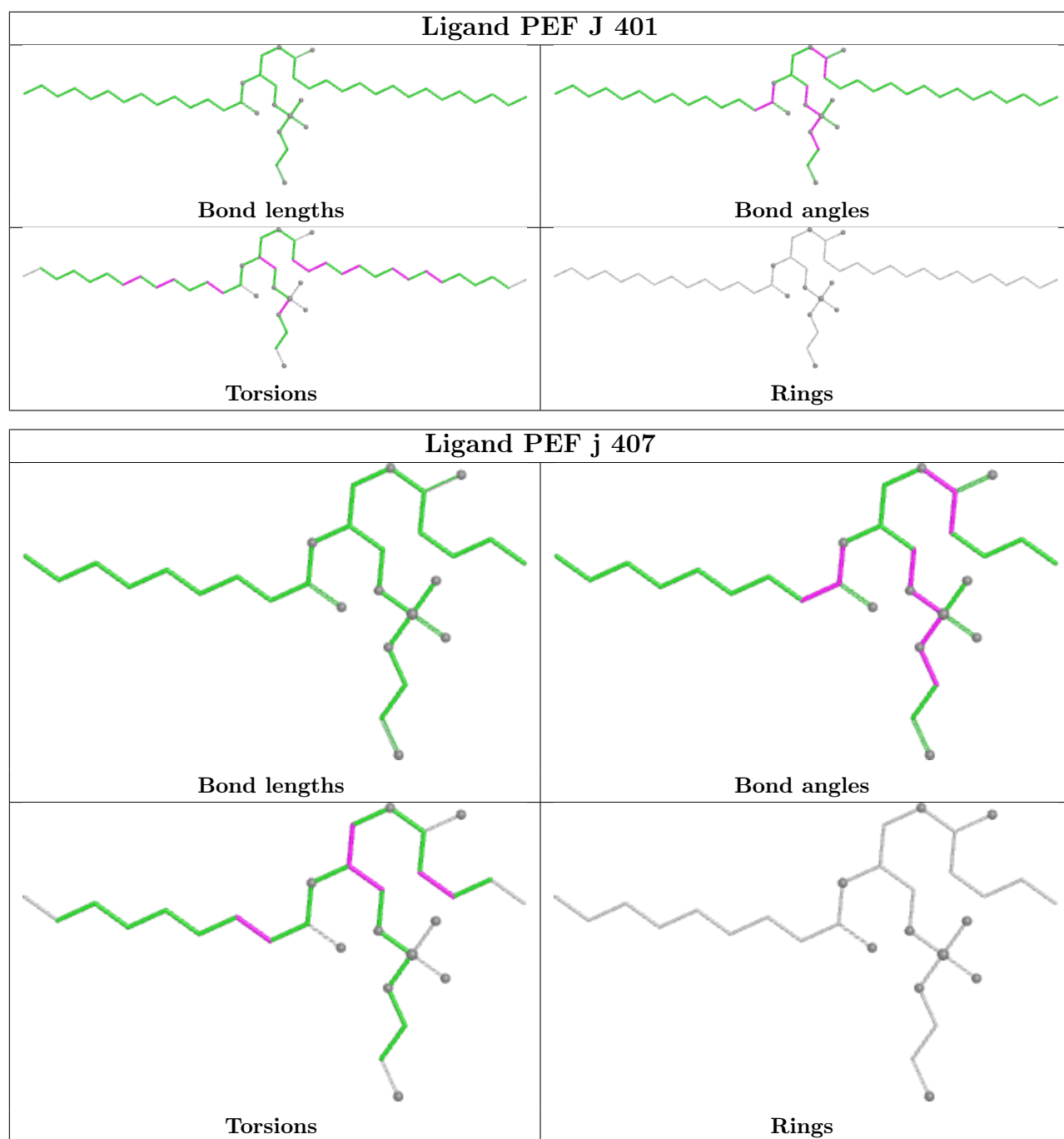
## Ligand PEF H 101

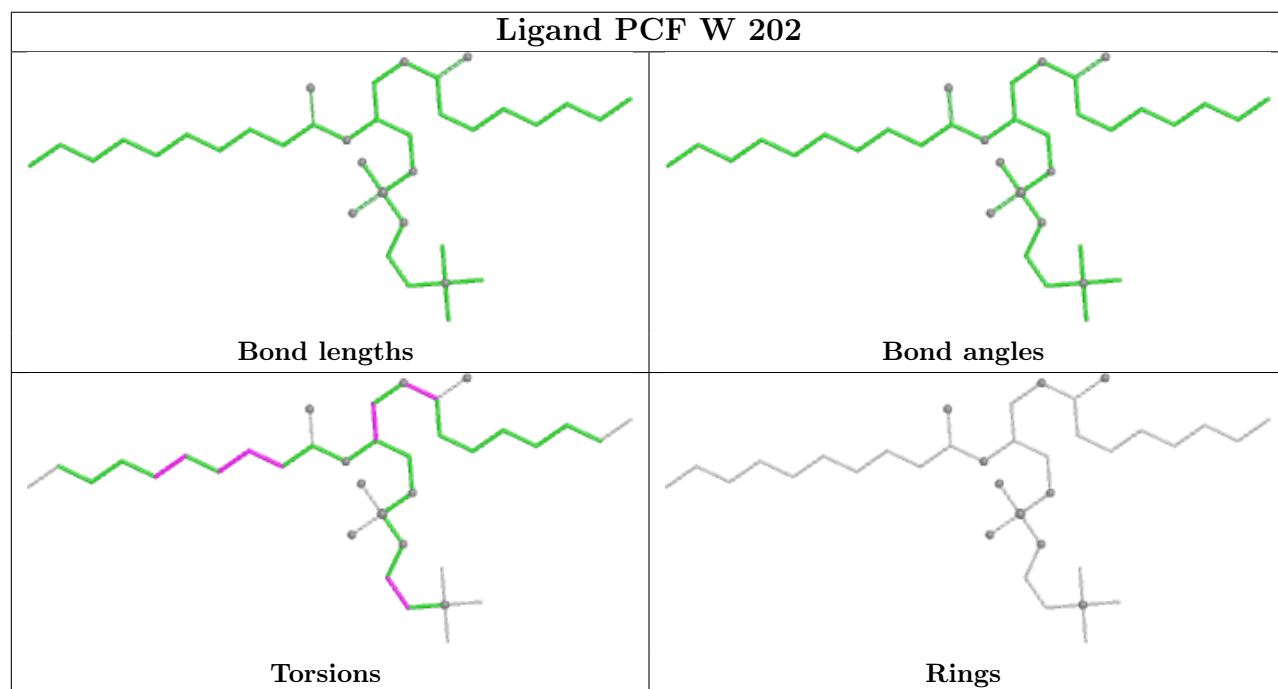
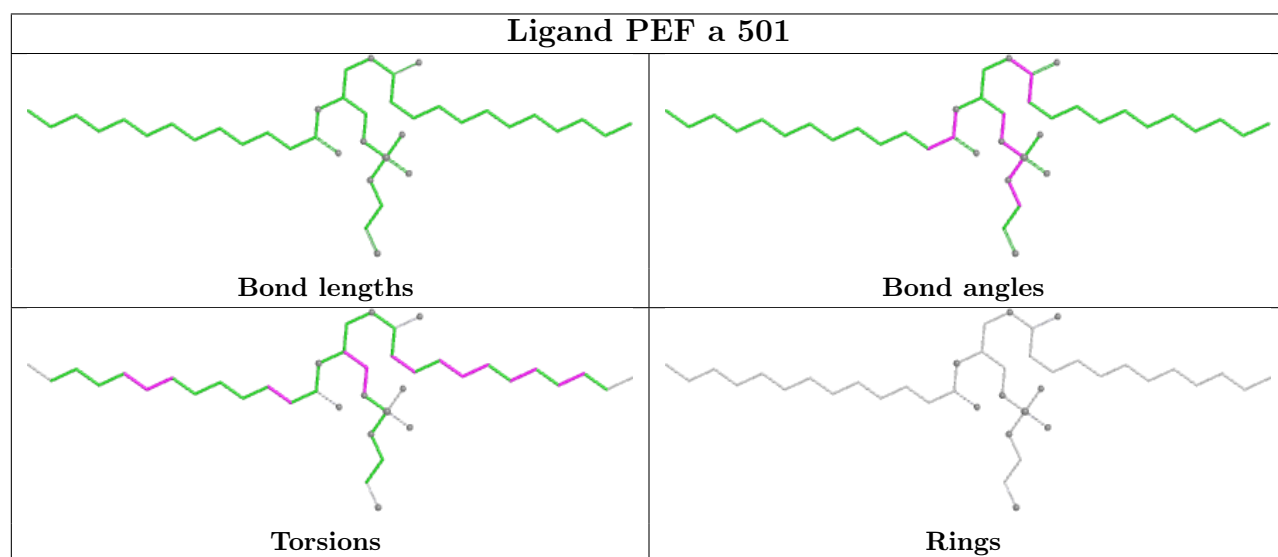
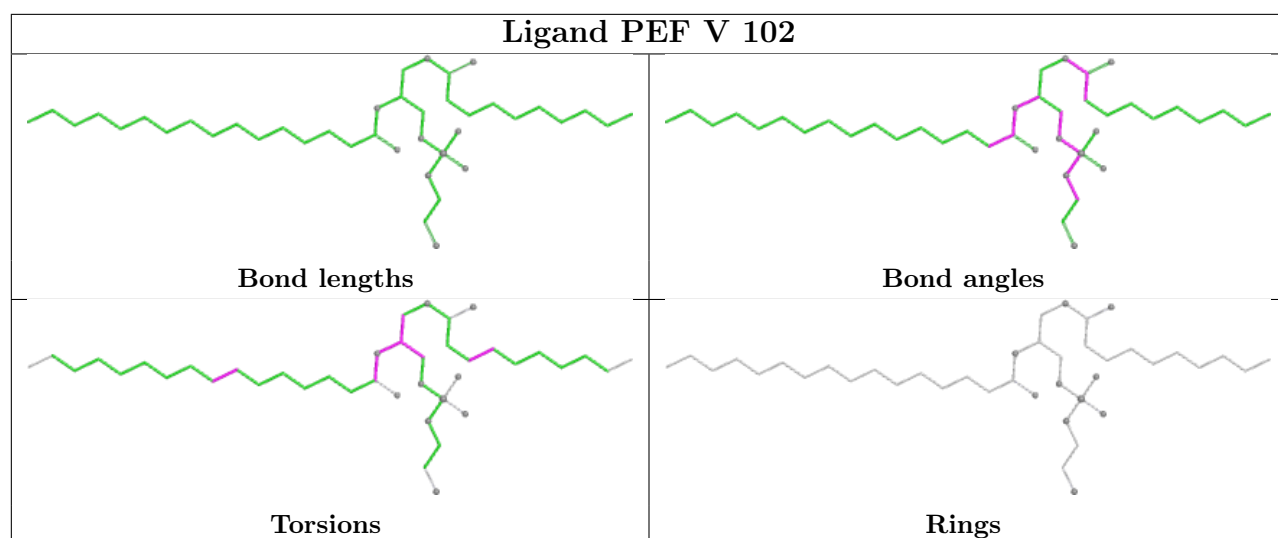


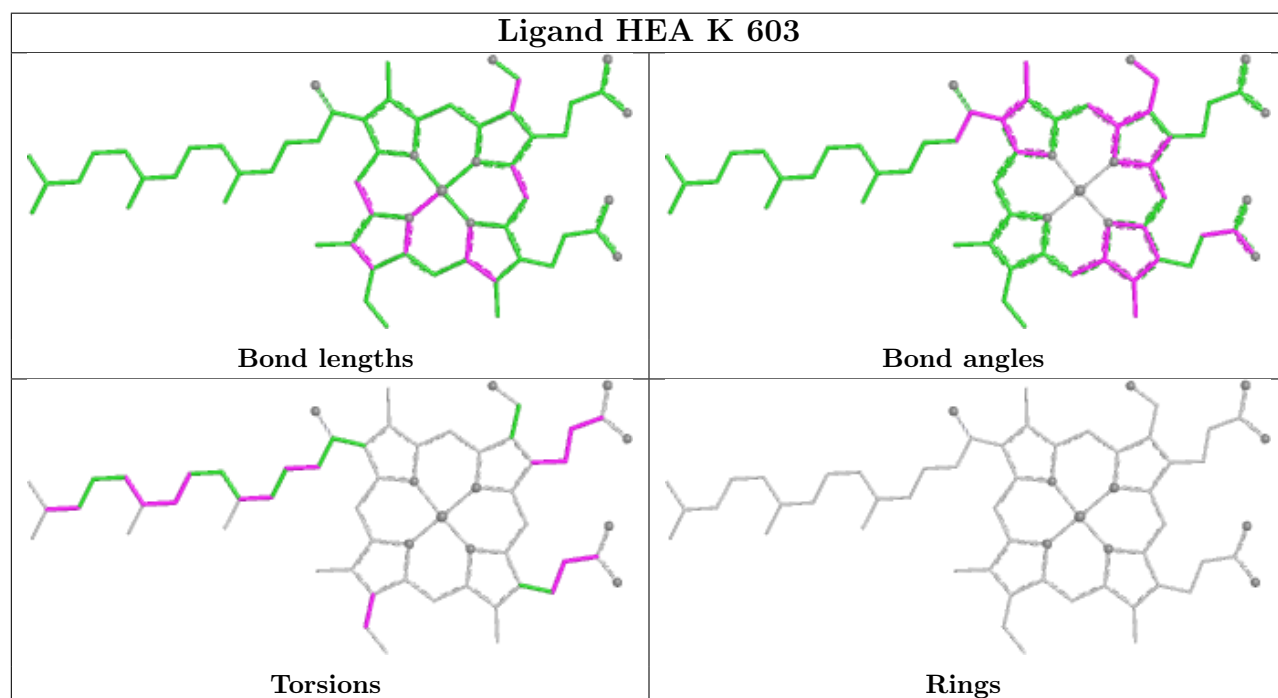
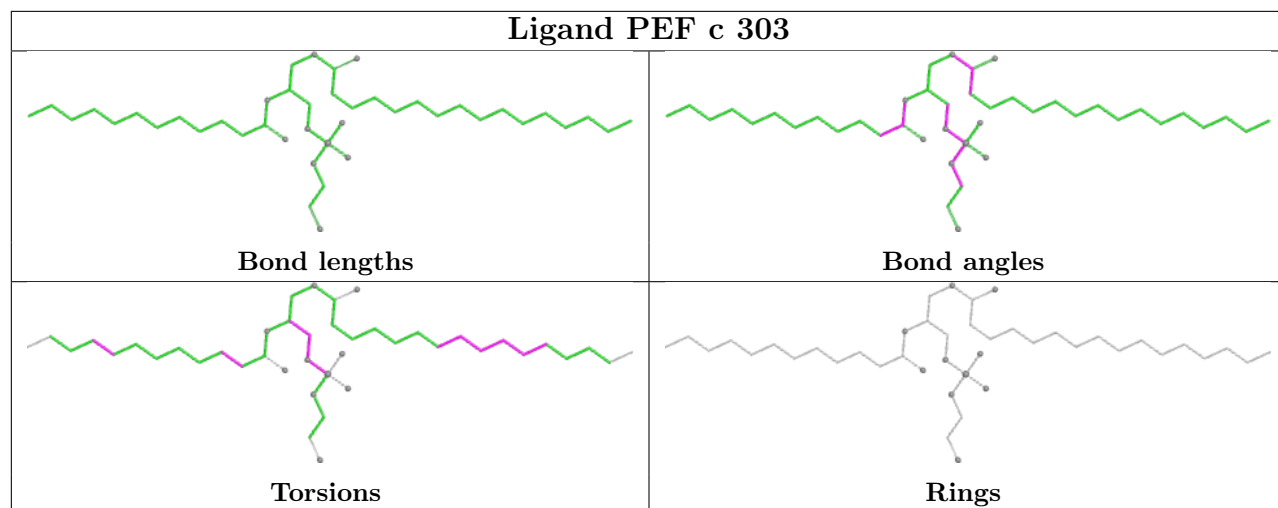
## Ligand HEM J 403

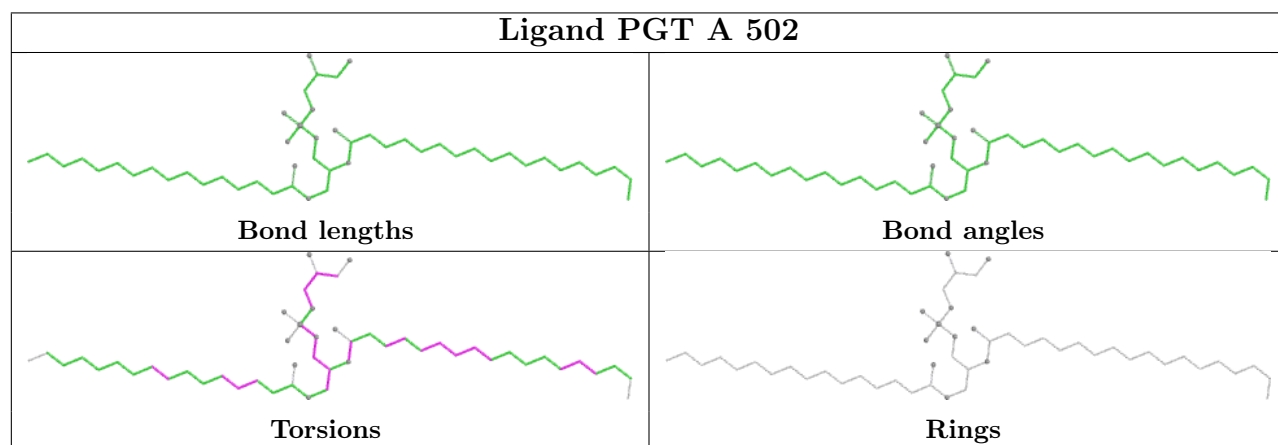
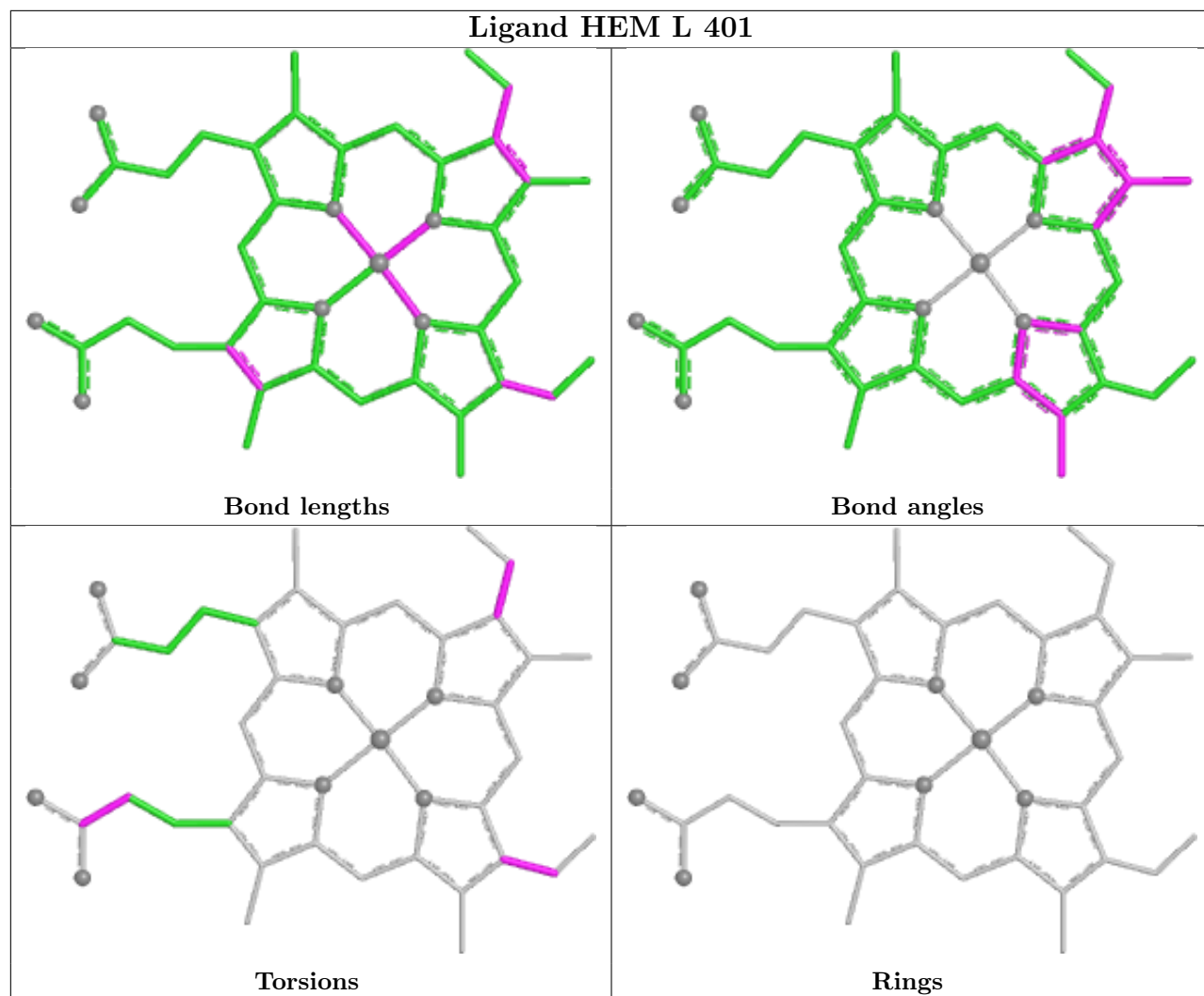


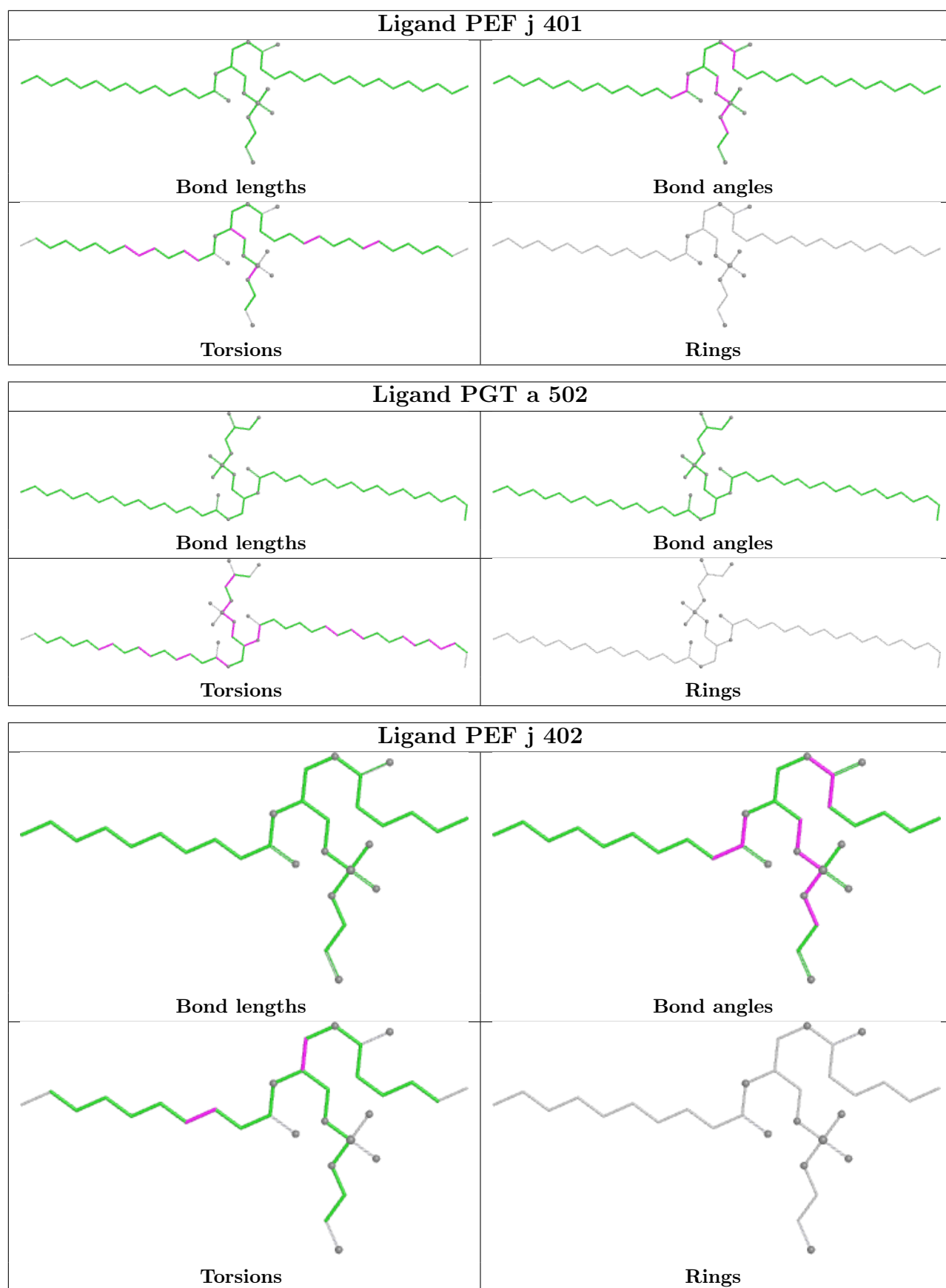




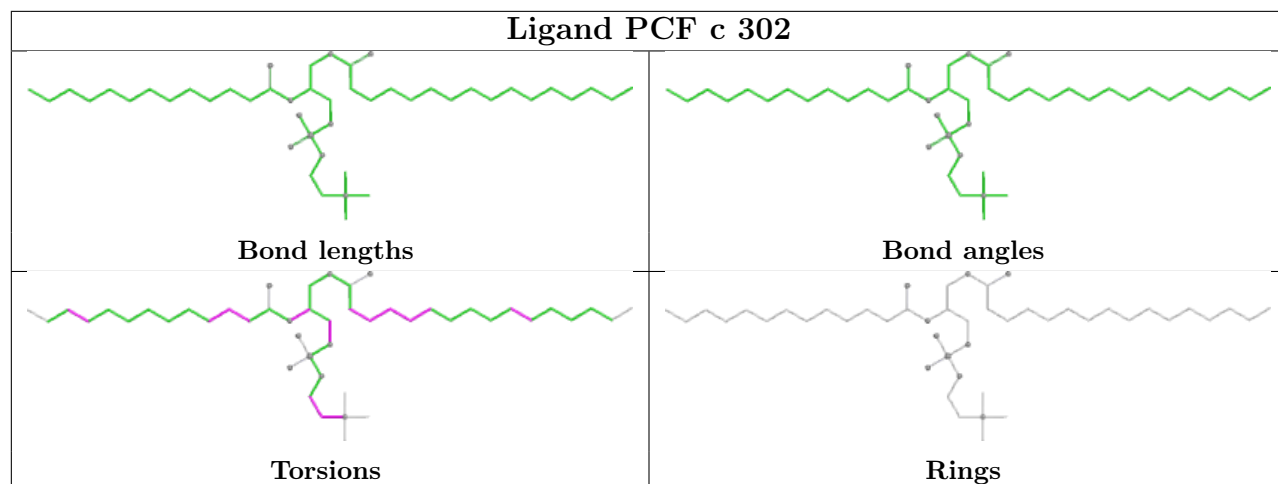




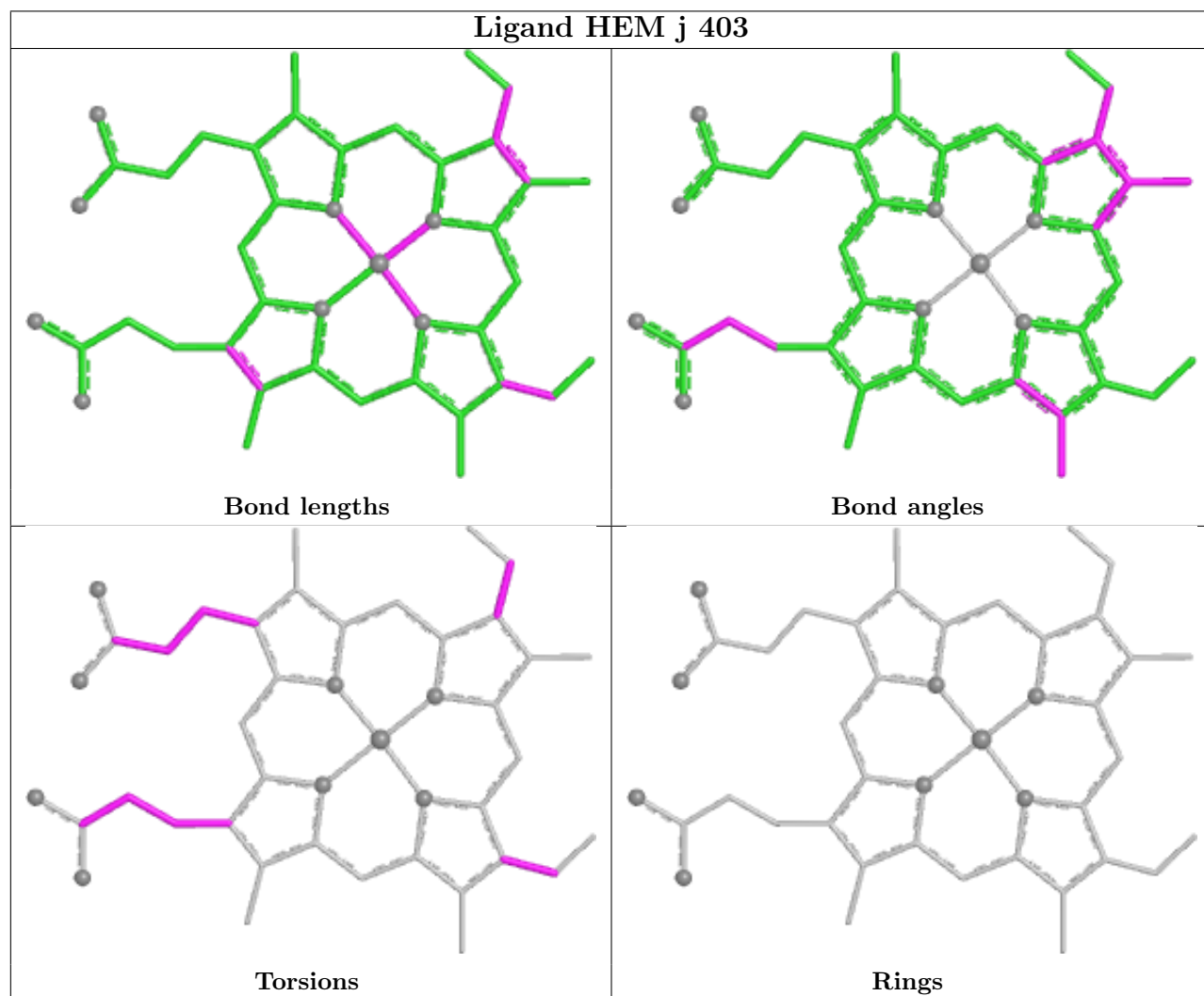


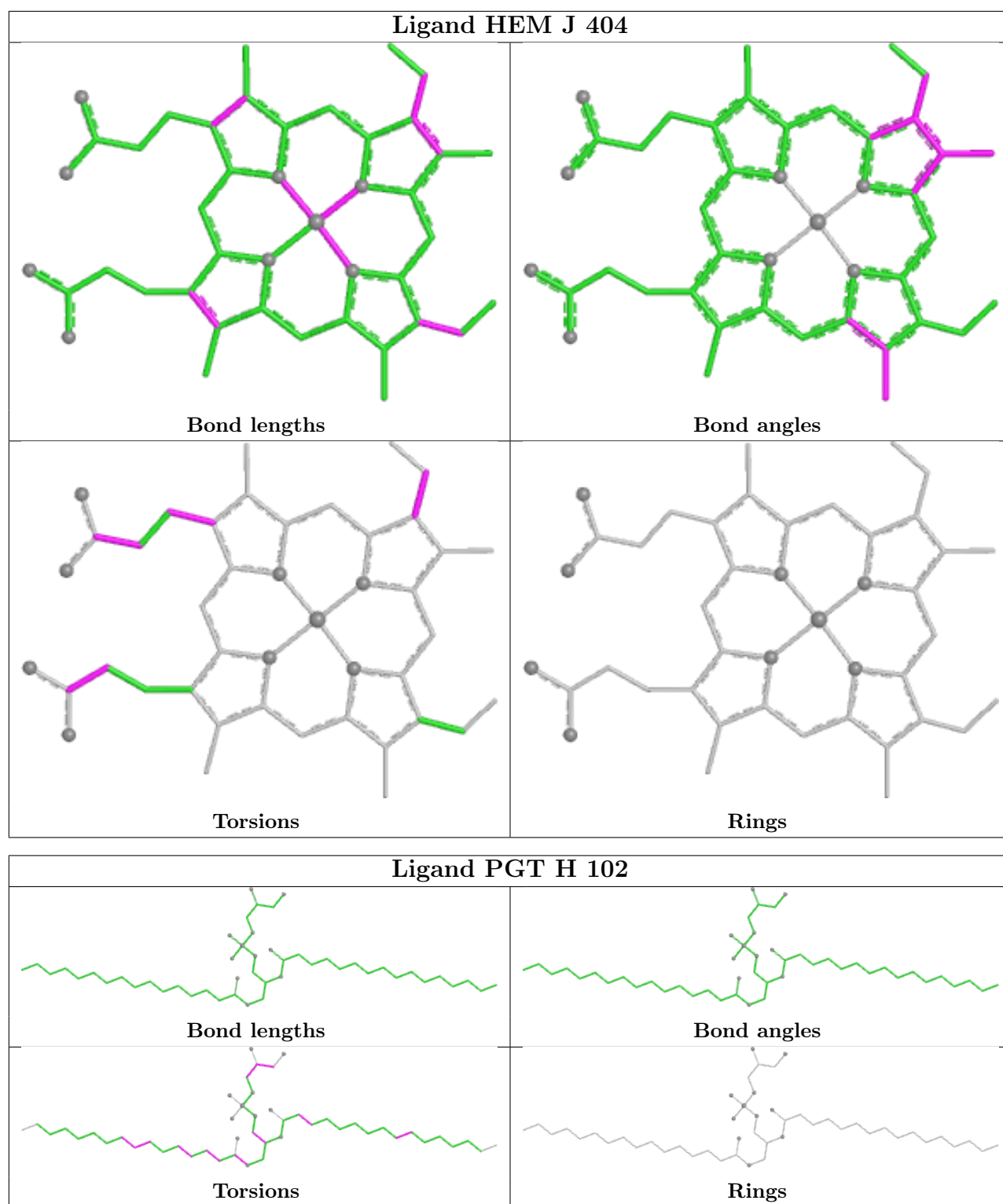


## Ligand PCF c 302



## Ligand HEM j 403





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

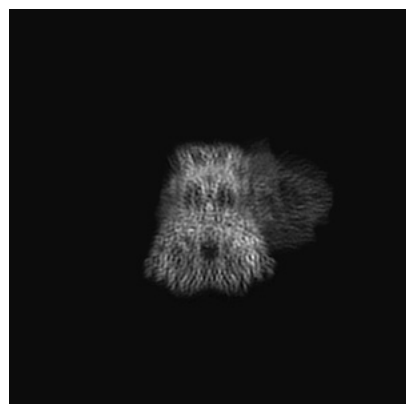
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28011. These allow visual inspection of the internal detail of the map and identification of artifacts.

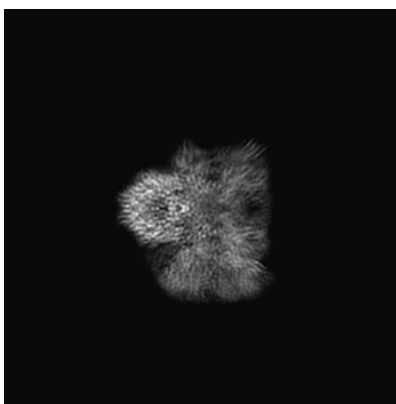
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

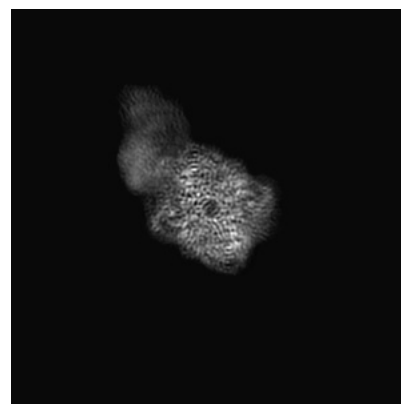
#### 6.1.1 Primary map



X

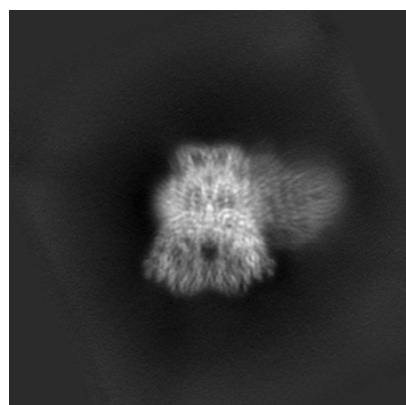


Y

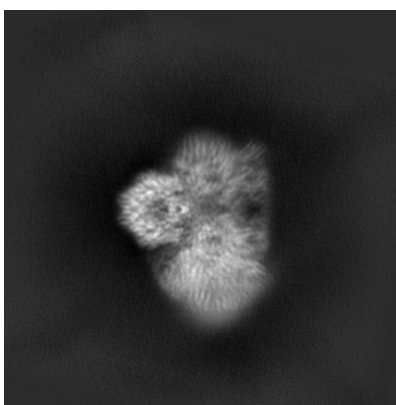


Z

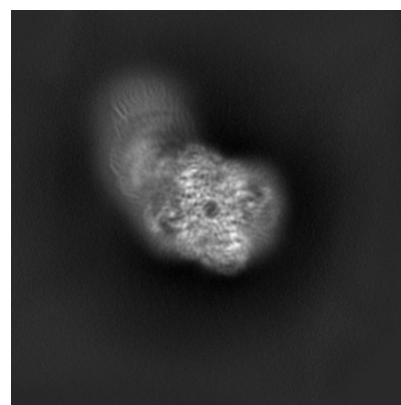
#### 6.1.2 Raw map



X



Y

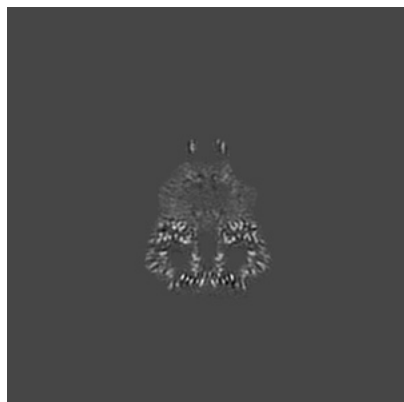


Z

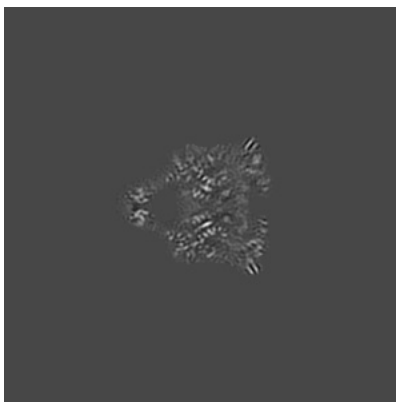
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

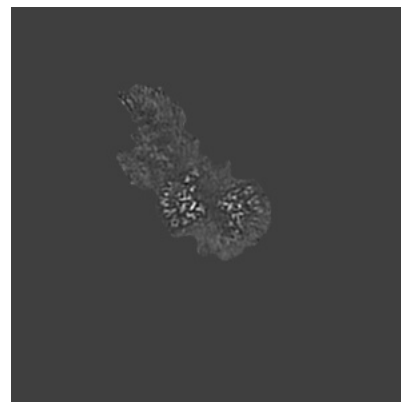
### 6.2.1 Primary map



X Index: 180

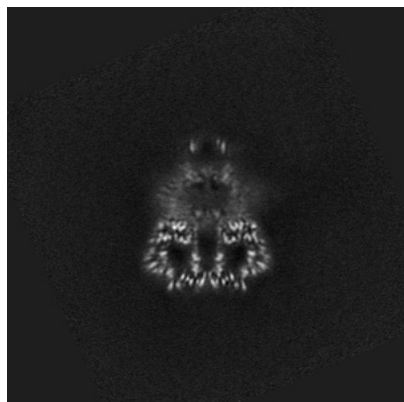


Y Index: 180

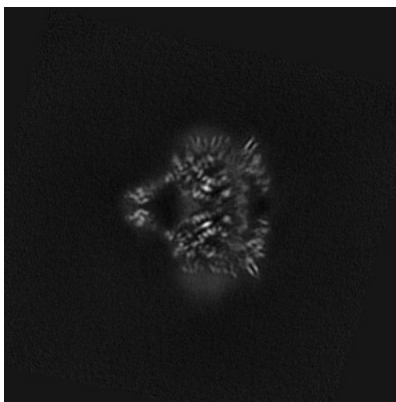


Z Index: 180

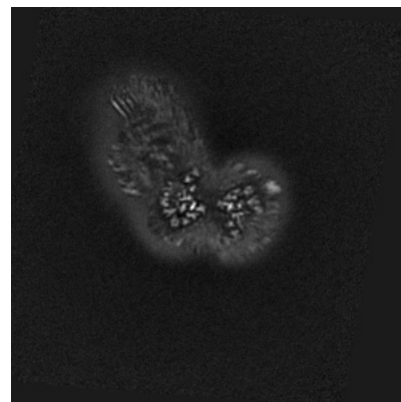
### 6.2.2 Raw map



X Index: 180



Y Index: 180

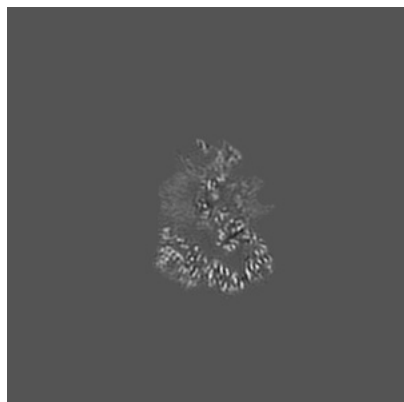


Z Index: 180

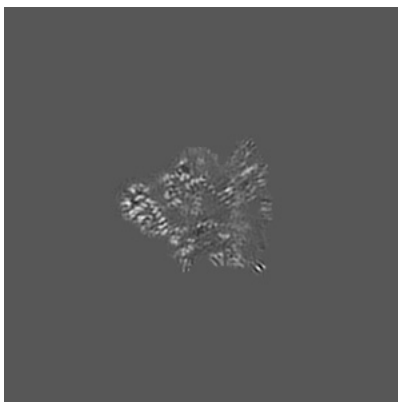
The images above show central slices of the map in three orthogonal directions.

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

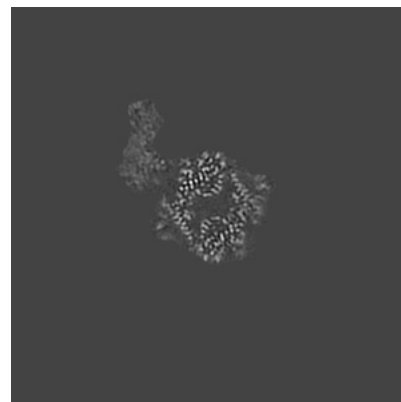
### 6.3.1 Primary map



X Index: 168

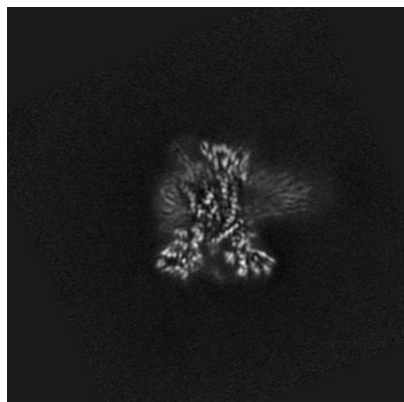


Y Index: 170

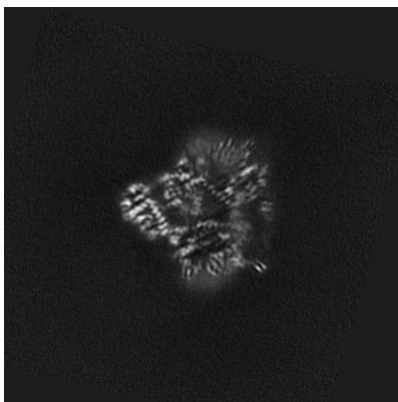


Z Index: 155

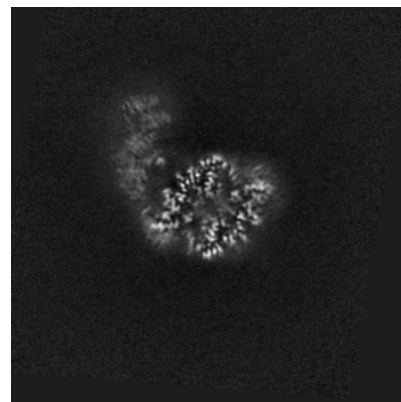
### 6.3.2 Raw map



X Index: 158



Y Index: 170

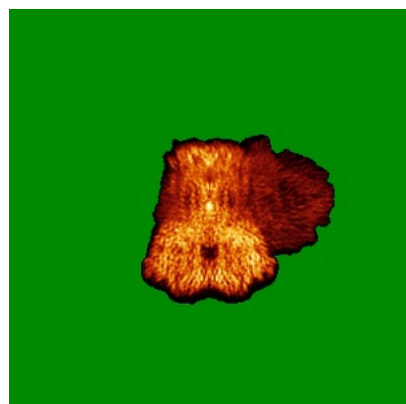


Z Index: 160

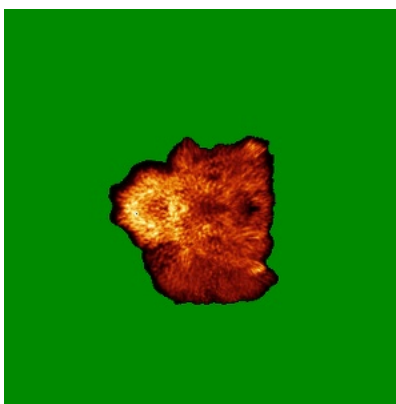
The images above show the largest variance slices of the map in three orthogonal directions.

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

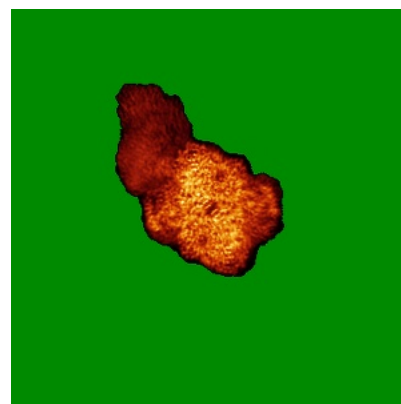
### 6.4.1 Primary map



X

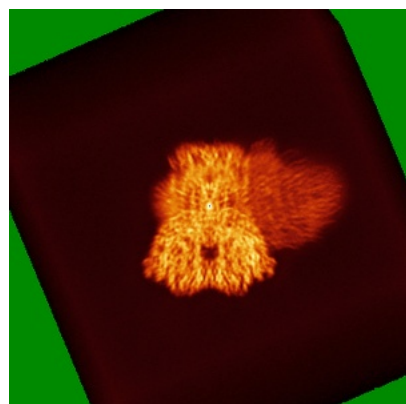


Y

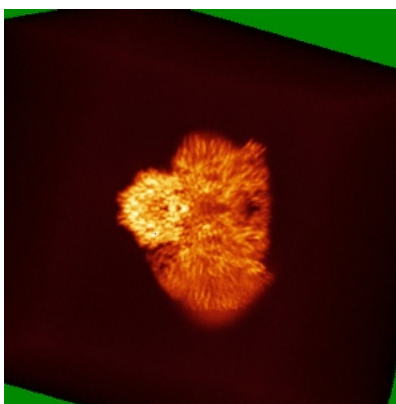


Z

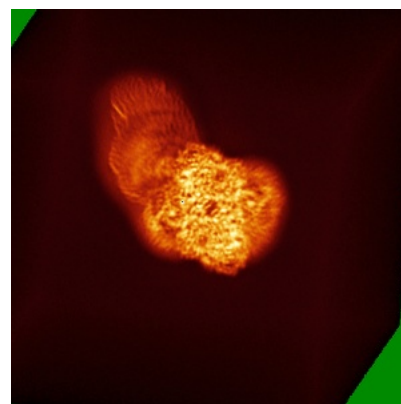
### 6.4.2 Raw map



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.

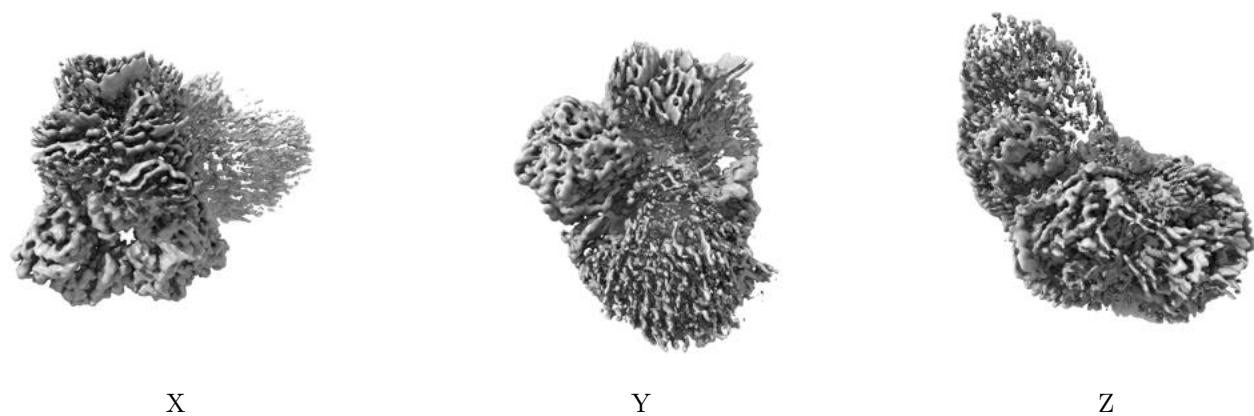
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

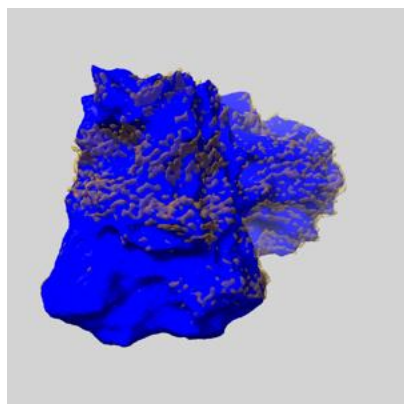
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

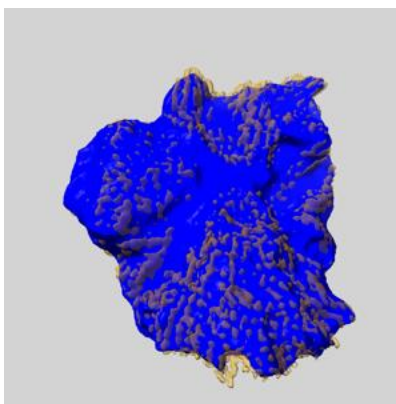
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

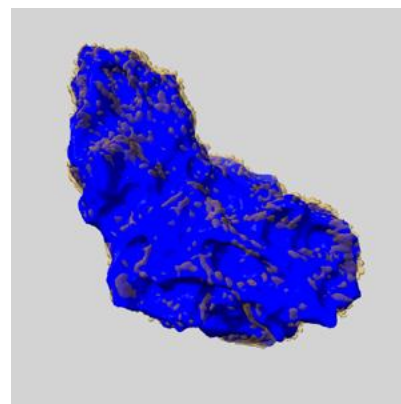
### 6.6.1 emd\_28011\_msk\_1.map [i](#)



X



Y

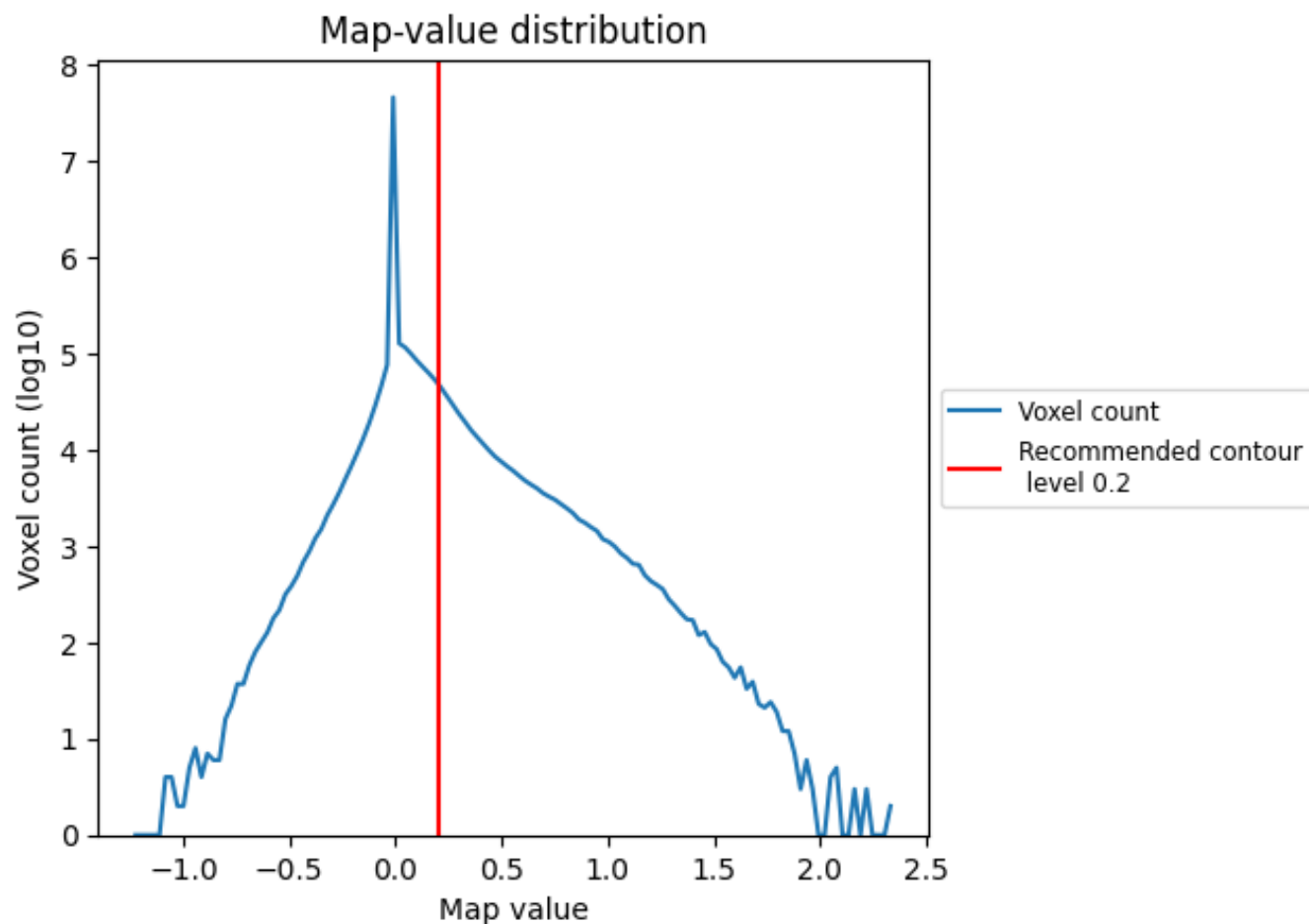


Z

## 7 Map analysis [i](#)

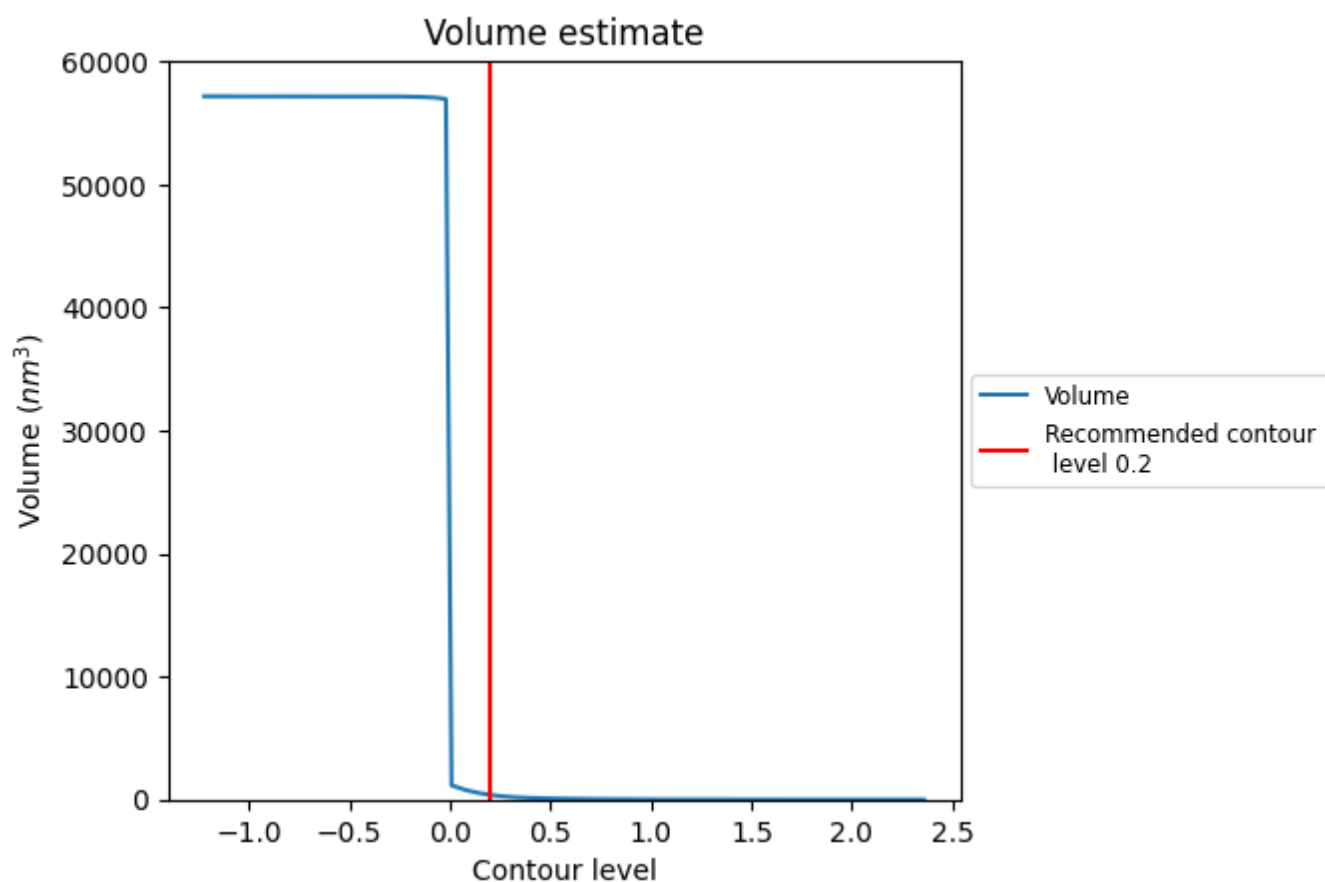
This section contains the results of statistical analysis of the map.

### 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.

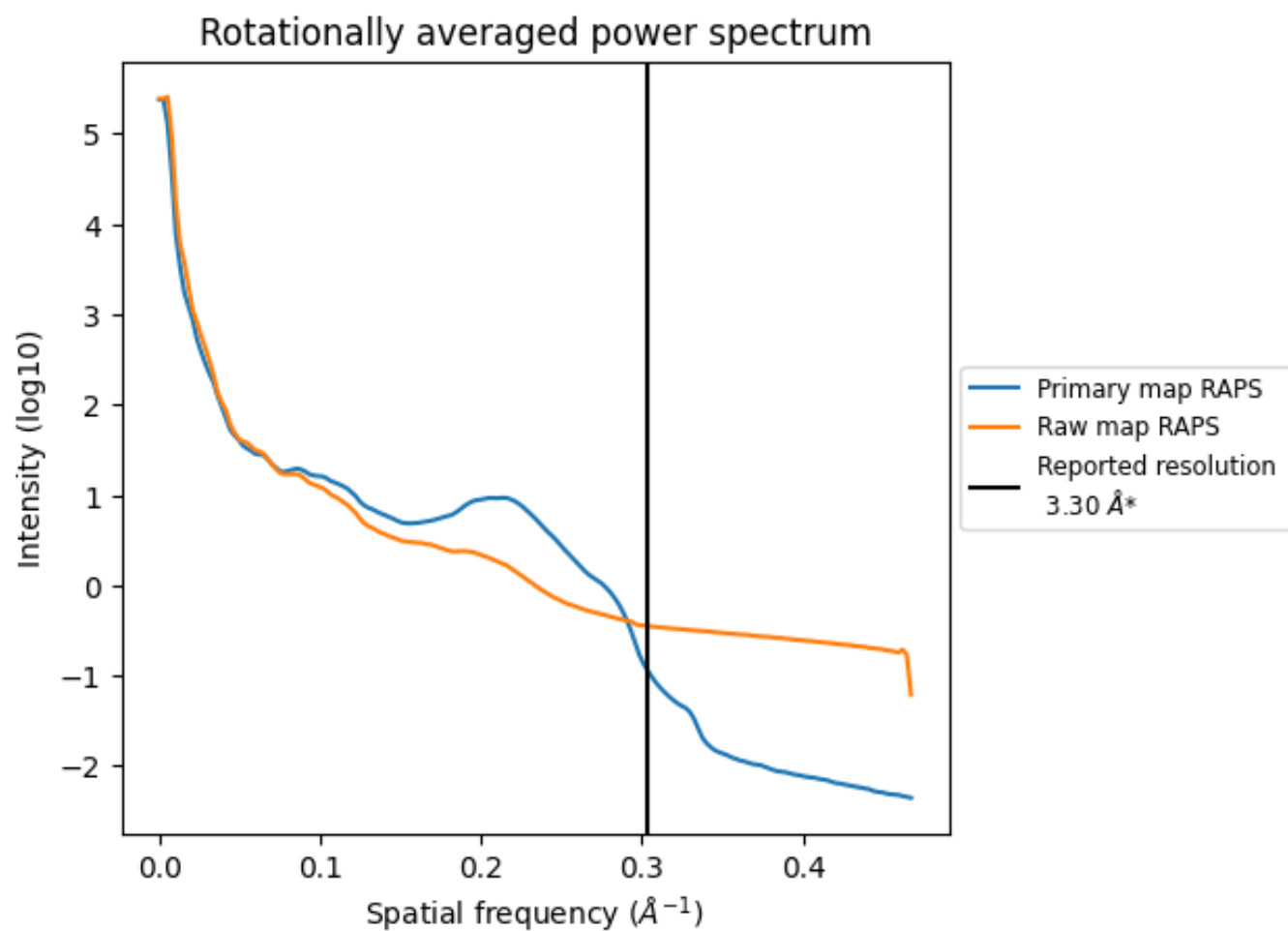
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 380 nm<sup>3</sup>; this corresponds to an approximate mass of 343 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 ⓘ

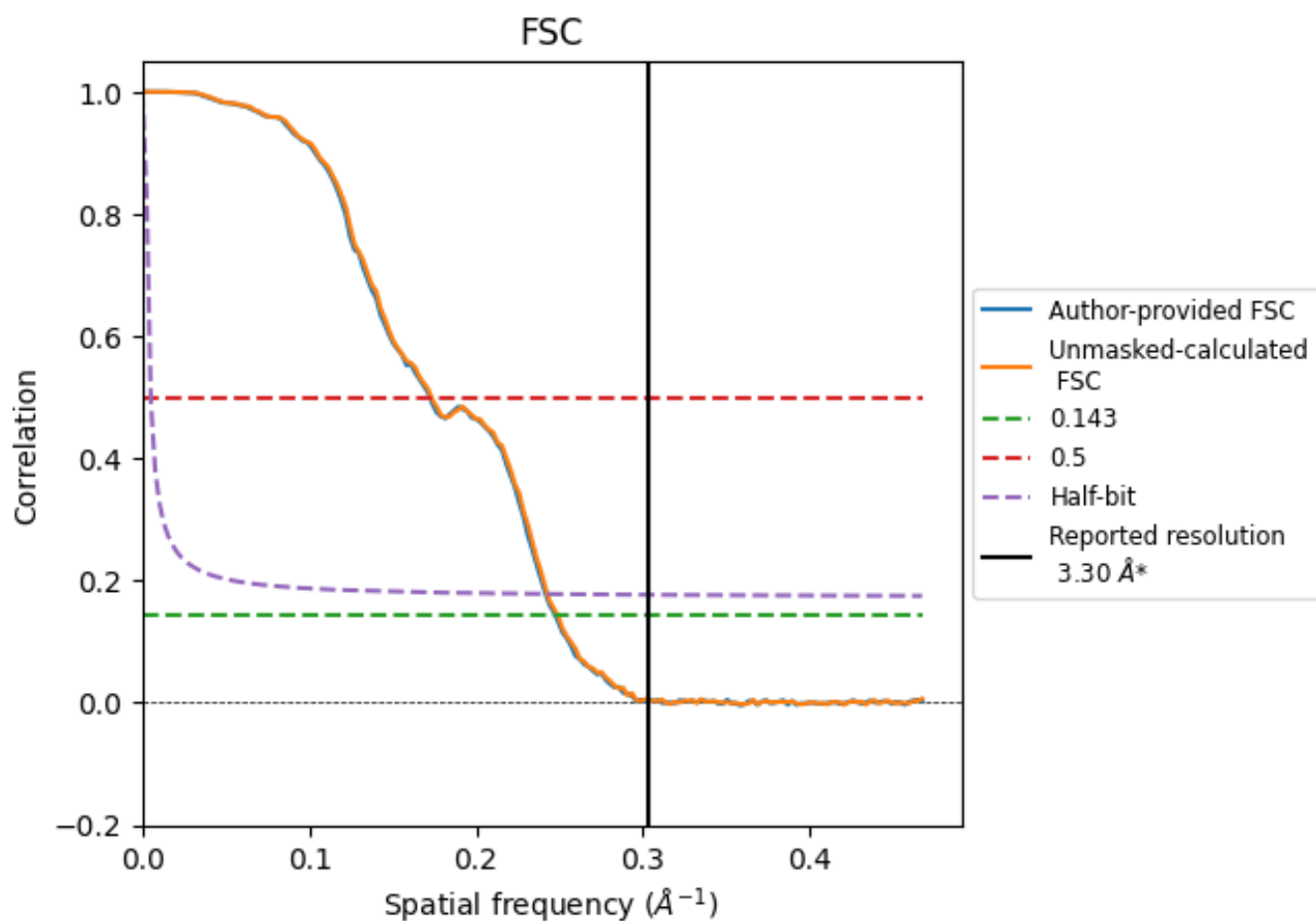


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 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 0.303 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        | 3.30                               | -    | -        |
| Author-provided FSC curve | 4.04                               | 5.80 | 4.14     |
| Unmasked-calculated*      | 4.02                               | 5.77 | 4.12     |

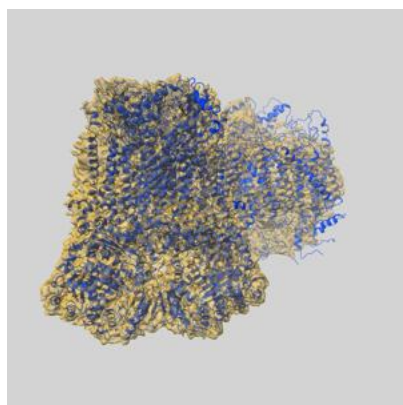
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.04 differs from the reported value 3.3 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.3 by more than 10 %

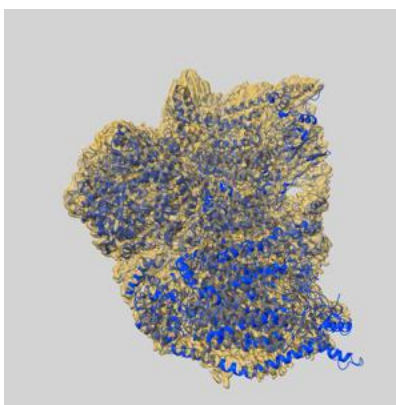
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-28011 and PDB model 8EC0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

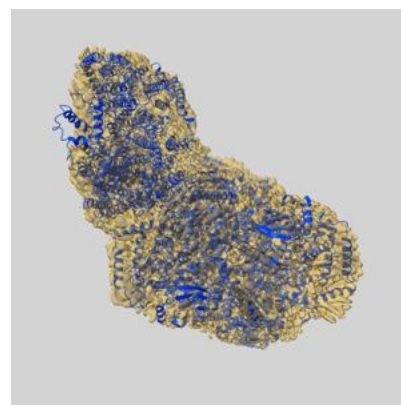
### 9.1 Map-model overlay [i](#)



X



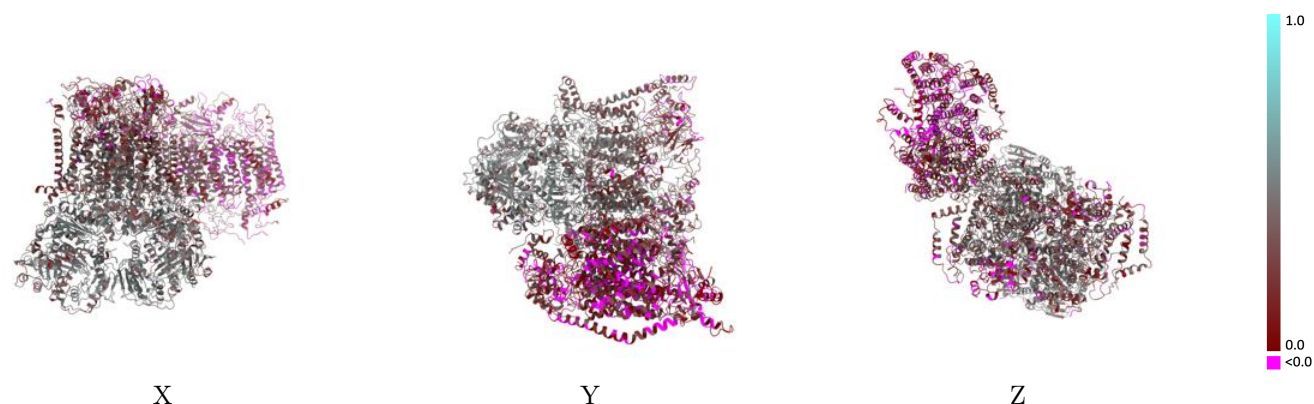
Y



Z

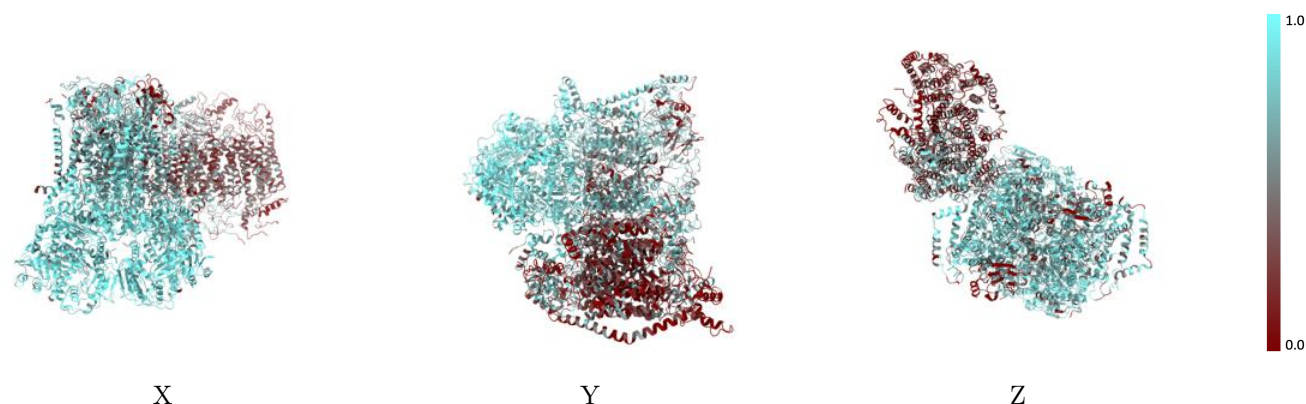
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



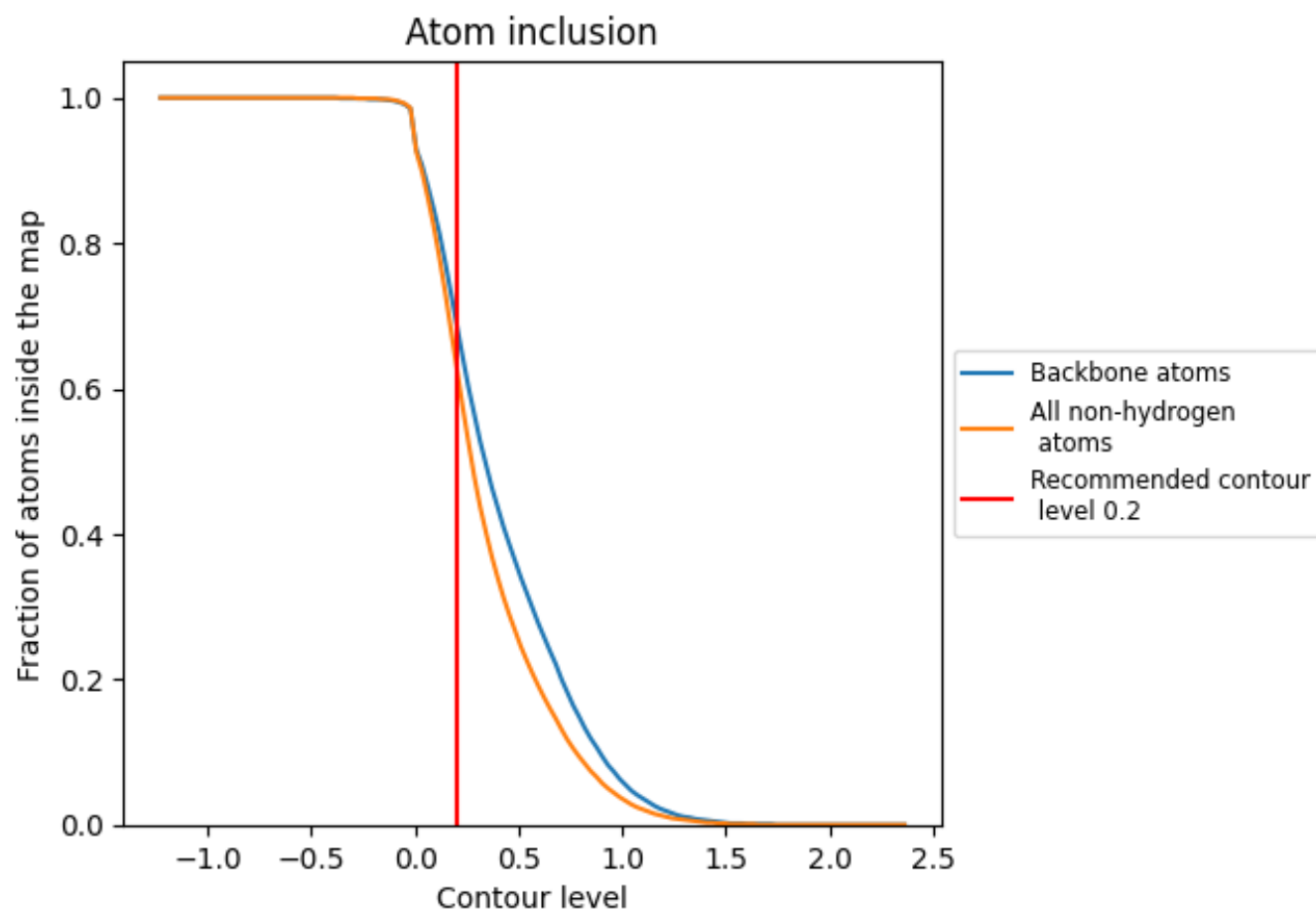
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 63% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6320   |  0.3070   |
| A     |  0.8630   |  0.4430   |
| B     |  0.9030   |  0.4560   |
| C     |  0.4320   |  0.2220   |
| E     |  0.5560   |  0.2890   |
| F     |  0.8650   |  0.4390   |
| G     |  0.6620   |  0.2540   |
| H     |  0.7350   |  0.3930   |
| J     |  0.7270   |  0.3870   |
| K     |  0.3270   |  0.1480   |
| L     |  0.7750   |  0.3630   |
| M     |  0.1990   |  0.1340   |
| N     |  0.1800   |  0.1080   |
| O     |  0.2700   |  0.1390   |
| P     |  0.4140  |  0.1460  |
| Q     |  0.5600 |  0.2060 |
| R     |  0.3710 |  0.1330 |
| S     |  0.1110 |  0.0390 |
| T     |  0.3650 |  0.1360 |
| U     |  0.1050 |  0.0640 |
| V     |  0.4880 |  0.2790 |
| W     |  0.5720 |  0.2760 |
| a     |  0.8700 |  0.4390 |
| b     |  0.8860 |  0.4460 |
| c     |  0.4160 |  0.1840 |
| e     |  0.6430 |  0.2290 |
| f     |  0.8540 |  0.4190 |
| g     |  0.6470 |  0.2620 |
| h     |  0.8100 |  0.3540 |
| j     |  0.7370 |  0.3660 |
| l     |  0.7200 |  0.3220 |

