



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:55 AM UTC

PDB ID : 8Q1B / pdb\_00008q1b  
EMDB ID : EMD-18062  
Title : III2-IV1 respiratory supercomplex from *S. pombe*  
Authors : Moe, A.; Brzezinski, P.  
Deposited on : 2023-07-31  
Resolution : 3.40 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:

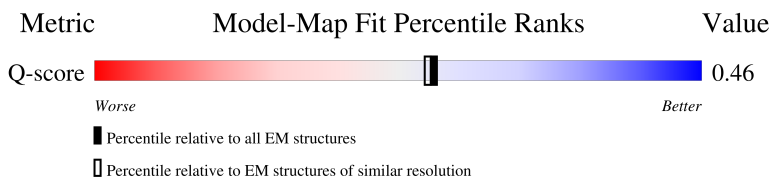
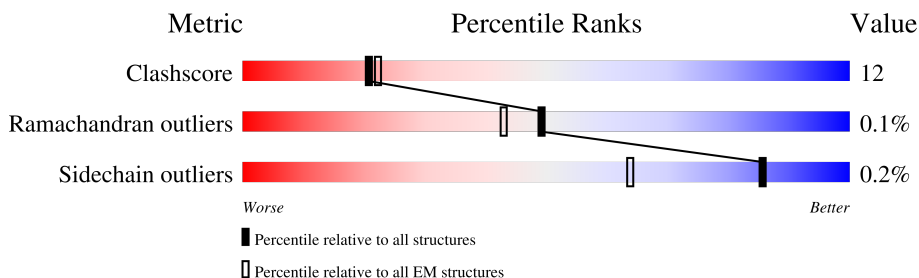
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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                       | 14717 ( 2.90 - 3.90 )                                    |

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   | L     | 457    |                  |
| 2   | B     | 426    |                  |
| 2   | M     | 426    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 387    |                  |
| 3   | N     | 387    |                  |
| 4   | D     | 307    |                  |
| 4   | O     | 307    |                  |
| 5   | E     | 228    |                  |
| 5   | P     | 228    |                  |
| 6   | F     | 214    |                  |
| 6   | Q     | 214    |                  |
| 7   | G     | 137    |                  |
| 7   | R     | 137    |                  |
| 8   | H     | 92     |                  |
| 8   | S     | 92     |                  |
| 9   | I     | 67     |                  |
| 9   | T     | 67     |                  |
| 10  | J     | 79     |                  |
| 10  | U     | 79     |                  |
| 11  | a     | 538    |                  |
| 12  | b     | 248    |                  |
| 13  | c     | 269    |                  |
| 14  | d     | 159    |                  |
| 15  | e     | 228    |                  |
| 16  | f     | 140    |                  |
| 17  | g     | 59     |                  |
| 18  | h     | 66     |                  |
| 19  | i     | 58     |                  |

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| Mol | Chain | Length | Quality of chain                                   |
|-----|-------|--------|----------------------------------------------------|
| 20  | j     | 86     | <div> <div>79%</div> <div>81% 6% 13%</div> </div>  |
| 21  | k     | 130    | <div> <div>53%</div> <div>55% 12% 32%</div> </div> |
| 22  | l     | 242    | <div> <div>22%</div> <div>23% 5% 71%</div> </div>  |
| 23  | m     | 26     | <div> <div>100%</div> <div>100%</div> </div>       |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 31  | FES  | E     | 301 | -         | -        | X       | -                |
| 31  | FES  | P     | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 48686 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 Probable mitochondrial-processing peptidase subunit beta.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 443      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3449  | 2151 | 618 | 671 | 9 |         |       |
| 1   | L     | 443      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3449  | 2151 | 618 | 671 | 9 |         |       |

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | B     | 406      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3044  | 1943 | 500 | 596 | 5 |         |       |
| 2   | M     | 406      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3043  | 1943 | 500 | 595 | 5 |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 387      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3101  | 2101 | 473 | 510 | 17 |         |       |
| 3   | N     | 387      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3101  | 2101 | 473 | 510 | 17 |         |       |

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | D     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1943  | 1241 | 336 | 357 | 9 |         |       |
| 4   | O     | 245      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1943  | 1241 | 336 | 357 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | E     | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1384  | 871 | 240 | 264 | 9 |         |       |
| 5   | P     | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1384  | 871 | 240 | 264 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 6   | F     | 66       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 536   | 334 | 90 | 104 | 8 |         |       |
| 6   | Q     | 66       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 536   | 334 | 90 | 104 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | G     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 657 | 176 | 184 | 4 |         |       |
| 7   | R     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 657 | 176 | 184 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 697   | 454 | 124 | 115 | 4 |         |       |
| 8   | S     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 455 | 124 | 115 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 9   | I     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 497   | 328 | 82 | 86 | 1 |         |       |
| 9   | T     | 60       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 497   | 328 | 82 | 86 | 1 |         |       |

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 629   | 421 | 102 | 103 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | U     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 629   | 421 | 102 | 103 | 3 |         |       |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | a     | 537      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4212  | 2827 | 652 | 711 | 22 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| a     | 400     | TYR      | -      | insertion | UNP P07657 |

- Molecule 12 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | b     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1902  | 1242 | 297 | 354 | 9 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | c     | 268      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2156  | 1452 | 332 | 365 | 7 |         |       |

- Molecule 14 is a protein called Cytochrome c oxidase subunit 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | d     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 922   | 573 | 160 | 182 | 7 |         |       |

- Molecule 15 is a protein called Cytochrome c oxidase polypeptide 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | e     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 728 | 202 | 212 | 4 |         |       |

There are 42 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| e     | 187     | GLU      | -      | expression tag | UNP O74988 |
| e     | 188     | ASN      | -      | expression tag | UNP O74988 |
| e     | 189     | LEU      | -      | expression tag | UNP O74988 |
| e     | 190     | TYR      | -      | expression tag | UNP O74988 |
| e     | 191     | PHE      | -      | expression tag | UNP O74988 |
| e     | 192     | GLN      | -      | expression tag | UNP O74988 |
| e     | 193     | GLY      | -      | expression tag | UNP O74988 |
| e     | 194     | GLY      | -      | expression tag | UNP O74988 |
| e     | 195     | GLY      | -      | expression tag | UNP O74988 |
| e     | 196     | GLY      | -      | expression tag | UNP O74988 |
| e     | 197     | GLY      | -      | expression tag | UNP O74988 |
| e     | 198     | GLY      | -      | expression tag | UNP O74988 |
| e     | 199     | SER      | -      | expression tag | UNP O74988 |
| e     | 200     | ALA      | -      | expression tag | UNP O74988 |
| e     | 201     | TRP      | -      | expression tag | UNP O74988 |
| e     | 202     | SER      | -      | expression tag | UNP O74988 |
| e     | 203     | HIS      | -      | expression tag | UNP O74988 |
| e     | 204     | PRO      | -      | expression tag | UNP O74988 |
| e     | 205     | GLN      | -      | expression tag | UNP O74988 |
| e     | 206     | PHE      | -      | expression tag | UNP O74988 |
| e     | 207     | GLU      | -      | expression tag | UNP O74988 |
| e     | 208     | LYS      | -      | expression tag | UNP O74988 |
| e     | 209     | GLY      | -      | expression tag | UNP O74988 |
| e     | 210     | GLY      | -      | expression tag | UNP O74988 |
| e     | 211     | GLY      | -      | expression tag | UNP O74988 |
| e     | 212     | SER      | -      | expression tag | UNP O74988 |
| e     | 213     | GLY      | -      | expression tag | UNP O74988 |
| e     | 214     | GLY      | -      | expression tag | UNP O74988 |
| e     | 215     | GLY      | -      | expression tag | UNP O74988 |
| e     | 216     | SER      | -      | expression tag | UNP O74988 |
| e     | 217     | GLY      | -      | expression tag | UNP O74988 |
| e     | 218     | GLY      | -      | expression tag | UNP O74988 |
| e     | 219     | SER      | -      | expression tag | UNP O74988 |
| e     | 220     | ALA      | -      | expression tag | UNP O74988 |
| e     | 221     | TRP      | -      | expression tag | UNP O74988 |
| e     | 222     | SER      | -      | expression tag | UNP O74988 |
| e     | 223     | HIS      | -      | expression tag | UNP O74988 |
| e     | 224     | PRO      | -      | expression tag | UNP O74988 |
| e     | 225     | GLN      | -      | expression tag | UNP O74988 |
| e     | 226     | PHE      | -      | expression tag | UNP O74988 |
| e     | 227     | GLU      | -      | expression tag | UNP O74988 |
| e     | 228     | LYS      | -      | expression tag | UNP O74988 |

- Molecule 16 is a protein called Cytochrome c oxidase subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | f     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 813   | 520 | 137 | 154 | 2 |         |       |

- Molecule 17 is a protein called Cytochrome c oxidase subunit 7.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 17  | g     | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 457   | 301 | 78 | 77 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 18  | h     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 363   | 249 | 57 | 57 |   |         |       |

- Molecule 19 is a protein called Cytochrome c oxidase subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 19  | i     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 445   | 292 | 77 | 73 | 3 |         |       |

- Molecule 20 is a protein called Cytochrome c oxidase subunit 12, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | j     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 411 | 107 | 113 | 5 |         |       |

- Molecule 21 is a protein called Cytochrome c oxidase subunit 13, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | k     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 480 | 124 | 136 | 1 |         |       |

- Molecule 22 is a protein called Respiratory supercomplex factor 2 homolog C1565.01.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 22  | l     | 69       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 550   | 356 | 95 | 97 | 2 |         |       |

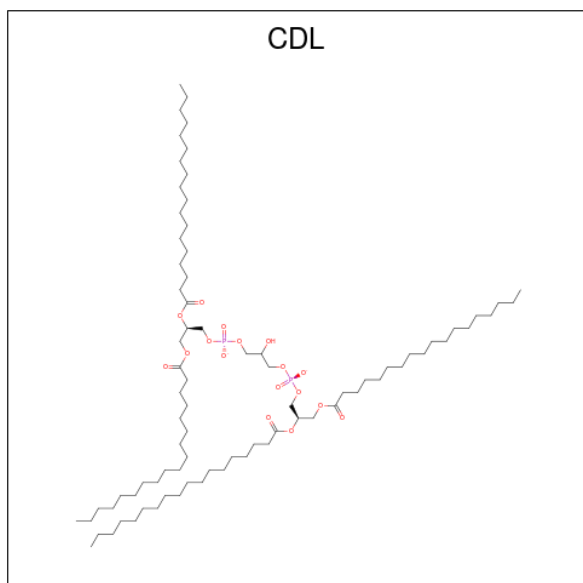
- Molecule 23 is a protein called Unknown polypeptide.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 23  | m     | 26       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 130   | 78 | 26 | 26 |         |       |

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

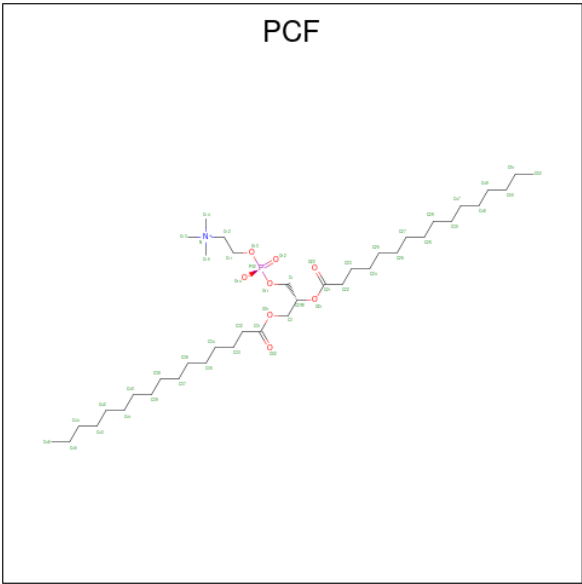
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 24  | A     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 24  | L     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 24  | d     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



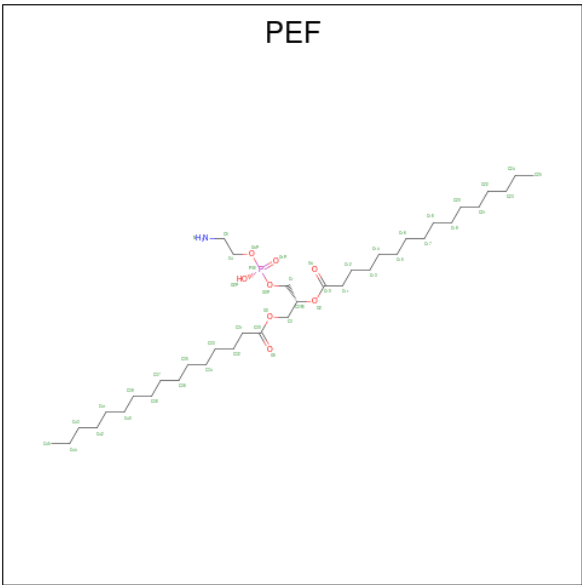
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 25  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 25  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 79    | 60 | 17 | 2 |         |
| 25  | H     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |
| 25  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 25  | S     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 77    | 58 | 17 | 2 |         |
| 25  | S     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 73    | 54 | 17 | 2 |         |

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (CCD ID: PCF) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



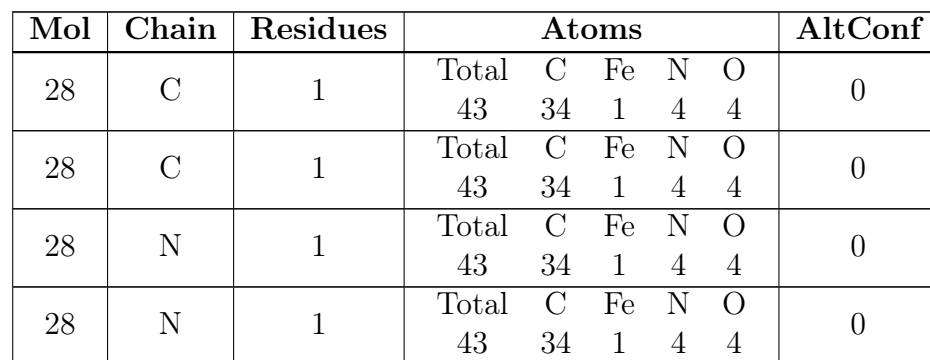
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 26  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 26  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 26  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |
| 26  | T     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |

- Molecule 27 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (CCD ID: PEF) (formula: C<sub>37</sub>H<sub>74</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 27  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | O     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | c     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 27  | k     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |

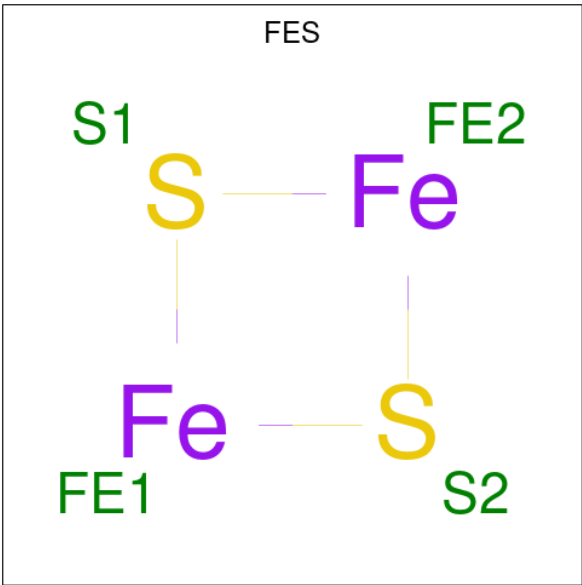
- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



- Molecule 29 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ).

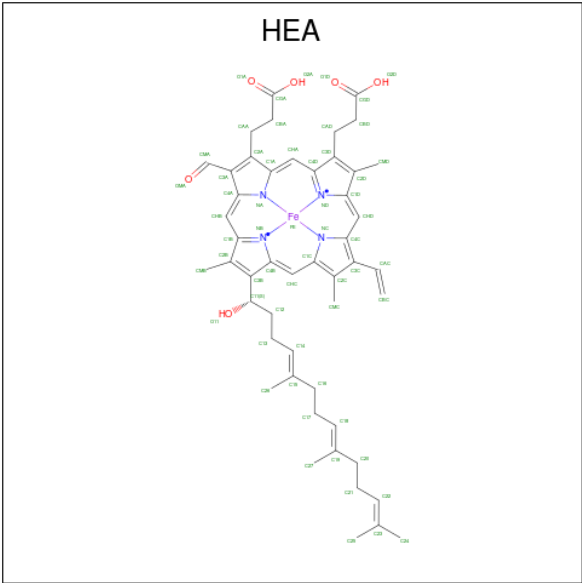






| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 31  | E     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 31  | P     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 32 is HEME-A (CCD ID: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 32  | a     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |
| 32  | a     | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 60    | 49 | 1  | 4 | 6 |         |

- Molecule 33 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

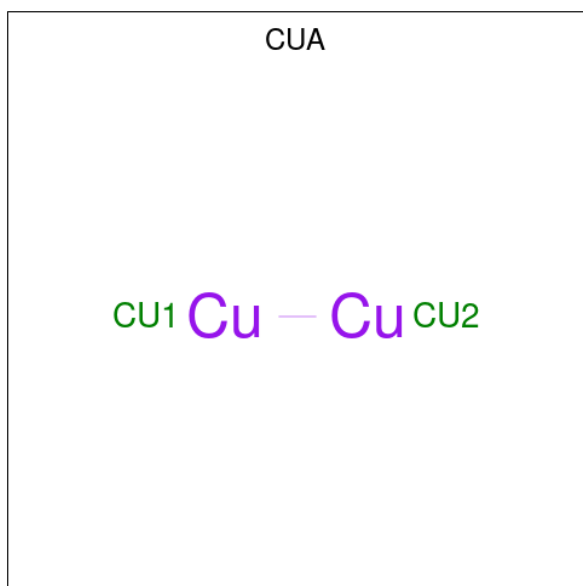
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 34  | a     | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 35  | b     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 36 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).

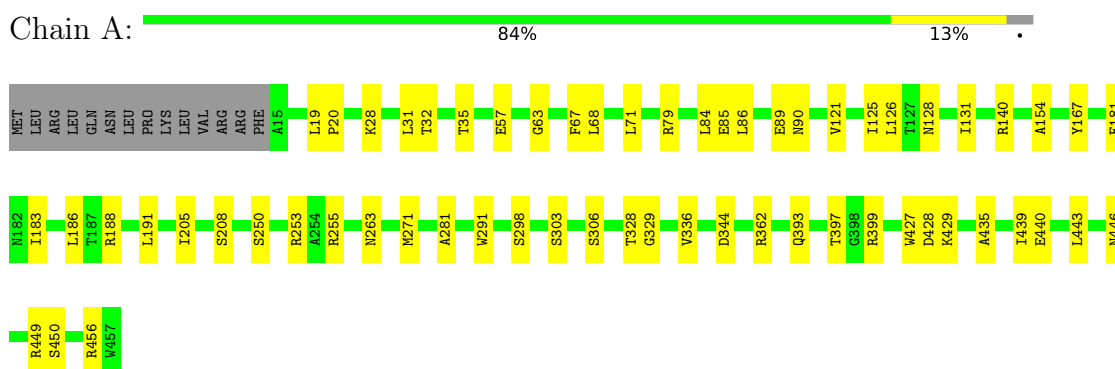


| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 36  | b     | 1        | Total | Cu | 0       |
|     |       |          | 2     | 2  |         |

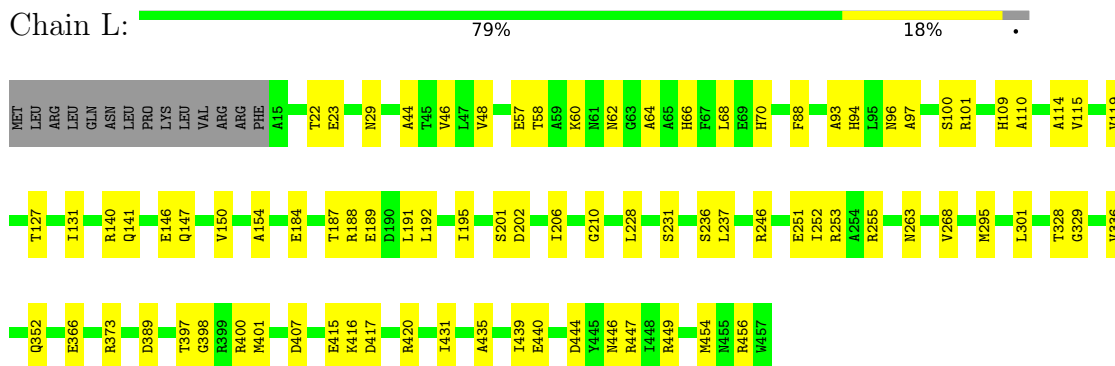
### 3 Residue-property plots

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.

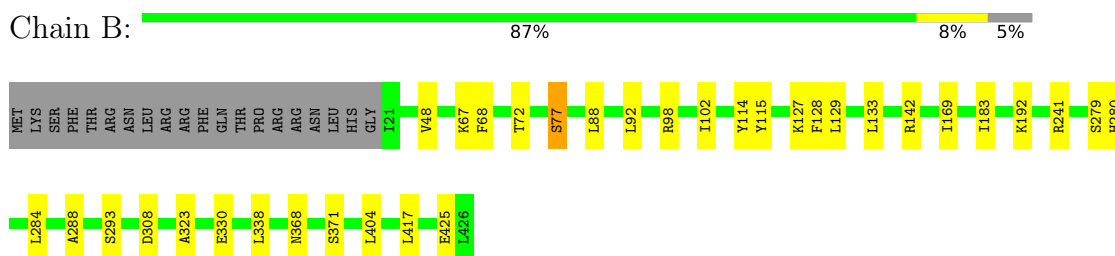
- Molecule 1: Probable mitochondrial-processing peptidase subunit beta



- Molecule 1: Probable mitochondrial-processing peptidase subunit beta

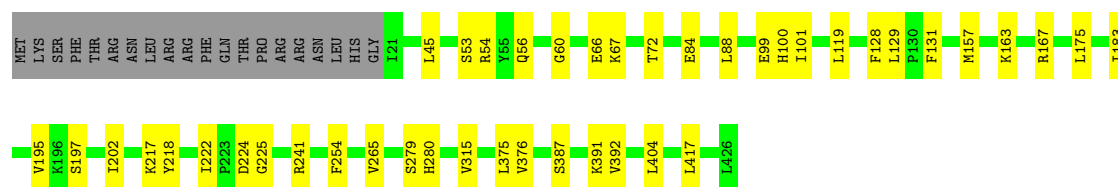


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



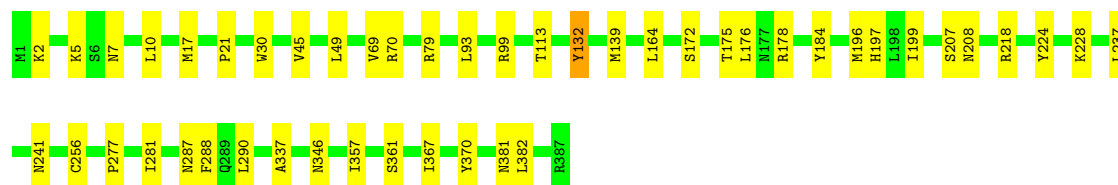
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:  85% 10% 5%



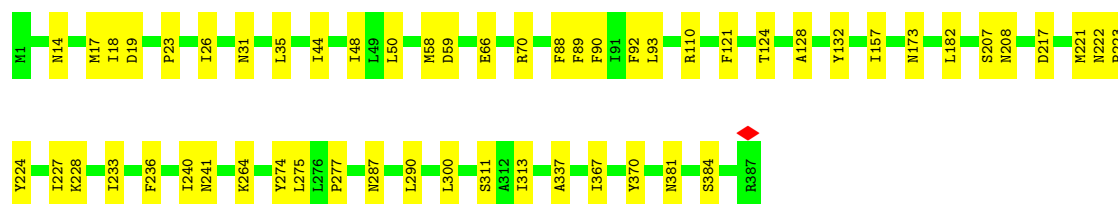
• Molecule 3: Cytochrome b

Chain C:  88% 12%



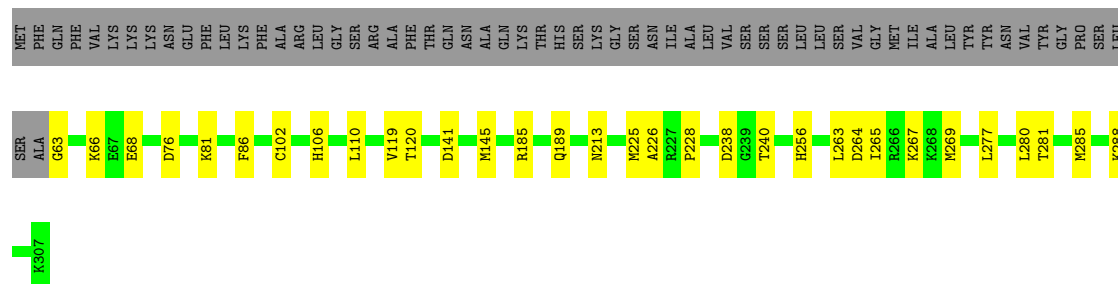
• Molecule 3: Cytochrome b

Chain N:  86% 14%



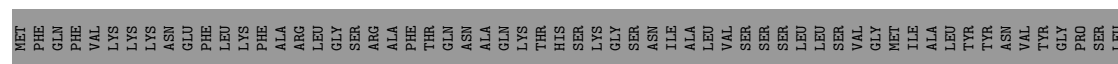
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:  69% 10% 20%



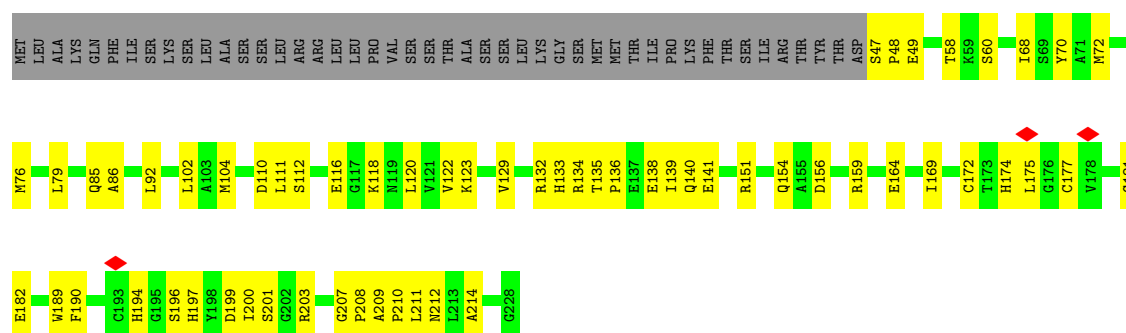
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:  72% 7% 20%

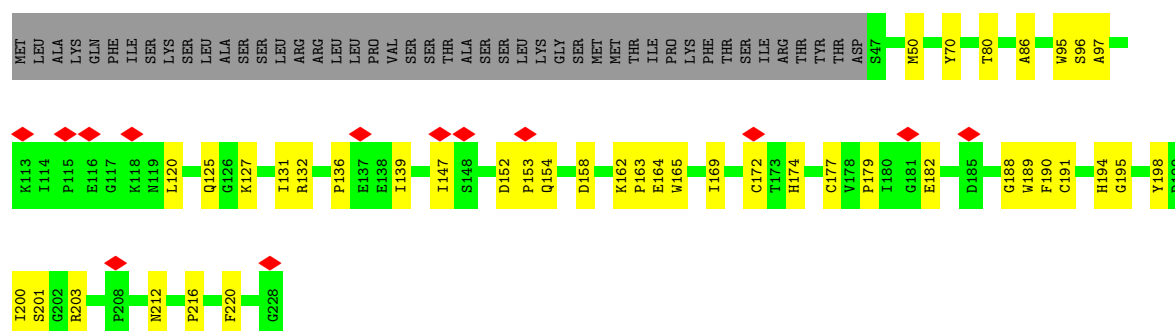




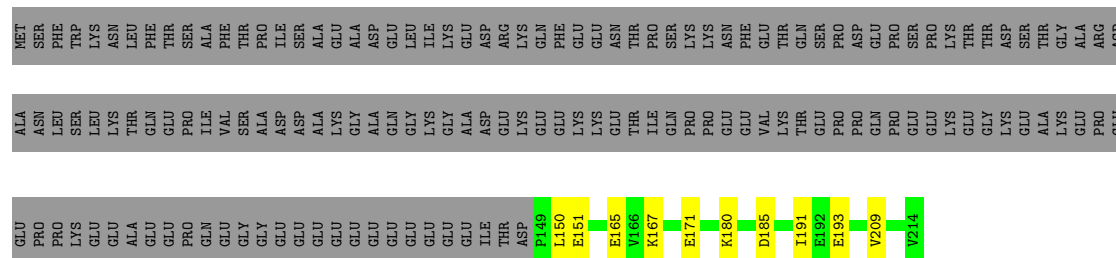
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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

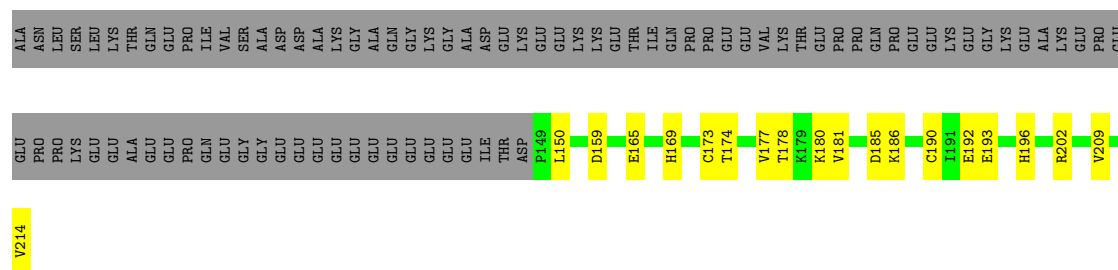


- Molecule 6: Cytochrome b-c1 complex subunit 6



- Molecule 6: Cytochrome b-c1 complex subunit 6





- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G: 71% 18% 11%



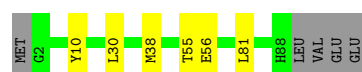
- Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R: 79% 9% 11%



- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H: 88% 7% 5%



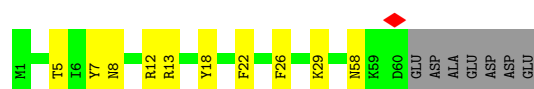
- Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S: 79% 15% 5%



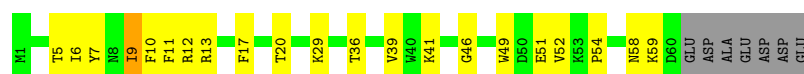
- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I: 75% 15% 10%



- Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T: 58% 30% 10%



- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain J:  85% 13%



- Molecule 10: Cytochrome b-c1 complex subunit 10

Chain U:  77% 20%



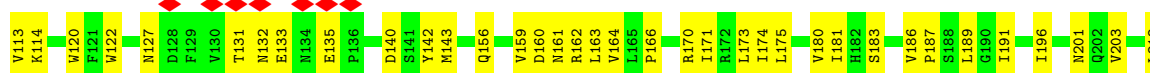
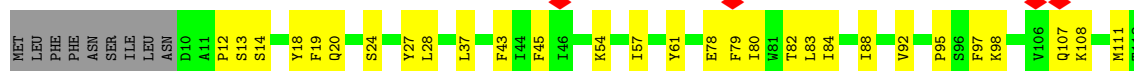
- Molecule 11: Cytochrome c oxidase subunit 1

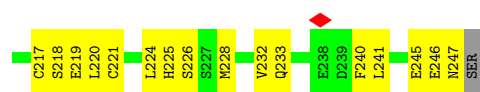
Chain a:  63% 36%



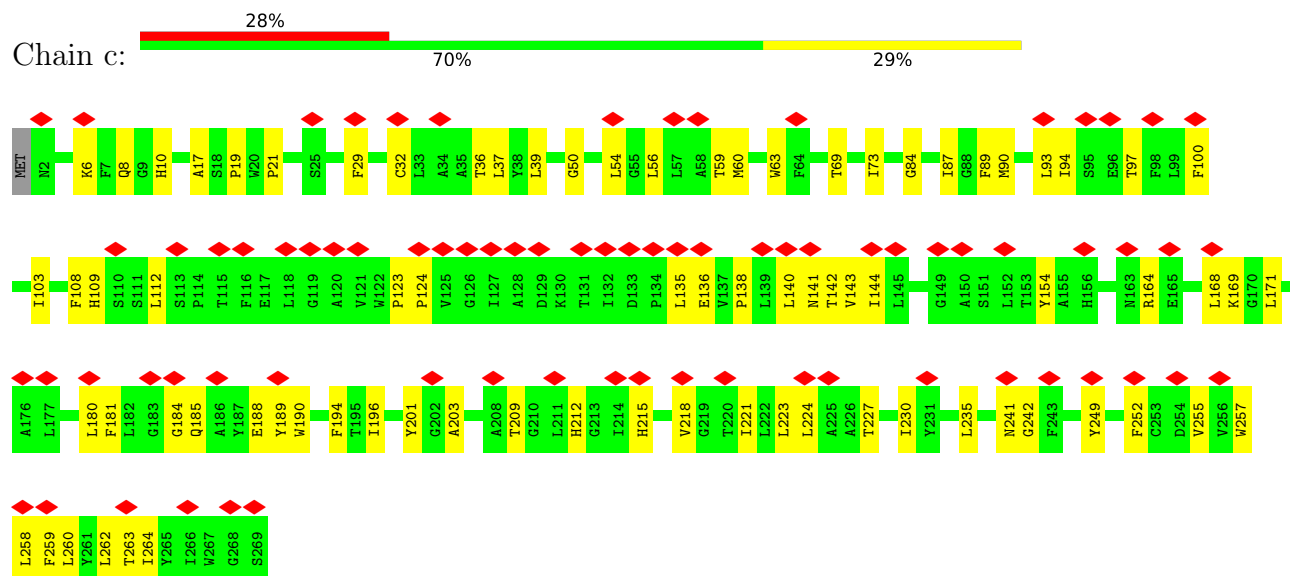
- Molecule 12: Cytochrome c oxidase subunit 2

Chain b:  5% 63% 33%

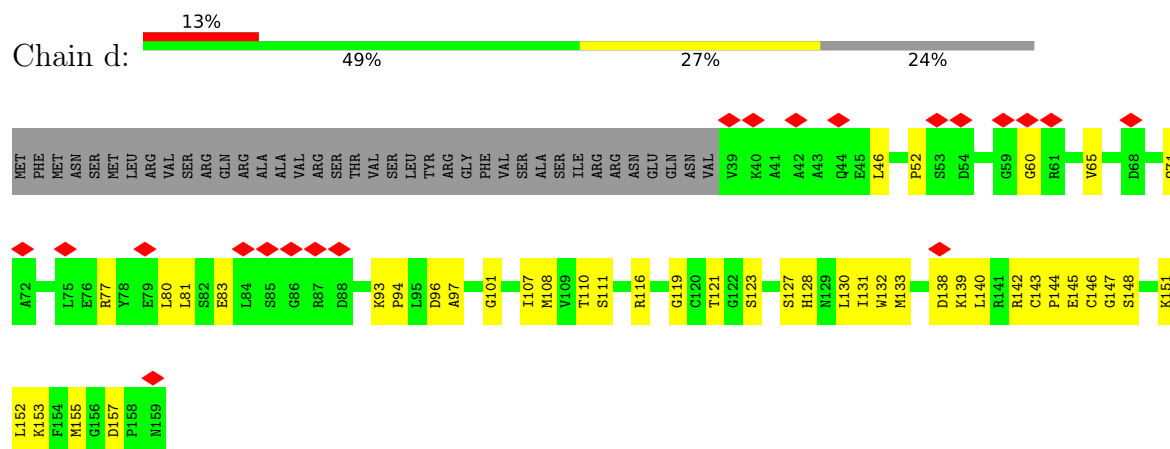




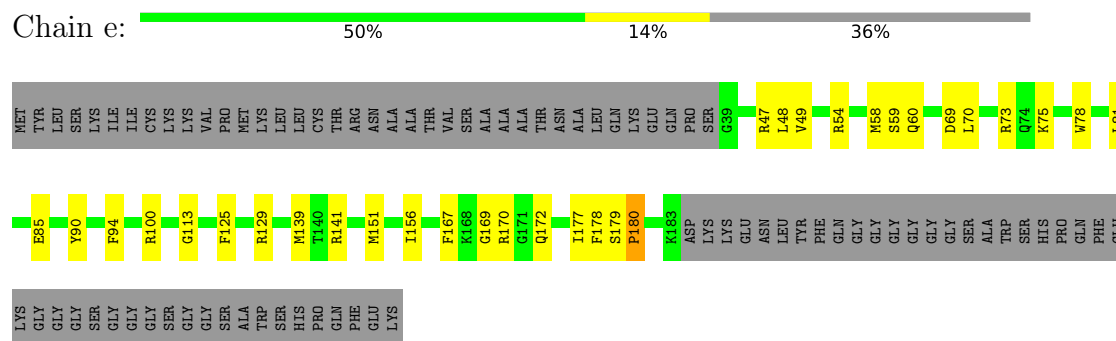
• Molecule 13: Cytochrome c oxidase subunit 3



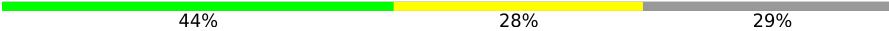
• Molecule 14: Cytochrome c oxidase subunit 4, mitochondrial

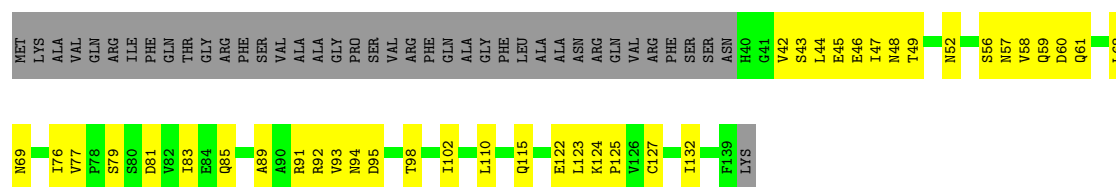


• Molecule 15: Cytochrome c oxidase polypeptide 5, mitochondrial



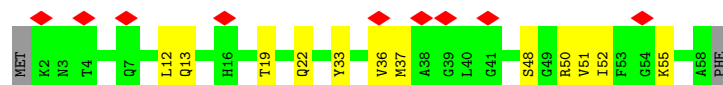
• Molecule 16: Cytochrome c oxidase subunit 6, mitochondrial

Chain f: 



• Molecule 17: Cytochrome c oxidase subunit 7

Chain g: 



• Molecule 18: Cytochrome c oxidase polypeptide VIII, mitochondrial

Chain h: 



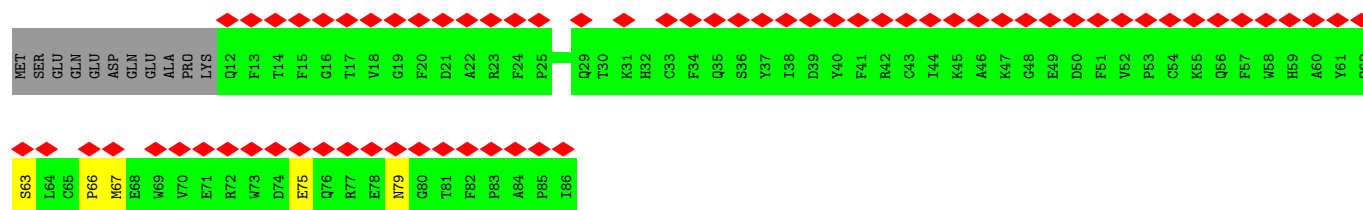
• Molecule 19: Cytochrome c oxidase subunit 9, mitochondrial

Chain i: 



• Molecule 20: Cytochrome c oxidase subunit 12, mitochondrial

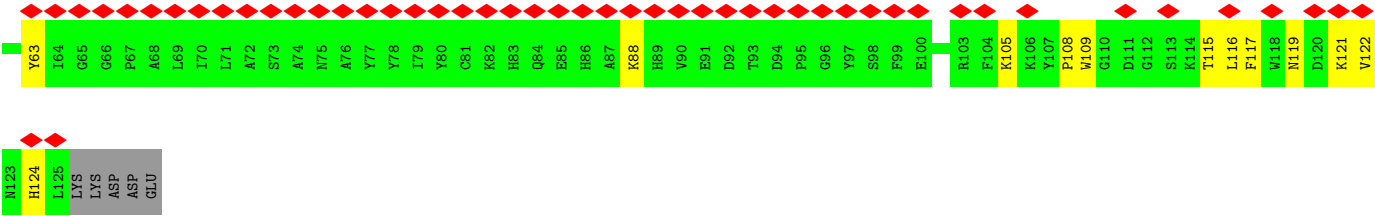
Chain j: 



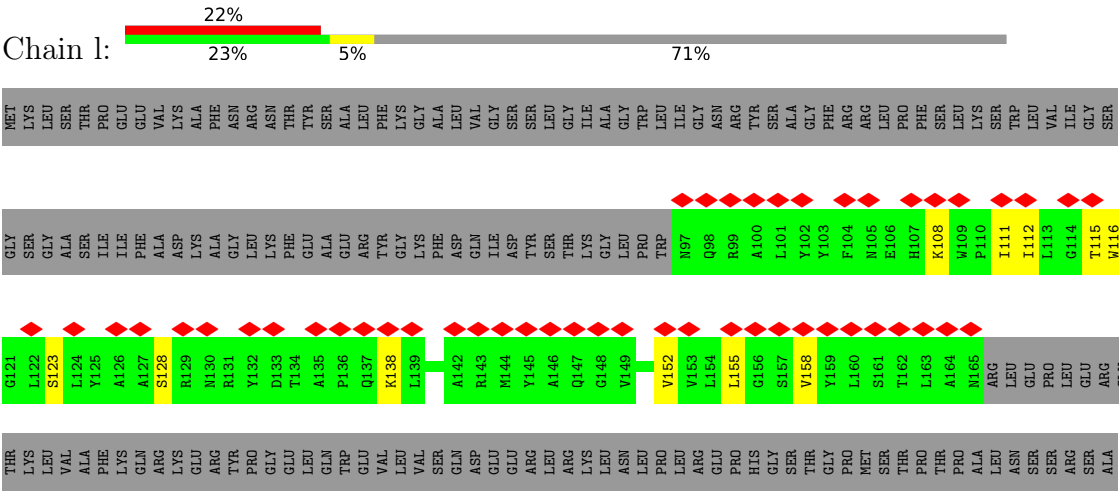
• Molecule 21: Cytochrome c oxidase subunit 13, mitochondrial

Chain k: 

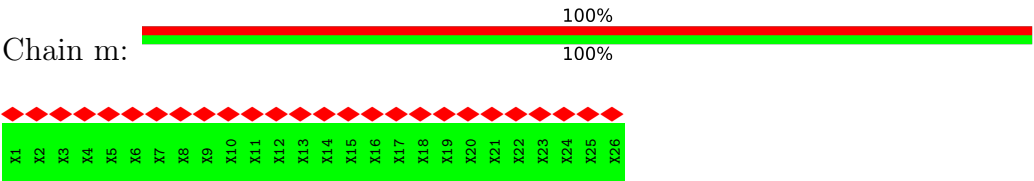




• Molecule 22: Respiratory supercomplex factor 2 homolog C1565.01



• Molecule 23: Unknown polypeptide



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 125752                                  | 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 ( $e^-/\text{\AA}^2$ ) | 41.0                                    | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | 105000                                  | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.727                                   | Depositor |
| Minimum map value                    | -0.342                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.08                                    | Depositor |
| Map size (Å)                         | 433.3568, 433.3568, 433.3568            | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.8464, 0.8464, 0.8464                  | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEA, CA, PCF, HEM, HEC, MG, CU, CDL, CUA, U10, ZN, PEF, FES

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     | 0.08         | 0/3510        | 0.25        | 0/4759      |
| 1   | L     | 0.14         | 0/3510        | 0.25        | 0/4759      |
| 2   | B     | 0.08         | 0/3104        | 0.23        | 0/4212      |
| 2   | M     | 0.08         | 0/3103        | 0.24        | 0/4212      |
| 3   | C     | 0.16         | 0/3204        | 0.32        | 0/4378      |
| 3   | N     | 0.11         | 0/3204        | 0.29        | 0/4378      |
| 4   | D     | 0.10         | 0/2002        | 0.26        | 0/2721      |
| 4   | O     | 0.10         | 0/2002        | 0.25        | 0/2721      |
| 5   | E     | 0.15         | 0/1418        | 0.35        | 0/1925      |
| 5   | P     | 0.16         | 0/1418        | 0.31        | 0/1925      |
| 6   | F     | 0.17         | 0/547         | 0.40        | 0/731       |
| 6   | Q     | 0.26         | 0/547         | 0.45        | 0/731       |
| 7   | G     | 0.26         | 0/1042        | 0.37        | 0/1402      |
| 7   | R     | 0.19         | 0/1042        | 0.30        | 0/1402      |
| 8   | H     | 0.09         | 0/719         | 0.27        | 0/963       |
| 8   | S     | 0.10         | 0/722         | 0.30        | 0/971       |
| 9   | I     | 0.11         | 0/512         | 0.25        | 0/691       |
| 9   | T     | 0.27         | 0/512         | 0.39        | 0/691       |
| 10  | J     | 0.19         | 0/653         | 0.41        | 0/888       |
| 10  | U     | 0.11         | 0/653         | 0.29        | 0/888       |
| 11  | a     | 0.16         | 0/4353        | 0.35        | 0/5950      |
| 12  | b     | 0.16         | 0/1953        | 0.34        | 0/2668      |
| 13  | c     | 0.11         | 0/2237        | 0.30        | 0/3057      |
| 14  | d     | 0.13         | 0/940         | 0.38        | 0/1270      |
| 15  | e     | 0.44         | 1/1173 (0.1%) | 0.34        | 0/1580      |
| 16  | f     | 0.22         | 0/828         | 0.39        | 0/1119      |
| 17  | g     | 0.09         | 0/469         | 0.23        | 0/633       |
| 18  | h     | 0.28         | 0/377         | 0.50        | 0/514       |
| 19  | i     | 0.11         | 0/458         | 0.27        | 0/618       |
| 20  | j     | 0.11         | 0/660         | 0.28        | 0/893       |
| 21  | k     | 0.08         | 0/767         | 0.25        | 0/1039      |
| 22  | l     | 0.11         | 0/563         | 0.32        | 0/767       |

| Mol | Chain | Bond lengths |                | Bond angles |         |
|-----|-------|--------------|----------------|-------------|---------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5 |
| All | All   | 0.15         | 1/48202 (0.0%) | 0.30        | 0/65456 |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | G     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | e     | 180 | PRO  | N-CD  | 14.53 | 1.68        | 1.47     |

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 7   | G     | 112 | ARG  | Sidechain |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3449  | 0        | 3416     | 54      | 0            |
| 1   | L     | 3449  | 0        | 3416     | 63      | 0            |
| 2   | B     | 3044  | 0        | 3091     | 23      | 0            |
| 2   | M     | 3043  | 0        | 3091     | 25      | 0            |
| 3   | C     | 3101  | 0        | 3146     | 39      | 0            |
| 3   | N     | 3101  | 0        | 3147     | 71      | 0            |
| 4   | D     | 1943  | 0        | 1877     | 48      | 0            |
| 4   | O     | 1943  | 0        | 1877     | 27      | 0            |
| 5   | E     | 1384  | 0        | 1349     | 45      | 0            |
| 5   | P     | 1384  | 0        | 1349     | 53      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | F     | 536   | 0        | 507      | 7       | 0            |
| 6   | Q     | 536   | 0        | 507      | 16      | 0            |
| 7   | G     | 1021  | 0        | 1059     | 19      | 0            |
| 7   | R     | 1021  | 0        | 1059     | 20      | 0            |
| 8   | H     | 697   | 0        | 676      | 6       | 0            |
| 8   | S     | 698   | 0        | 679      | 25      | 0            |
| 9   | I     | 497   | 0        | 483      | 9       | 0            |
| 9   | T     | 497   | 0        | 483      | 27      | 0            |
| 10  | J     | 629   | 0        | 630      | 25      | 0            |
| 10  | U     | 629   | 0        | 630      | 25      | 0            |
| 11  | a     | 4212  | 0        | 4233     | 248     | 0            |
| 12  | b     | 1902  | 0        | 1872     | 88      | 0            |
| 13  | c     | 2156  | 0        | 2101     | 112     | 0            |
| 14  | d     | 922   | 0        | 907      | 70      | 0            |
| 15  | e     | 1146  | 0        | 1140     | 33      | 0            |
| 16  | f     | 813   | 0        | 805      | 29      | 0            |
| 17  | g     | 457   | 0        | 467      | 8       | 0            |
| 18  | h     | 363   | 0        | 379      | 18      | 0            |
| 19  | i     | 445   | 0        | 444      | 8       | 0            |
| 20  | j     | 636   | 0        | 575      | 4       | 0            |
| 21  | k     | 741   | 0        | 689      | 31      | 0            |
| 22  | l     | 550   | 0        | 554      | 9       | 0            |
| 23  | m     | 130   | 0        | 29       | 0       | 0            |
| 24  | A     | 1     | 0        | 0        | 0       | 0            |
| 24  | L     | 1     | 0        | 0        | 0       | 0            |
| 24  | d     | 1     | 0        | 0        | 0       | 0            |
| 25  | A     | 57    | 0        | 58       | 5       | 0            |
| 25  | H     | 157   | 0        | 208      | 9       | 0            |
| 25  | L     | 57    | 0        | 58       | 5       | 0            |
| 25  | S     | 150   | 0        | 191      | 6       | 0            |
| 26  | A     | 100   | 0        | 160      | 11      | 0            |
| 26  | L     | 50    | 0        | 80       | 3       | 0            |
| 26  | T     | 50    | 0        | 80       | 3       | 0            |
| 27  | A     | 47    | 0        | 73       | 7       | 0            |
| 27  | D     | 47    | 0        | 73       | 2       | 0            |
| 27  | J     | 47    | 0        | 73       | 6       | 0            |
| 27  | N     | 94    | 0        | 146      | 7       | 0            |
| 27  | O     | 47    | 0        | 73       | 1       | 0            |
| 27  | a     | 47    | 0        | 73       | 2       | 0            |
| 27  | b     | 47    | 0        | 73       | 3       | 0            |
| 27  | c     | 47    | 0        | 73       | 3       | 0            |
| 27  | k     | 47    | 0        | 73       | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 28  | C     | 86    | 0        | 60       | 7       | 0            |
| 28  | N     | 86    | 0        | 60       | 6       | 0            |
| 29  | C     | 63    | 0        | 90       | 7       | 0            |
| 29  | N     | 63    | 0        | 90       | 5       | 0            |
| 30  | D     | 43    | 0        | 32       | 6       | 0            |
| 30  | O     | 43    | 0        | 32       | 3       | 0            |
| 31  | E     | 4     | 0        | 0        | 4       | 0            |
| 31  | P     | 4     | 0        | 0        | 2       | 0            |
| 32  | a     | 120   | 0        | 108      | 10      | 0            |
| 33  | a     | 1     | 0        | 0        | 0       | 0            |
| 34  | a     | 1     | 0        | 0        | 0       | 0            |
| 35  | b     | 1     | 0        | 0        | 0       | 0            |
| 36  | b     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 48686 | 0        | 48704    | 1170    | 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 12.

All (1170) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 11:a:13:PHE:CE1  | 13:c:19:PRO:HB3   | 1.26                     | 1.67              |
| 21:k:109:TRP:CH2 | 27:k:201:PEF:H112 | 1.39                     | 1.57              |
| 11:a:13:PHE:HE1  | 13:c:19:PRO:CB    | 1.18                     | 1.51              |
| 1:L:252:ILE:CD1  | 8:S:28:TYR:HE1    | 1.25                     | 1.50              |
| 5:P:162:LYS:HD2  | 5:P:165:TRP:CH2   | 1.47                     | 1.50              |
| 21:k:109:TRP:CE2 | 21:k:116:LEU:HD21 | 1.48                     | 1.44              |
| 15:e:180:PRO:CD  | 15:e:180:PRO:N    | 1.68                     | 1.44              |
| 3:N:89:PHE:CE2   | 3:N:124:THR:HG21  | 1.55                     | 1.41              |
| 11:a:381:VAL:HA  | 11:a:384:PHE:CE2  | 1.54                     | 1.40              |
| 11:a:420:GLN:NE2 | 11:a:474:LEU:HB3  | 1.10                     | 1.38              |
| 1:L:252:ILE:CD1  | 8:S:28:TYR:CE1    | 2.03                     | 1.38              |
| 11:a:515:GLN:O   | 14:d:132:TRP:CZ3  | 1.83                     | 1.32              |
| 11:a:515:GLN:O   | 14:d:132:TRP:HZ3  | 1.04                     | 1.29              |
| 4:D:86:PHE:CE2   | 4:D:263:LEU:HB3   | 1.68                     | 1.28              |
| 3:N:92:PHE:CE2   | 3:N:236:PHE:CE1   | 2.23                     | 1.27              |
| 11:a:516:SER:HA  | 14:d:132:TRP:CZ3  | 1.68                     | 1.26              |
| 3:N:92:PHE:CZ    | 3:N:236:PHE:CD1   | 2.28                     | 1.22              |
| 7:R:111:GLU:CG   | 7:R:115:PHE:HE2   | 1.53                     | 1.22              |
| 5:P:50:MET:HE1   | 8:S:28:TYR:CZ     | 1.75                     | 1.21              |
| 3:N:92:PHE:HE2   | 3:N:236:PHE:CE1   | 1.59                     | 1.18              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:420:GLN:NE2  | 11:a:474:LEU:CB   | 2.05                     | 1.18              |
| 21:k:109:TRP:CH2  | 27:k:201:PEF:C11  | 2.27                     | 1.17              |
| 13:c:97:THR:CG2   | 13:c:252:PHE:CZ   | 2.29                     | 1.17              |
| 1:L:252:ILE:HD11  | 8:S:28:TYR:CE1    | 1.73                     | 1.16              |
| 13:c:255:VAL:CG1  | 13:c:259:PHE:HE2  | 1.55                     | 1.16              |
| 3:C:70:ARG:NH2    | 4:D:110:LEU:HD13  | 1.58                     | 1.15              |
| 21:k:109:TRP:CD2  | 21:k:116:LEU:HD21 | 1.81                     | 1.15              |
| 3:N:89:PHE:HE2    | 3:N:124:THR:CG2   | 1.60                     | 1.14              |
| 12:b:79:PHE:CE2   | 12:b:83:LEU:HD11  | 1.81                     | 1.14              |
| 11:a:13:PHE:CZ    | 13:c:19:PRO:HB3   | 1.83                     | 1.14              |
| 11:a:380:VAL:O    | 11:a:384:PHE:CD2  | 2.01                     | 1.13              |
| 3:N:92:PHE:HZ     | 3:N:236:PHE:CD1   | 1.65                     | 1.13              |
| 13:c:97:THR:HG23  | 13:c:252:PHE:CZ   | 1.83                     | 1.12              |
| 11:a:13:PHE:HE1   | 13:c:19:PRO:CA    | 1.63                     | 1.11              |
| 3:N:227:ILE:HD12  | 4:O:291:LYS:HD3   | 1.17                     | 1.10              |
| 12:b:79:PHE:CZ    | 12:b:83:LEU:HD11  | 1.87                     | 1.10              |
| 4:D:189:GLN:NE2   | 4:D:256:HIS:CD2   | 2.19                     | 1.09              |
| 1:L:252:ILE:HD13  | 8:S:28:TYR:CE1    | 1.77                     | 1.09              |
| 11:a:13:PHE:CE1   | 13:c:19:PRO:CB    | 2.04                     | 1.09              |
| 11:a:381:VAL:HA   | 11:a:384:PHE:CZ   | 1.86                     | 1.09              |
| 13:c:97:THR:CG2   | 13:c:252:PHE:HZ   | 1.65                     | 1.09              |
| 5:P:162:LYS:CD    | 5:P:165:TRP:HH2   | 1.64                     | 1.08              |
| 11:a:323:GLY:O    | 11:a:327:PHE:CD2  | 2.06                     | 1.08              |
| 13:c:255:VAL:HG12 | 13:c:259:PHE:HE2  | 1.10                     | 1.08              |
| 3:C:70:ARG:HH22   | 4:D:110:LEU:HD13  | 0.91                     | 1.08              |
| 4:D:189:GLN:HE21  | 4:D:256:HIS:CG    | 1.72                     | 1.07              |
| 13:c:108:PHE:CE2  | 13:c:112:LEU:CD2  | 2.38                     | 1.07              |
| 21:k:109:TRP:CZ2  | 21:k:116:LEU:HD21 | 1.87                     | 1.07              |
| 1:A:67:PHE:HZ     | 1:A:183:ILE:HG12  | 1.19                     | 1.07              |
| 11:a:440:LEU:CD1  | 12:b:19:PHE:CE1   | 2.37                     | 1.07              |
| 3:N:88:PHE:HD2    | 3:N:236:PHE:CE1   | 1.73                     | 1.06              |
| 3:N:89:PHE:CE2    | 3:N:124:THR:CG2   | 2.36                     | 1.06              |
| 11:a:440:LEU:HD12 | 12:b:19:PHE:CE1   | 1.91                     | 1.06              |
| 11:a:381:VAL:CA   | 11:a:384:PHE:CE2  | 2.39                     | 1.05              |
| 9:T:10:PHE:HD1    | 9:T:20:THR:OG1    | 1.39                     | 1.04              |
| 13:c:56:LEU:HD11  | 13:c:60:MET:CE    | 1.85                     | 1.04              |
| 13:c:194:PHE:CZ   | 13:c:201:TYR:CE2  | 2.45                     | 1.04              |
| 1:A:67:PHE:CZ     | 1:A:183:ILE:HG12  | 1.93                     | 1.04              |
| 5:E:194:HIS:HB2   | 31:E:301:FES:S2   | 1.97                     | 1.04              |
| 13:c:194:PHE:CZ   | 13:c:201:TYR:HE2  | 1.76                     | 1.04              |
| 10:U:54:LYS:O     | 10:U:59:GLN:HG2   | 1.57                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:162:LYS:CD    | 5:P:165:TRP:CH2   | 2.39                     | 1.03              |
| 7:R:111:GLU:CG    | 7:R:115:PHE:CE2   | 2.43                     | 1.02              |
| 21:k:109:TRP:CE2  | 21:k:116:LEU:CD2  | 2.43                     | 1.02              |
| 11:a:323:GLY:O    | 11:a:327:PHE:HD2  | 1.38                     | 1.02              |
| 21:k:109:TRP:CD2  | 21:k:116:LEU:CD2  | 2.43                     | 1.01              |
| 1:L:252:ILE:HD11  | 8:S:28:TYR:HE1    | 0.85                     | 1.01              |
| 7:R:111:GLU:HG2   | 7:R:115:PHE:HE2   | 1.22                     | 1.01              |
| 14:d:110:THR:HG23 | 14:d:155:MET:HE1  | 1.41                     | 1.00              |
| 13:c:255:VAL:HG12 | 13:c:259:PHE:CE2  | 1.95                     | 1.00              |
| 1:L:263:ASN:OD1   | 1:L:336:VAL:HG22  | 1.60                     | 1.00              |
| 18:h:33:TYR:OH    | 18:h:44:TYR:CE2   | 2.16                     | 0.98              |
| 7:R:111:GLU:HG3   | 7:R:115:PHE:CE2   | 1.97                     | 0.98              |
| 13:c:56:LEU:HD11  | 13:c:60:MET:HE1   | 1.45                     | 0.98              |
| 4:D:189:GLN:HE21  | 4:D:256:HIS:CD2   | 1.78                     | 0.98              |
| 4:D:86:PHE:CZ     | 4:D:263:LEU:HB3   | 1.99                     | 0.98              |
| 3:N:222:ASN:OD1   | 3:N:223:PRO:HA    | 1.62                     | 0.98              |
| 13:c:255:VAL:CG1  | 13:c:259:PHE:CE2  | 2.45                     | 0.98              |
| 5:P:165:TRP:CZ2   | 5:P:220:PHE:CZ    | 2.52                     | 0.97              |
| 1:A:63:GLY:O      | 1:A:67:PHE:CD2    | 2.16                     | 0.97              |
| 18:h:33:TYR:OH    | 18:h:44:TYR:HE2   | 1.47                     | 0.96              |
| 3:N:92:PHE:HE2    | 3:N:236:PHE:HE1   | 0.97                     | 0.96              |
| 13:c:100:PHE:CZ   | 13:c:260:LEU:HD21 | 2.00                     | 0.96              |
| 13:c:56:LEU:CD1   | 13:c:60:MET:CE    | 2.43                     | 0.96              |
| 4:D:86:PHE:HE2    | 4:D:263:LEU:HB3   | 1.20                     | 0.95              |
| 21:k:109:TRP:HH2  | 27:k:201:PEF:C11  | 1.71                     | 0.95              |
| 3:N:227:ILE:CD1   | 4:O:291:LYS:HD3   | 1.97                     | 0.95              |
| 5:P:165:TRP:HZ2   | 5:P:220:PHE:CZ    | 1.85                     | 0.95              |
| 3:N:92:PHE:HZ     | 3:N:236:PHE:HD1   | 1.02                     | 0.94              |
| 12:b:107:GLN:HB2  | 12:b:170:ARG:CZ   | 1.98                     | 0.94              |
| 5:P:162:LYS:HB2   | 5:P:165:TRP:CZ2   | 2.01                     | 0.94              |
| 11:a:420:GLN:HE21 | 11:a:474:LEU:HB3  | 1.12                     | 0.94              |
| 11:a:440:LEU:HD12 | 12:b:19:PHE:HE1   | 1.32                     | 0.94              |
| 10:J:5:PHE:CD2    | 10:J:8:LYS:HB2    | 2.02                     | 0.94              |
| 11:a:13:PHE:CE1   | 13:c:19:PRO:CA    | 2.44                     | 0.93              |
| 11:a:516:SER:CA   | 14:d:132:TRP:CZ3  | 2.52                     | 0.93              |
| 11:a:440:LEU:HD11 | 12:b:19:PHE:CZ    | 2.03                     | 0.92              |
| 13:c:97:THR:CG2   | 13:c:252:PHE:CE1  | 2.52                     | 0.92              |
| 13:c:97:THR:HG22  | 13:c:252:PHE:CZ   | 2.04                     | 0.92              |
| 3:C:70:ARG:HH22   | 4:D:110:LEU:CD1   | 1.80                     | 0.92              |
| 5:P:177:CYS:HB2   | 31:P:301:FES:S2   | 2.08                     | 0.92              |
| 4:D:86:PHE:CZ     | 4:D:263:LEU:CB    | 2.53                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:86:PHE:CZ     | 4:D:263:LEU:HD23  | 2.04                     | 0.92              |
| 11:a:380:VAL:O    | 11:a:384:PHE:HD2  | 1.51                     | 0.91              |
| 11:a:338:ILE:HG23 | 11:a:345:MET:HE2  | 1.52                     | 0.91              |
| 1:L:252:ILE:HG12  | 8:S:28:TYR:CD1    | 2.05                     | 0.91              |
| 14:d:110:THR:HG23 | 14:d:155:MET:CE   | 2.00                     | 0.90              |
| 9:I:18:TYR:O      | 9:I:22:PHE:CD2    | 2.25                     | 0.90              |
| 21:k:109:TRP:HH2  | 27:k:201:PEF:H112 | 1.15                     | 0.90              |
| 3:N:88:PHE:CD2    | 3:N:236:PHE:CE1   | 2.59                     | 0.89              |
| 3:N:227:ILE:HD12  | 4:O:291:LYS:CD    | 2.01                     | 0.89              |
| 10:U:59:GLN:OE1   | 10:U:68:PHE:HB3   | 1.72                     | 0.89              |
| 1:L:94:HIS:HB2    | 1:L:109:HIS:CE1   | 2.08                     | 0.88              |
| 3:N:128:ALA:HB1   | 3:N:274:TYR:OH    | 1.74                     | 0.88              |
| 3:N:88:PHE:HD2    | 3:N:236:PHE:HE1   | 1.19                     | 0.87              |
| 12:b:140:ASP:CG   | 12:b:142:TYR:CE2  | 2.46                     | 0.87              |
| 1:A:63:GLY:O      | 1:A:67:PHE:HD2    | 1.53                     | 0.87              |
| 16:f:68:LEU:HD11  | 16:f:102:ILE:HD11 | 1.55                     | 0.87              |
| 4:D:86:PHE:HD2    | 4:D:264:ASP:OD1   | 1.57                     | 0.86              |
| 21:k:109:TRP:CZ2  | 27:k:201:PEF:H112 | 2.10                     | 0.86              |
| 1:A:271:MET:CE    | 1:A:281:ALA:HB2   | 2.07                     | 0.85              |
| 11:a:515:GLN:C    | 14:d:132:TRP:CZ3  | 2.54                     | 0.85              |
| 15:e:177:ILE:O    | 15:e:180:PRO:HD3  | 1.75                     | 0.85              |
| 12:b:108:LYS:O    | 12:b:170:ARG:NH2  | 2.08                     | 0.85              |
| 11:a:515:GLN:C    | 14:d:132:TRP:HZ3  | 1.83                     | 0.85              |
| 9:I:18:TYR:O      | 9:I:22:PHE:HD2    | 1.58                     | 0.85              |
| 3:N:274:TYR:CE1   | 3:N:275:LEU:HD21  | 2.12                     | 0.85              |
| 21:k:109:TRP:HH2  | 27:k:201:PEF:C12  | 1.88                     | 0.85              |
| 11:a:420:GLN:HE22 | 11:a:474:LEU:CB   | 1.74                     | 0.85              |
| 13:c:215:HIS:ND1  | 13:c:249:TYR:OH   | 2.09                     | 0.85              |
| 11:a:115:ALA:HB2  | 11:a:159:LEU:HD11 | 1.58                     | 0.85              |
| 4:D:86:PHE:CD2    | 4:D:264:ASP:OD1   | 2.30                     | 0.84              |
| 11:a:536:LYS:HD2  | 14:d:130:LEU:HD21 | 1.59                     | 0.84              |
| 10:J:5:PHE:CZ     | 10:J:7:ASN:HB2    | 2.12                     | 0.84              |
| 5:P:50:MET:HE1    | 8:S:28:TYR:CE1    | 2.12                     | 0.84              |
| 10:U:59:GLN:OE1   | 10:U:68:PHE:O     | 1.97                     | 0.83              |
| 4:D:225:MET:SD    | 30:D:401:HEC:NA   | 2.51                     | 0.83              |
| 11:a:479:MET:HE2  | 11:a:483:PHE:HZ   | 1.43                     | 0.83              |
| 13:c:108:PHE:CE2  | 13:c:112:LEU:HD22 | 2.14                     | 0.83              |
| 11:a:479:MET:HE2  | 11:a:483:PHE:CZ   | 2.14                     | 0.83              |
| 11:a:534:PRO:HA   | 14:d:116:ARG:HH12 | 1.44                     | 0.83              |
| 13:c:255:VAL:O    | 13:c:259:PHE:CD2  | 2.31                     | 0.83              |
| 7:R:111:GLU:O     | 7:R:115:PHE:CD2   | 2.32                     | 0.82              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:50:MET:HE1    | 8:S:28:TYR:OH     | 1.79                     | 0.82              |
| 3:N:92:PHE:CZ     | 3:N:236:PHE:CE1   | 2.62                     | 0.82              |
| 9:T:11:PHE:CE1    | 9:T:17:PHE:CE1    | 2.68                     | 0.82              |
| 13:c:56:LEU:HG    | 13:c:60:MET:HE3   | 1.62                     | 0.82              |
| 12:b:166:PRO:HD3  | 12:b:240:PHE:CE1  | 2.15                     | 0.81              |
| 13:c:194:PHE:HZ   | 13:c:201:TYR:CE2  | 1.93                     | 0.81              |
| 7:R:111:GLU:HG2   | 7:R:115:PHE:CE2   | 2.10                     | 0.81              |
| 13:c:194:PHE:HZ   | 13:c:201:TYR:HE2  | 1.24                     | 0.81              |
| 11:a:440:LEU:HD11 | 12:b:19:PHE:CE1   | 2.13                     | 0.81              |
| 11:a:536:LYS:CD   | 14:d:119:GLY:HA3  | 2.10                     | 0.81              |
| 5:P:162:LYS:HB2   | 5:P:165:TRP:CH2   | 2.16                     | 0.80              |
| 11:a:536:LYS:HZ1  | 14:d:132:TRP:CD1  | 2.00                     | 0.80              |
| 11:a:310:TYR:CD2  | 11:a:311:PHE:CD1  | 2.70                     | 0.80              |
| 12:b:131:THR:HG22 | 12:b:132:ASN:H    | 1.46                     | 0.80              |
| 1:A:456:ARG:NH1   | 25:A:502:CDL:OB4  | 2.15                     | 0.80              |
| 9:T:10:PHE:CD1    | 9:T:20:THR:OG1    | 2.22                     | 0.80              |
| 11:a:310:TYR:CE2  | 11:a:311:PHE:HE1  | 1.97                     | 0.80              |
| 1:A:67:PHE:HZ     | 1:A:183:ILE:CG1   | 1.93                     | 0.80              |
| 4:D:86:PHE:CZ     | 4:D:263:LEU:CD2   | 2.65                     | 0.80              |
| 10:J:5:PHE:CD2    | 10:J:8:LYS:N      | 2.49                     | 0.80              |
| 11:a:310:TYR:HD2  | 11:a:311:PHE:CD1  | 2.00                     | 0.80              |
| 12:b:143:MET:HE1  | 12:b:156:GLN:HA   | 1.64                     | 0.80              |
| 4:D:213:ASN:ND2   | 4:D:226:ALA:HA    | 1.98                     | 0.79              |
| 1:L:252:ILE:CG1   | 8:S:28:TYR:CE1    | 2.65                     | 0.79              |
| 12:b:140:ASP:CG   | 12:b:142:TYR:HE2  | 1.91                     | 0.79              |
| 4:D:86:PHE:CE2    | 4:D:263:LEU:CB    | 2.59                     | 0.79              |
| 5:E:140:GLN:NE2   | 5:E:141:GLU:OE1   | 2.16                     | 0.79              |
| 4:O:287:TYR:CE2   | 4:O:291:LYS:HD2   | 2.18                     | 0.79              |
| 13:c:136:GLU:HG3  | 13:c:138:PRO:HD2  | 1.63                     | 0.79              |
| 5:P:165:TRP:CZ2   | 5:P:220:PHE:CE1   | 2.71                     | 0.78              |
| 11:a:381:VAL:HG22 | 11:a:384:PHE:HZ   | 1.48                     | 0.78              |
| 11:a:388:LEU:HD13 | 32:a:601:HEA:HAC  | 1.65                     | 0.78              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:CA   | 2.32                     | 0.78              |
| 13:c:255:VAL:O    | 13:c:259:PHE:HD2  | 1.67                     | 0.78              |
| 15:e:167:PHE:HZ   | 15:e:170:ARG:O    | 1.66                     | 0.77              |
| 9:T:11:PHE:CE1    | 9:T:17:PHE:HE1    | 2.02                     | 0.77              |
| 11:a:358:GLY:N    | 11:a:386:TYR:HE2  | 1.83                     | 0.77              |
| 28:N:402:HEM:HHC  | 28:N:402:HEM:HBB2 | 1.67                     | 0.77              |
| 3:N:89:PHE:HE2    | 3:N:124:THR:HG21  | 0.69                     | 0.77              |
| 5:P:165:TRP:CE2   | 5:P:220:PHE:CE1   | 2.72                     | 0.77              |
| 3:N:92:PHE:CE2    | 3:N:236:PHE:HE1   | 1.82                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:479:MET:HG3  | 11:a:483:PHE:CE2  | 2.21                     | 0.77              |
| 13:c:108:PHE:CZ   | 13:c:112:LEU:HD22 | 2.20                     | 0.77              |
| 11:a:535:THR:HG23 | 14:d:116:ARG:HH22 | 1.50                     | 0.76              |
| 12:b:108:LYS:C    | 12:b:170:ARG:NH2  | 2.42                     | 0.76              |
| 11:a:310:TYR:HE2  | 11:a:311:PHE:HE1  | 1.33                     | 0.76              |
| 13:c:97:THR:HG23  | 13:c:252:PHE:HZ   | 1.24                     | 0.76              |
| 11:a:310:TYR:CE2  | 11:a:311:PHE:CE1  | 2.74                     | 0.75              |
| 6:Q:193:GLU:OE1   | 6:Q:193:GLU:N     | 2.20                     | 0.75              |
| 3:C:381:ASN:HB2   | 7:G:24:SER:HB2    | 1.67                     | 0.75              |
| 11:a:235:PRO:HG2  | 12:b:196:ILE:HD11 | 1.67                     | 0.75              |
| 11:a:420:GLN:HE22 | 11:a:474:LEU:HB3  | 0.94                     | 0.75              |
| 12:b:79:PHE:CE2   | 12:b:83:LEU:CD1   | 2.66                     | 0.75              |
| 13:c:56:LEU:CD1   | 13:c:60:MET:HE2   | 2.14                     | 0.75              |
| 1:A:303:SER:OG    | 1:A:306:SER:OG    | 2.05                     | 0.75              |
| 1:A:435:ALA:HB1   | 1:A:439:ILE:HG21  | 1.69                     | 0.75              |
| 4:D:86:PHE:HZ     | 4:D:263:LEU:CB    | 2.00                     | 0.74              |
| 11:a:345:MET:HE3  | 11:a:349:ILE:HD11 | 1.67                     | 0.74              |
| 13:c:100:PHE:HZ   | 13:c:260:LEU:HD21 | 1.48                     | 0.74              |
| 13:c:108:PHE:CD2  | 13:c:112:LEU:HD23 | 2.22                     | 0.74              |
| 13:c:108:PHE:CE2  | 13:c:112:LEU:HD23 | 2.22                     | 0.74              |
| 11:a:420:GLN:CD   | 11:a:471:SER:O    | 2.30                     | 0.74              |
| 13:c:141:ASN:HD22 | 13:c:185:GLN:NE2  | 1.86                     | 0.74              |
| 7:R:111:GLU:O     | 7:R:115:PHE:HD2   | 1.69                     | 0.73              |
| 1:A:271:MET:HE1   | 1:A:281:ALA:HB2   | 1.70                     | 0.73              |
| 11:a:310:TYR:CD2  | 11:a:311:PHE:HD1  | 2.07                     | 0.73              |
| 21:k:109:TRP:CE3  | 21:k:116:LEU:CD2  | 2.71                     | 0.73              |
| 13:c:255:VAL:HG13 | 13:c:259:PHE:CE2  | 2.23                     | 0.73              |
| 5:P:162:LYS:CB    | 5:P:165:TRP:CH2   | 2.72                     | 0.73              |
| 13:c:97:THR:HG22  | 13:c:252:PHE:HZ   | 1.45                     | 0.73              |
| 11:a:532:THR:HG21 | 14:d:116:ARG:HD3  | 1.71                     | 0.72              |
| 11:a:393:LEU:HD21 | 32:a:601:HEA:H171 | 1.72                     | 0.72              |
| 5:P:165:TRP:NE1   | 5:P:220:PHE:CE1   | 2.57                     | 0.72              |
| 13:c:141:ASN:HD22 | 13:c:185:GLN:HE21 | 1.35                     | 0.72              |
| 13:c:100:PHE:HZ   | 13:c:260:LEU:CD2  | 2.02                     | 0.72              |
| 10:U:59:GLN:OE1   | 10:U:68:PHE:CB    | 2.38                     | 0.71              |
| 5:P:179:PRO:HG3   | 5:P:191:CYS:SG    | 2.29                     | 0.71              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:O    | 2.08                     | 0.71              |
| 15:e:179:SER:C    | 15:e:180:PRO:CD   | 2.62                     | 0.71              |
| 3:N:227:ILE:CD1   | 4:O:291:LYS:CD    | 2.64                     | 0.71              |
| 21:k:59:LYS:O     | 21:k:63:TYR:HB2   | 1.91                     | 0.70              |
| 13:c:100:PHE:CE1  | 13:c:103:ILE:HD11 | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:354:LEU:HA   | 11:a:386:TYR:OH   | 1.91                     | 0.70              |
| 12:b:162:ARG:HH12 | 12:b:233:GLN:HG2  | 1.56                     | 0.70              |
| 2:B:88:LEU:HD21   | 10:J:5:PHE:HZ     | 1.57                     | 0.70              |
| 11:a:274:PHE:HE2  | 12:b:78:GLU:OE2   | 1.74                     | 0.70              |
| 11:a:13:PHE:CE1   | 13:c:19:PRO:HA    | 2.26                     | 0.70              |
| 27:A:504:PEF:H351 | 26:A:505:PCF:H232 | 1.73                     | 0.69              |
| 11:a:536:LYS:CD   | 14:d:130:LEU:HD21 | 2.21                     | 0.69              |
| 1:A:154:ALA:HB1   | 1:A:263:ASN:HD22  | 1.55                     | 0.69              |
| 10:U:76:ASP:OD1   | 10:U:77:LYS:N     | 2.25                     | 0.69              |
| 13:c:100:PHE:CE1  | 13:c:260:LEU:HD21 | 2.27                     | 0.69              |
| 3:N:274:TYR:CE1   | 3:N:275:LEU:CD2   | 2.76                     | 0.69              |
| 11:a:381:VAL:HG22 | 11:a:384:PHE:CZ   | 2.27                     | 0.69              |
| 1:A:79:ARG:NH2    | 1:A:121:VAL:HG22  | 2.08                     | 0.69              |
| 10:U:76:ASP:CG    | 10:U:77:LYS:H     | 2.01                     | 0.69              |
| 12:b:127:ASN:ND2  | 20:j:67:MET:SD    | 2.64                     | 0.69              |
| 16:f:91:ARG:NH2   | 16:f:94:ASN:OD1   | 2.26                     | 0.69              |
| 21:k:109:TRP:CZ2  | 21:k:116:LEU:CD2  | 2.74                     | 0.69              |
| 11:a:310:TYR:CD2  | 11:a:311:PHE:CE1  | 2.81                     | 0.68              |
| 13:c:154:TYR:HB2  | 21:k:57:TRP:HB3   | 1.76                     | 0.68              |
| 3:N:274:TYR:HE1   | 3:N:275:LEU:HD21  | 1.55                     | 0.68              |
| 10:J:5:PHE:CE2    | 10:J:7:ASN:HB2    | 2.28                     | 0.67              |
| 1:L:154:ALA:HB1   | 1:L:263:ASN:HD22  | 1.58                     | 0.67              |
| 4:O:304:ARG:HH21  | 7:R:61:MET:HE3    | 1.60                     | 0.67              |
| 11:a:37:VAL:HG22  | 18:h:52:PHE:CE1   | 2.30                     | 0.67              |
| 12:b:108:LYS:C    | 12:b:170:ARG:HH22 | 2.03                     | 0.67              |
| 5:E:129:VAL:HG12  | 5:E:169:ILE:HA    | 1.74                     | 0.67              |
| 3:N:274:TYR:CD1   | 3:N:275:LEU:CD2   | 2.77                     | 0.67              |
| 11:a:5:TRP:NE1    | 11:a:9:ASN:HD21   | 1.91                     | 0.67              |
| 3:N:88:PHE:CD2    | 3:N:236:PHE:HE1   | 2.05                     | 0.67              |
| 11:a:247:HIS:CG   | 11:a:296:HIS:HE1  | 2.13                     | 0.67              |
| 3:N:35:LEU:HD13   | 3:N:92:PHE:CE1    | 2.30                     | 0.66              |
| 10:U:59:GLN:HE22  | 10:U:69:LYS:CG    | 2.09                     | 0.66              |
| 11:a:43:ARG:NH2   | 32:a:601:HEA:OMA  | 2.28                     | 0.66              |
| 11:a:57:ASN:OD1   | 11:a:59:GLN:HG2   | 1.95                     | 0.66              |
| 2:B:88:LEU:HD21   | 10:J:5:PHE:CZ     | 2.29                     | 0.66              |
| 6:F:193:GLU:N     | 6:F:193:GLU:OE1   | 2.28                     | 0.66              |
| 11:a:532:THR:HG21 | 14:d:116:ARG:CD   | 2.26                     | 0.66              |
| 13:c:36:THR:HA    | 13:c:39:LEU:HD12  | 1.76                     | 0.66              |
| 10:J:5:PHE:CE2    | 10:J:8:LYS:N      | 2.62                     | 0.66              |
| 2:M:128:PHE:HB3   | 2:M:183:ILE:HD11  | 1.78                     | 0.66              |
| 11:a:357:ILE:HB   | 11:a:386:TYR:OH   | 1.95                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:534:PRO:HA   | 14:d:116:ARG:NH1  | 2.10                     | 0.66              |
| 13:c:56:LEU:HD11  | 13:c:60:MET:HE2   | 1.75                     | 0.66              |
| 3:N:92:PHE:CZ     | 3:N:236:PHE:HD1   | 1.88                     | 0.66              |
| 11:a:536:LYS:HD3  | 14:d:119:GLY:HA3  | 1.78                     | 0.66              |
| 13:c:194:PHE:CE2  | 13:c:201:TYR:HE2  | 2.13                     | 0.66              |
| 4:D:86:PHE:HZ     | 4:D:263:LEU:HB2   | 1.59                     | 0.66              |
| 11:a:209:LEU:HD12 | 11:a:245:PHE:CD2  | 2.30                     | 0.66              |
| 2:B:128:PHE:HB3   | 2:B:183:ILE:HD11  | 1.79                     | 0.65              |
| 5:P:162:LYS:HD2   | 5:P:165:TRP:HH2   | 0.74                     | 0.65              |
| 13:c:108:PHE:CD2  | 13:c:112:LEU:CD2  | 2.79                     | 0.65              |
| 12:b:12:PRO:O     | 15:e:172:GLN:NE2  | 2.29                     | 0.65              |
| 12:b:18:TYR:CE1   | 19:i:36:TYR:CE1   | 2.84                     | 0.65              |
| 4:D:63:GLY:N      | 4:D:68:GLU:OE2    | 2.29                     | 0.65              |
| 11:a:345:MET:HE3  | 11:a:349:ILE:CD1  | 2.26                     | 0.65              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:HA   | 1.97                     | 0.65              |
| 16:f:52:ASN:ND2   | 16:f:81:ASP:OD2   | 2.29                     | 0.65              |
| 11:a:447:ILE:HG22 | 12:b:226:SER:HB3  | 1.79                     | 0.65              |
| 11:a:29:LEU:HD11  | 11:a:476:MET:HE1  | 1.77                     | 0.65              |
| 1:A:255:ARG:NH2   | 1:A:440:GLU:OE1   | 2.29                     | 0.65              |
| 10:J:55:THR:HA    | 10:J:59:GLN:NE2   | 2.11                     | 0.65              |
| 9:T:11:PHE:CD1    | 9:T:17:PHE:CE1    | 2.85                     | 0.65              |
| 16:f:52:ASN:O     | 16:f:85:GLN:NE2   | 2.22                     | 0.65              |
| 4:D:225:MET:SD    | 30:D:401:HEC:FE   | 1.89                     | 0.65              |
| 13:c:196:ILE:HG13 | 13:c:203:ALA:HA   | 1.79                     | 0.65              |
| 11:a:420:GLN:HE21 | 11:a:474:LEU:CB   | 1.87                     | 0.64              |
| 15:e:73:ARG:NH1   | 15:e:85:GLU:OE2   | 2.29                     | 0.64              |
| 1:A:140:ARG:NH2   | 1:A:186:LEU:O     | 2.31                     | 0.64              |
| 10:J:5:PHE:HD2    | 10:J:8:LYS:HB2    | 1.60                     | 0.64              |
| 8:S:52:ARG:NH2    | 25:S:102:CDL:OA4  | 2.30                     | 0.64              |
| 11:a:536:LYS:CE   | 14:d:130:LEU:HD21 | 2.27                     | 0.64              |
| 13:c:108:PHE:CZ   | 13:c:112:LEU:CD2  | 2.80                     | 0.64              |
| 11:a:194:ALA:O    | 11:a:198:THR:HG23 | 1.97                     | 0.64              |
| 10:U:70:ASP:OD1   | 10:U:71:LYS:N     | 2.31                     | 0.64              |
| 15:e:49:VAL:O     | 15:e:54:ARG:NH2   | 2.29                     | 0.64              |
| 2:M:45:LEU:HD23   | 2:M:119:LEU:HD12  | 1.80                     | 0.64              |
| 1:L:252:ILE:HG12  | 8:S:28:TYR:CE1    | 2.31                     | 0.64              |
| 6:Q:165:GLU:OE1   | 6:Q:165:GLU:N     | 2.25                     | 0.64              |
| 11:a:48:ALA:HB3   | 11:a:52:GLN:HE22  | 1.62                     | 0.64              |
| 5:E:49:GLU:OE2    | 5:E:49:GLU:N      | 2.30                     | 0.64              |
| 14:d:142:ARG:NH1  | 16:f:60:ASP:OD2   | 2.31                     | 0.64              |
| 28:C:401:HEM:HBC2 | 28:C:401:HEM:HMC1 | 1.79                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:536:LYS:HE3  | 14:d:132:TRP:CD1  | 2.33                     | 0.63              |
| 5:E:85:GLN:HE22   | 10:J:49:GLN:HG3   | 1.62                     | 0.63              |
| 11:a:358:GLY:N    | 11:a:386:TYR:CE2  | 2.64                     | 0.63              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:C    | 2.41                     | 0.63              |
| 5:E:194:HIS:CB    | 31:E:301:FES:S2   | 2.75                     | 0.63              |
| 5:E:174:HIS:HB2   | 5:E:209:ALA:HA    | 1.80                     | 0.63              |
| 4:O:185:ARG:NH2   | 30:O:401:HEC:O1A  | 2.31                     | 0.63              |
| 1:A:263:ASN:OD1   | 1:A:336:VAL:HG22  | 1.97                     | 0.63              |
| 11:a:5:TRP:CD1    | 11:a:9:ASN:ND2    | 2.66                     | 0.63              |
| 13:c:73:ILE:HD11  | 17:g:13:GLN:HG3   | 1.80                     | 0.63              |
| 1:A:253:ARG:NH2   | 1:A:443:LEU:O     | 2.28                     | 0.63              |
| 10:J:5:PHE:CE2    | 10:J:8:LYS:HB2    | 2.32                     | 0.63              |
| 5:E:196:SER:HB3   | 5:E:208:PRO:HD2   | 1.79                     | 0.62              |
| 7:R:67:VAL:HG11   | 8:S:22:GLN:HG2    | 1.81                     | 0.62              |
| 13:c:37:LEU:HD11  | 17:g:51:VAL:HG21  | 1.80                     | 0.62              |
| 13:c:194:PHE:CE2  | 13:c:201:TYR:CE2  | 2.86                     | 0.62              |
| 27:J:101:PEF:H453 | 3:N:157:ILE:HD11  | 1.81                     | 0.62              |
| 1:L:389:ASP:OD2   | 1:L:400:ARG:NH1   | 2.33                     | 0.62              |
| 1:A:131:ILE:O     | 1:A:188:ARG:NH1   | 2.30                     | 0.62              |
| 5:P:165:TRP:CE2   | 5:P:220:PHE:CZ    | 2.87                     | 0.62              |
| 11:a:118:LEU:HB3  | 13:c:29:PHE:HE1   | 1.63                     | 0.62              |
| 1:A:291:TRP:NE1   | 1:A:298:SER:OG    | 2.33                     | 0.62              |
| 12:b:111:MET:HE2  | 12:b:171:ILE:HG12 | 1.80                     | 0.62              |
| 3:C:237:LEU:O     | 3:C:241:ASN:ND2   | 2.28                     | 0.62              |
| 1:L:68:LEU:HD11   | 1:L:195:ILE:HD11  | 1.80                     | 0.62              |
| 13:c:84:GLY:HA2   | 13:c:87:ILE:HD12  | 1.81                     | 0.62              |
| 1:L:23:GLU:N      | 1:L:23:GLU:OE1    | 2.32                     | 0.62              |
| 5:P:165:TRP:NE1   | 5:P:220:PHE:HE1   | 1.97                     | 0.61              |
| 5:P:179:PRO:HB2   | 5:P:189:TRP:HB3   | 1.82                     | 0.61              |
| 10:J:5:PHE:HE2    | 10:J:8:LYS:HG3    | 1.66                     | 0.61              |
| 14:d:121:THR:O    | 14:d:127:SER:OG   | 2.19                     | 0.61              |
| 3:N:222:ASN:OD1   | 3:N:223:PRO:CA    | 2.44                     | 0.61              |
| 11:a:255:MET:HA   | 11:a:258:PHE:HD2  | 1.66                     | 0.61              |
| 11:a:535:THR:HG23 | 14:d:116:ARG:NH2  | 2.16                     | 0.61              |
| 1:A:67:PHE:CZ     | 1:A:183:ILE:HA    | 2.35                     | 0.61              |
| 6:Q:177:VAL:O     | 6:Q:181:VAL:HG22  | 2.01                     | 0.61              |
| 11:a:420:GLN:NE2  | 11:a:471:SER:O    | 2.34                     | 0.61              |
| 13:c:194:PHE:CZ   | 13:c:201:TYR:CD2  | 2.87                     | 0.61              |
| 1:L:435:ALA:HB1   | 1:L:439:ILE:HG21  | 1.81                     | 0.61              |
| 11:a:113:PRO:O    | 11:a:117:MET:HG2  | 2.01                     | 0.61              |
| 11:a:310:TYR:HD2  | 11:a:311:PHE:HD1  | 1.42                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:i:16:THR:O     | 19:i:20:VAL:HG23  | 2.01                     | 0.61              |
| 6:F:167:LYS:NZ    | 6:F:171:GLU:OE2   | 2.33                     | 0.60              |
| 11:a:77:ILE:HG22  | 11:a:253:LEU:HD11 | 1.82                     | 0.60              |
| 13:c:56:LEU:CG    | 13:c:60:MET:HE3   | 2.31                     | 0.60              |
| 1:A:67:PHE:CE1    | 1:A:183:ILE:HG23  | 2.36                     | 0.60              |
| 1:L:417:ASP:OD1   | 1:L:420:ARG:NH2   | 2.33                     | 0.60              |
| 11:a:260:VAL:HG21 | 11:a:399:ALA:HB2  | 1.83                     | 0.60              |
| 21:k:109:TRP:CD2  | 21:k:116:LEU:HD22 | 2.35                     | 0.60              |
| 10:U:59:GLN:NE2   | 10:U:69:LYS:HG3   | 2.17                     | 0.60              |
| 10:J:5:PHE:CD2    | 10:J:8:LYS:CB     | 2.82                     | 0.60              |
| 11:a:517:ILE:HG21 | 11:a:530:PHE:HZ   | 1.66                     | 0.60              |
| 21:k:109:TRP:CH2  | 21:k:116:LEU:HD21 | 2.36                     | 0.60              |
| 4:D:81:LYS:O      | 4:D:267:LYS:NZ    | 2.33                     | 0.60              |
| 10:U:59:GLN:NE2   | 10:U:69:LYS:CG    | 2.65                     | 0.60              |
| 10:U:59:GLN:HE22  | 10:U:69:LYS:HG3   | 1.67                     | 0.60              |
| 6:F:165:GLU:OE2   | 6:F:165:GLU:N     | 2.30                     | 0.60              |
| 3:N:221:MET:HE1   | 29:N:403:U10:H3M3 | 1.84                     | 0.60              |
| 11:a:5:TRP:CD1    | 11:a:9:ASN:HD21   | 2.20                     | 0.60              |
| 11:a:219:ASP:OD1  | 11:a:224:THR:OG1  | 2.20                     | 0.60              |
| 16:f:42:VAL:HG11  | 16:f:47:ILE:HD13  | 1.83                     | 0.60              |
| 28:C:402:HEM:HBC2 | 28:C:402:HEM:HMC2 | 1.83                     | 0.60              |
| 4:D:213:ASN:HD21  | 4:D:226:ALA:HA    | 1.67                     | 0.60              |
| 1:L:58:THR:OG1    | 1:L:60:LYS:NZ     | 2.35                     | 0.60              |
| 3:N:90:PHE:CE2    | 3:N:274:TYR:CD1   | 2.90                     | 0.59              |
| 9:T:5:THR:O       | 9:T:9:ILE:HG13    | 2.02                     | 0.59              |
| 9:T:10:PHE:HD1    | 9:T:20:THR:HG1    | 0.73                     | 0.59              |
| 28:N:401:HEM:HMC1 | 28:N:401:HEM:HBC2 | 1.84                     | 0.59              |
| 15:e:75:LYS:HA    | 16:f:94:ASN:HD21  | 1.67                     | 0.59              |
| 7:G:115:PHE:HA    | 7:G:118:LEU:HG    | 1.83                     | 0.59              |
| 16:f:61:GLN:NE2   | 16:f:95:ASP:OD2   | 2.35                     | 0.59              |
| 1:L:94:HIS:CB     | 1:L:109:HIS:CE1   | 2.84                     | 0.59              |
| 3:N:90:PHE:CZ     | 3:N:274:TYR:CE1   | 2.90                     | 0.59              |
| 10:U:52:LYS:O     | 10:U:56:THR:OG1   | 2.15                     | 0.59              |
| 14:d:157:ASP:OD1  | 14:d:157:ASP:N    | 2.36                     | 0.59              |
| 5:P:70:TYR:CB     | 9:T:11:PHE:CD2    | 2.85                     | 0.59              |
| 1:A:63:GLY:O      | 1:A:67:PHE:CE2    | 2.55                     | 0.59              |
| 3:C:287:ASN:OD1   | 3:C:288:PHE:N     | 2.35                     | 0.59              |
| 3:C:69:VAL:HG12   | 3:C:70:ARG:HG3    | 1.85                     | 0.59              |
| 3:N:17:MET:HE1    | 26:T:101:PCF:H441 | 1.85                     | 0.59              |
| 12:b:166:PRO:HD3  | 12:b:240:PHE:CD1  | 2.38                     | 0.59              |
| 1:L:252:ILE:CG1   | 8:S:28:TYR:CD1    | 2.79                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:P:70:TYR:HB3    | 9:T:11:PHE:CE2    | 2.38                     | 0.59              |
| 11:a:176:ILE:O    | 11:a:179:ARG:NH1  | 2.36                     | 0.58              |
| 11:a:274:PHE:CE2  | 12:b:78:GLU:OE2   | 2.55                     | 0.58              |
| 15:e:177:ILE:O    | 15:e:180:PRO:CD   | 2.51                     | 0.58              |
| 11:a:247:HIS:ND1  | 11:a:296:HIS:HE1  | 1.96                     | 0.58              |
| 25:H:101:CDL:H742 | 25:H:102:CDL:H111 | 1.85                     | 0.58              |
| 1:L:131:ILE:O     | 1:L:188:ARG:NH1   | 2.34                     | 0.58              |
| 1:L:446:ASN:ND2   | 3:N:224:TYR:OH    | 2.33                     | 0.58              |
| 11:a:365:LEU:HD22 | 11:a:380:VAL:HG12 | 1.85                     | 0.58              |
| 11:a:536:LYS:CE   | 14:d:132:TRP:CD1  | 2.86                     | 0.58              |
| 1:A:399:ARG:HE    | 15:e:54:ARG:HE    | 1.49                     | 0.58              |
| 7:G:120:VAL:HG21  | 1:L:366:GLU:HG3   | 1.85                     | 0.58              |
| 1:L:251:GLU:OE1   | 1:L:253:ARG:NH1   | 2.36                     | 0.58              |
| 11:a:536:LYS:NZ   | 14:d:132:TRP:CD1  | 2.71                     | 0.58              |
| 1:L:252:ILE:HD13  | 8:S:28:TYR:CZ     | 2.32                     | 0.58              |
| 11:a:47:SER:OG    | 15:e:129:ARG:NH1  | 2.37                     | 0.58              |
| 11:a:122:SER:HB2  | 11:a:152:LEU:HB2  | 1.86                     | 0.58              |
| 11:a:135:VAL:O    | 11:a:238:TYR:OH   | 2.17                     | 0.58              |
| 5:P:162:LYS:HD2   | 5:P:165:TRP:CZ3   | 2.27                     | 0.58              |
| 12:b:113:VAL:HG23 | 12:b:171:ILE:HG21 | 1.84                     | 0.58              |
| 2:B:72:THR:HG23   | 2:B:77:SER:HA     | 1.85                     | 0.58              |
| 4:O:285:MET:HB3   | 25:S:102:CDL:H512 | 1.85                     | 0.58              |
| 11:a:516:SER:HA   | 14:d:132:TRP:CH2  | 2.35                     | 0.58              |
| 13:c:97:THR:CG2   | 13:c:252:PHE:HE1  | 2.14                     | 0.58              |
| 12:b:18:TYR:CZ    | 19:i:36:TYR:CE1   | 2.92                     | 0.57              |
| 3:C:381:ASN:ND2   | 7:G:25:ASN:OD1    | 2.37                     | 0.57              |
| 6:Q:174:THR:O     | 6:Q:178:THR:OG1   | 2.19                     | 0.57              |
| 11:a:381:VAL:N    | 11:a:384:PHE:CE2  | 2.72                     | 0.57              |
| 6:F:180:LYS:NZ    | 6:F:185:ASP:OD2   | 2.38                     | 0.57              |
| 7:G:118:LEU:HD11  | 10:U:4:PHE:CE2    | 2.40                     | 0.57              |
| 21:k:88:LYS:HE3   | 21:k:121:LYS:HB3  | 1.86                     | 0.57              |
| 1:A:344:ASP:OD1   | 1:A:344:ASP:N     | 2.36                     | 0.57              |
| 11:a:515:GLN:C    | 14:d:132:TRP:CE3  | 2.82                     | 0.57              |
| 28:N:402:HEM:HBC2 | 28:N:402:HEM:HMC1 | 1.85                     | 0.57              |
| 4:O:304:ARG:NH2   | 7:R:61:MET:CE     | 2.68                     | 0.57              |
| 5:P:165:TRP:NE1   | 5:P:220:PHE:CZ    | 2.73                     | 0.57              |
| 3:N:88:PHE:O      | 3:N:92:PHE:HD2    | 1.87                     | 0.57              |
| 10:U:59:GLN:CD    | 10:U:68:PHE:O     | 2.47                     | 0.57              |
| 28:C:401:HEM:HBB2 | 28:C:401:HEM:HMB2 | 1.87                     | 0.57              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:OG   | 2.20                     | 0.57              |
| 5:P:201:SER:OG    | 5:P:203:ARG:NH2   | 2.36                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:364:ILE:HD13 | 12:b:37:LEU:HD22  | 1.85                     | 0.57              |
| 13:c:56:LEU:CG    | 13:c:60:MET:CE    | 2.82                     | 0.57              |
| 13:c:257:TRP:HA   | 13:c:260:LEU:HD12 | 1.86                     | 0.57              |
| 11:a:385:HIS:CE1  | 32:a:601:HEA:NA   | 2.72                     | 0.57              |
| 4:D:189:GLN:NE2   | 4:D:256:HIS:CG    | 2.51                     | 0.56              |
| 3:N:217:ASP:OD2   | 4:O:298:ARG:NH2   | 2.38                     | 0.56              |
| 5:P:70:TYR:HB3    | 9:T:11:PHE:CD2    | 2.40                     | 0.56              |
| 12:b:108:LYS:N    | 12:b:170:ARG:NH2  | 2.53                     | 0.56              |
| 4:D:238:ASP:OD1   | 4:D:240:THR:OG1   | 2.21                     | 0.56              |
| 11:a:380:VAL:C    | 11:a:384:PHE:CD2  | 2.83                     | 0.56              |
| 3:C:164:LEU:HD23  | 29:N:403:U10:H452 | 1.86                     | 0.56              |
| 5:E:58:THR:HG23   | 5:E:60:SER:H      | 1.71                     | 0.56              |
| 1:L:187:THR:HG23  | 1:L:189:GLU:H     | 1.70                     | 0.56              |
| 28:N:401:HEM:HMB2 | 28:N:401:HEM:HBB2 | 1.87                     | 0.56              |
| 4:O:304:ARG:HH21  | 7:R:61:MET:CE     | 2.18                     | 0.56              |
| 11:a:265:ILE:HD12 | 11:a:333:LEU:HD21 | 1.87                     | 0.56              |
| 11:a:476:MET:HE2  | 11:a:476:MET:HA   | 1.86                     | 0.56              |
| 21:k:117:PHE:HB2  | 27:k:201:PEF:H51  | 1.87                     | 0.56              |
| 1:A:181:GLU:OE1   | 1:A:181:GLU:N     | 2.36                     | 0.56              |
| 9:T:11:PHE:CD1    | 9:T:17:PHE:CD1    | 2.94                     | 0.56              |
| 4:D:281:THR:O     | 4:D:285:MET:HG3   | 2.05                     | 0.56              |
| 11:a:406:LYS:NZ   | 11:a:518:GLU:O    | 2.37                     | 0.56              |
| 1:L:140:ARG:HD3   | 1:L:184:GLU:HA    | 1.88                     | 0.56              |
| 11:a:310:TYR:HE2  | 11:a:311:PHE:CE1  | 2.17                     | 0.56              |
| 28:C:402:HEM:HBB2 | 28:C:402:HEM:HMB2 | 1.86                     | 0.56              |
| 11:a:5:TRP:NE1    | 11:a:9:ASN:ND2    | 2.54                     | 0.56              |
| 15:e:151:MET:HB2  | 15:e:156:ILE:HD12 | 1.88                     | 0.56              |
| 5:E:68:ILE:O      | 5:E:72:MET:HG2    | 2.06                     | 0.56              |
| 5:E:138:GLU:HB3   | 5:E:200:ILE:HG12  | 1.88                     | 0.56              |
| 1:A:167:TYR:HH    | 1:A:328:THR:HG1   | 1.54                     | 0.56              |
| 1:A:154:ALA:HB1   | 1:A:263:ASN:ND2   | 2.21                     | 0.56              |
| 12:b:191:ILE:HD11 | 12:b:203:VAL:HB   | 1.88                     | 0.56              |
| 1:A:362:ARG:HH21  | 7:R:119:ILE:HD11  | 1.71                     | 0.55              |
| 10:J:5:PHE:HD2    | 10:J:8:LYS:N      | 2.03                     | 0.55              |
| 11:a:154:ILE:HG12 | 11:a:213:LEU:HD11 | 1.86                     | 0.55              |
| 11:a:420:GLN:OE1  | 11:a:471:SER:CB   | 2.55                     | 0.55              |
| 11:a:380:VAL:C    | 11:a:384:PHE:CE2  | 2.84                     | 0.55              |
| 27:A:504:PEF:N    | 26:A:505:PCF:O14  | 2.40                     | 0.55              |
| 3:C:113:THR:HG22  | 3:C:197:HIS:CE1   | 2.41                     | 0.55              |
| 8:H:56:GLU:N      | 8:H:56:GLU:OE2    | 2.38                     | 0.55              |
| 11:a:538:ILE:HB   | 14:d:94:PRO:HB2   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:c:97:THR:HG21  | 13:c:252:PHE:HE1  | 1.72                     | 0.55              |
| 15:e:54:ARG:HG2   | 15:e:58:MET:HE2   | 1.89                     | 0.55              |
| 7:R:75:GLN:NE2    | 7:R:79:GLU:OE2    | 2.40                     | 0.55              |
| 9:T:11:PHE:CD1    | 9:T:17:PHE:HE1    | 2.23                     | 0.55              |
| 11:a:250:VAL:HB   | 32:a:602:HEA:CAC  | 2.35                     | 0.55              |
| 12:b:140:ASP:O    | 12:b:161:ASN:ND2  | 2.39                     | 0.55              |
| 18:h:56:PHE:O     | 18:h:59:VAL:HG12  | 2.06                     | 0.55              |
| 11:a:99:VAL:HG21  | 11:a:105:ASN:HD22 | 1.72                     | 0.55              |
| 11:a:536:LYS:CE   | 14:d:132:TRP:NE1  | 2.69                     | 0.55              |
| 12:b:43:PHE:HZ    | 19:i:22:MET:HE1   | 1.72                     | 0.55              |
| 12:b:246:GLU:OE1  | 12:b:247:ASN:ND2  | 2.39                     | 0.55              |
| 14:d:111:SER:OG   | 14:d:153:LYS:O    | 2.23                     | 0.55              |
| 5:E:172:CYS:HB3   | 5:E:177:CYS:H     | 1.70                     | 0.55              |
| 11:a:313:ALA:HB2  | 12:b:97:PHE:HZ    | 1.72                     | 0.55              |
| 2:B:425:GLU:OE2   | 2:M:167:ARG:NH2   | 2.40                     | 0.55              |
| 4:D:189:GLN:HE22  | 4:D:256:HIS:CD2   | 2.16                     | 0.55              |
| 5:E:159:ARG:HH12  | 5:E:203:ARG:HG2   | 1.70                     | 0.55              |
| 16:f:45:GLU:O     | 16:f:49:THR:HG23  | 2.07                     | 0.55              |
| 3:C:30:TRP:HA     | 3:C:99:ARG:NH1    | 2.22                     | 0.55              |
| 11:a:13:PHE:HB3   | 13:c:17:ALA:HA    | 1.89                     | 0.55              |
| 11:a:357:ILE:HD11 | 12:b:45:PHE:HE1   | 1.72                     | 0.55              |
| 13:c:56:LEU:HD12  | 13:c:60:MET:HE2   | 1.88                     | 0.55              |
| 13:c:260:LEU:O    | 13:c:264:ILE:HG22 | 2.06                     | 0.55              |
| 4:D:86:PHE:CE1    | 4:D:263:LEU:HD23  | 2.41                     | 0.55              |
| 14:d:107:ILE:H    | 14:d:107:ILE:HD12 | 1.72                     | 0.55              |
| 4:D:76:ASP:OD1    | 4:D:76:ASP:N      | 2.39                     | 0.54              |
| 5:P:70:TYR:HB2    | 9:T:11:PHE:CD2    | 2.43                     | 0.54              |
| 12:b:80:ILE:HG21  | 27:b:302:PEF:H381 | 1.89                     | 0.54              |
| 12:b:107:GLN:HB2  | 12:b:170:ARG:NE   | 2.22                     | 0.54              |
| 9:I:58:ASN:N      | 9:I:58:ASN:OD1    | 2.38                     | 0.54              |
| 10:J:5:PHE:CE2    | 10:J:8:LYS:HG3    | 2.42                     | 0.54              |
| 1:L:236:SER:OG    | 1:L:237:LEU:N     | 2.41                     | 0.54              |
| 6:Q:192:GLU:O     | 6:Q:196:HIS:ND1   | 2.27                     | 0.54              |
| 11:a:38:PHE:CE1   | 18:h:55:PRO:HB3   | 2.43                     | 0.54              |
| 14:d:143:CYS:CB   | 14:d:146:CYS:SG   | 2.94                     | 0.54              |
| 2:B:192:LYS:O     | 2:B:192:LYS:HG2   | 2.07                     | 0.54              |
| 11:a:312:SER:O    | 11:a:315:THR:OG1  | 2.25                     | 0.54              |
| 1:L:373:ARG:NH1   | 1:L:407:ASP:OD2   | 2.41                     | 0.54              |
| 1:L:449:ARG:HG2   | 27:N:404:PEF:HN1  | 1.72                     | 0.54              |
| 14:d:128:HIS:CD2  | 14:d:145:GLU:HG3  | 2.42                     | 0.54              |
| 7:G:109:ARG:O     | 7:G:113:GLU:HG3   | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:535:THR:HB   | 14:d:94:PRO:HA    | 1.90                     | 0.54              |
| 16:f:79:SER:OG    | 16:f:81:ASP:OD1   | 2.25                     | 0.54              |
| 4:D:189:GLN:NE2   | 4:D:256:HIS:NE2   | 2.53                     | 0.54              |
| 10:J:14:GLN:NE2   | 7:R:119:ILE:HB    | 2.23                     | 0.54              |
| 6:Q:165:GLU:O     | 6:Q:169:HIS:ND1   | 2.36                     | 0.54              |
| 12:b:108:LYS:N    | 12:b:108:LYS:HD2  | 2.22                     | 0.54              |
| 16:f:76:ILE:HA    | 19:i:7:THR:HG22   | 1.90                     | 0.54              |
| 1:L:44:ALA:HA     | 1:L:210:GLY:HA3   | 1.89                     | 0.54              |
| 11:a:221:ASN:HA   | 21:k:105:LYS:HD2  | 1.89                     | 0.54              |
| 6:Q:150:LEU:HD13  | 6:Q:209:VAL:HG11  | 1.89                     | 0.54              |
| 8:S:66:ILE:O      | 8:S:70:ILE:HG23   | 2.08                     | 0.54              |
| 5:E:151:ARG:NH1   | 5:E:207:GLY:O     | 2.41                     | 0.54              |
| 6:F:151:GLU:OE1   | 6:F:151:GLU:N     | 2.27                     | 0.54              |
| 9:I:26:PHE:HB2    | 10:J:45:VAL:HG22  | 1.89                     | 0.54              |
| 11:a:515:GLN:O    | 14:d:132:TRP:CE3  | 2.54                     | 0.54              |
| 1:L:328:THR:OG1   | 1:L:329:GLY:N     | 2.41                     | 0.53              |
| 11:a:33:ILE:HD13  | 18:h:51:ILE:HG23  | 1.90                     | 0.53              |
| 1:L:268:VAL:HG12  | 1:L:431:ILE:HG22  | 1.90                     | 0.53              |
| 3:N:128:ALA:CB    | 3:N:274:TYR:OH    | 2.54                     | 0.53              |
| 11:a:536:LYS:HD2  | 14:d:119:GLY:HA3  | 1.89                     | 0.53              |
| 12:b:88:ILE:O     | 12:b:92:VAL:HG12  | 2.08                     | 0.53              |
| 12:b:107:GLN:HB2  | 12:b:170:ARG:NH2  | 2.23                     | 0.53              |
| 13:c:97:THR:HG21  | 13:c:252:PHE:CE1  | 2.41                     | 0.53              |
| 1:L:141:GLN:OE1   | 1:L:141:GLN:N     | 2.36                     | 0.53              |
| 4:O:228:PRO:HB2   | 30:O:401:HEC:HBB2 | 1.90                     | 0.53              |
| 12:b:220:LEU:HA   | 12:b:225:HIS:CG   | 2.42                     | 0.53              |
| 16:f:124:LYS:HB3  | 16:f:125:PRO:HD3  | 1.90                     | 0.53              |
| 4:D:225:MET:SD    | 30:D:401:HEC:NB   | 2.82                     | 0.53              |
| 12:b:228:MET:HG3  | 12:b:228:MET:O    | 2.08                     | 0.53              |
| 1:L:202:ASP:OD2   | 1:L:231:SER:N     | 2.41                     | 0.53              |
| 11:a:159:LEU:HA   | 11:a:162:ILE:HG12 | 1.90                     | 0.53              |
| 12:b:160:ASP:OD1  | 12:b:160:ASP:N    | 2.41                     | 0.53              |
| 11:a:78:ILE:HG12  | 11:a:253:LEU:HD13 | 1.91                     | 0.53              |
| 13:c:262:LEU:HD13 | 22:l:116:TRP:HH2  | 1.74                     | 0.53              |
| 14:d:101:GLY:HA3  | 14:d:148:SER:HA   | 1.89                     | 0.53              |
| 11:a:440:LEU:O    | 12:b:19:PHE:CD1   | 2.62                     | 0.53              |
| 16:f:98:THR:O     | 16:f:102:ILE:HG12 | 2.08                     | 0.53              |
| 22:l:120:MET:HE3  | 22:l:120:MET:O    | 2.09                     | 0.53              |
| 3:C:139:MET:SD    | 3:C:256:CYS:SG    | 2.90                     | 0.53              |
| 3:N:277:PRO:HG3   | 3:N:337:ALA:HB2   | 1.91                     | 0.53              |
| 5:P:169:ILE:HG13  | 5:P:216:PRO:HD3   | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:e:151:MET:HE2  | 15:e:172:GLN:HG3  | 1.91                     | 0.53              |
| 3:C:79:ARG:NH1    | 28:C:401:HEM:O2A  | 2.43                     | 0.52              |
| 10:J:5:PHE:CE2    | 10:J:8:LYS:CB     | 2.92                     | 0.52              |
| 21:k:116:LEU:HB2  | 27:k:201:PEF:H11  | 1.89                     | 0.52              |
| 8:S:58:LEU:HA     | 8:S:61:ALA:HB3    | 1.91                     | 0.52              |
| 1:L:57:GLU:OE2    | 1:L:64:ALA:N      | 2.43                     | 0.52              |
| 2:M:88:LEU:HG     | 10:U:5:PHE:HZ     | 1.74                     | 0.52              |
| 6:Q:190:CYS:HB2   | 6:Q:193:GLU:CD    | 2.34                     | 0.52              |
| 11:a:247:HIS:CE1  | 11:a:296:HIS:CE1  | 2.94                     | 0.52              |
| 12:b:114:LYS:NZ   | 20:j:63:SER:O     | 2.42                     | 0.52              |
| 21:k:109:TRP:CE3  | 21:k:116:LEU:HD21 | 2.36                     | 0.52              |
| 2:B:48:VAL:HG22   | 2:B:102:ILE:HG12  | 1.89                     | 0.52              |
| 11:a:4:TRP:O      | 11:a:8:VAL:HG23   | 2.09                     | 0.52              |
| 8:S:56:GLU:HG2    | 25:S:101:CDL:HA61 | 1.90                     | 0.52              |
| 11:a:5:TRP:O      | 11:a:9:ASN:ND2    | 2.42                     | 0.52              |
| 11:a:380:VAL:O    | 11:a:384:PHE:CE2  | 2.58                     | 0.52              |
| 16:f:43:SER:OG    | 16:f:44:LEU:N     | 2.43                     | 0.52              |
| 1:A:328:THR:OG1   | 1:A:329:GLY:N     | 2.43                     | 0.52              |
| 26:A:505:PCF:H291 | 26:A:505:PCF:H391 | 1.92                     | 0.52              |
| 3:C:184:TYR:CZ    | 28:C:401:HEM:HBC1 | 2.44                     | 0.52              |
| 3:C:367:ILE:HA    | 3:C:370:TYR:CE2   | 2.45                     | 0.52              |
| 1:L:255:ARG:NH2   | 1:L:440:GLU:OE2   | 2.43                     | 0.52              |
| 3:N:110:ARG:HH21  | 3:N:207:SER:HB2   | 1.75                     | 0.52              |
| 5:P:154:GLN:HG3   | 5:P:158:ASP:HB3   | 1.92                     | 0.52              |
| 11:a:266:PRO:HD3  | 11:a:273:ILE:HD11 | 1.91                     | 0.52              |
| 14:d:110:THR:CG2  | 14:d:155:MET:HE1  | 2.28                     | 0.52              |
| 16:f:44:LEU:HD11  | 19:i:7:THR:HG21   | 1.91                     | 0.52              |
| 2:B:368:ASN:OD1   | 2:B:371:SER:OG    | 2.22                     | 0.52              |
| 4:D:66:LYS:HG3    | 6:F:191:ILE:HD12  | 1.90                     | 0.52              |
| 4:O:224:ALA:HB3   | 30:O:401:HEC:HBD2 | 1.91                     | 0.52              |
| 5:P:70:TYR:CB     | 9:T:11:PHE:CE2    | 2.93                     | 0.52              |
| 13:c:90:MET:O     | 13:c:94:ILE:HG12  | 2.09                     | 0.52              |
| 17:g:12:LEU:HD21  | 17:g:22:GLN:HB3   | 1.91                     | 0.52              |
| 3:N:132:TYR:HA    | 28:N:401:HEM:HAD2 | 1.91                     | 0.52              |
| 12:b:95:PRO:HA    | 12:b:98:LYS:HZ3   | 1.74                     | 0.52              |
| 13:c:215:HIS:HD1  | 13:c:249:TYR:HH   | 1.38                     | 0.52              |
| 3:C:357:ILE:O     | 3:C:361:SER:OG    | 2.25                     | 0.52              |
| 15:e:47:ARG:NH2   | 15:e:69:ASP:OD2   | 2.41                     | 0.52              |
| 11:a:501:ASP:O    | 15:e:100:ARG:NH2  | 2.43                     | 0.51              |
| 12:b:13:SER:OG    | 12:b:14:SER:N     | 2.42                     | 0.51              |
| 4:D:288:LYS:NZ    | 25:H:102:CDL:OB4  | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:46:VAL:HG11   | 1:L:119:VAL:HG22  | 1.92                     | 0.51              |
| 3:N:384:SER:O     | 3:N:384:SER:OG    | 2.26                     | 0.51              |
| 1:A:429:LYS:O     | 1:A:449:ARG:NH1   | 2.43                     | 0.51              |
| 7:G:8:LYS:HA      | 7:G:11:GLN:HE21   | 1.75                     | 0.51              |
| 4:O:81:LYS:O      | 4:O:267:LYS:NZ    | 2.43                     | 0.51              |
| 17:g:50:ARG:NH1   | 17:g:55:LYS:O     | 2.41                     | 0.51              |
| 9:I:18:TYR:HB3    | 9:I:22:PHE:HE2    | 1.76                     | 0.51              |
| 17:g:19:THR:HA    | 17:g:22:GLN:HG3   | 1.91                     | 0.51              |
| 2:M:60:GLY:HA3    | 2:M:175:LEU:HD12  | 1.92                     | 0.51              |
| 11:a:38:PHE:O     | 11:a:42:ILE:HG23  | 2.10                     | 0.51              |
| 11:a:536:LYS:HZ1  | 14:d:132:TRP:HD1  | 1.54                     | 0.51              |
| 12:b:181:ILE:HD12 | 12:b:181:ILE:H    | 1.75                     | 0.51              |
| 4:D:145:MET:HE3   | 4:D:145:MET:HA    | 1.93                     | 0.51              |
| 4:D:225:MET:SD    | 30:D:401:HEC:ND   | 2.84                     | 0.51              |
| 5:E:154:GLN:OE1   | 5:E:212:ASN:ND2   | 2.43                     | 0.51              |
| 11:a:154:ILE:HG21 | 11:a:217:PHE:HB2  | 1.92                     | 0.51              |
| 13:c:255:VAL:O    | 13:c:258:LEU:HG   | 2.11                     | 0.51              |
| 1:A:85:GLU:O      | 1:A:89:GLU:HG3    | 2.11                     | 0.51              |
| 25:A:502:CDL:H541 | 26:A:503:PCF:H482 | 1.92                     | 0.51              |
| 1:L:96:ASN:OD1    | 1:L:97:ALA:N      | 2.43                     | 0.51              |
| 3:N:367:ILE:HA    | 3:N:370:TYR:CE2   | 2.45                     | 0.51              |
| 1:A:450:SER:HB3   | 27:A:504:PEF:H51  | 1.93                     | 0.51              |
| 11:a:127:GLU:OE2  | 11:a:145:HIS:ND1  | 2.37                     | 0.51              |
| 13:c:212:HIS:NE2  | 13:c:257:TRP:HB2  | 2.26                     | 0.51              |
| 13:c:259:PHE:O    | 13:c:263:THR:HG22 | 2.11                     | 0.51              |
| 2:M:54:ARG:NH1    | 2:M:99:GLU:OE2    | 2.44                     | 0.50              |
| 11:a:140:SER:HA   | 11:a:145:HIS:CD2  | 2.46                     | 0.50              |
| 11:a:247:HIS:CD2  | 11:a:293:VAL:O    | 2.64                     | 0.50              |
| 21:k:109:TRP:CZ3  | 21:k:116:LEU:CD2  | 2.95                     | 0.50              |
| 11:a:502:ASP:OD1  | 11:a:503:ASN:N    | 2.44                     | 0.50              |
| 12:b:164:VAL:HG22 | 12:b:233:GLN:HE21 | 1.76                     | 0.50              |
| 14:d:123:SER:HB3  | 14:d:127:SER:HB3  | 1.94                     | 0.50              |
| 1:L:22:THR:HG21   | 1:L:400:ARG:HE    | 1.75                     | 0.50              |
| 10:U:59:GLN:OE1   | 10:U:68:PHE:C     | 2.54                     | 0.50              |
| 1:A:57:GLU:OE1    | 1:A:63:GLY:N      | 2.37                     | 0.50              |
| 5:P:147:ILE:HB    | 5:P:153:PRO:HB3   | 1.92                     | 0.50              |
| 10:U:76:ASP:CG    | 10:U:77:LYS:N     | 2.70                     | 0.50              |
| 9:I:12:ARG:HG3    | 9:I:13:ARG:HD2    | 1.92                     | 0.50              |
| 25:L:502:CDL:H112 | 25:L:502:CDL:H711 | 1.93                     | 0.50              |
| 2:M:387:SER:O     | 2:M:391:LYS:NZ    | 2.44                     | 0.50              |
| 11:a:480:TYR:O    | 11:a:484:THR:HG22 | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:b:221:CYS:H    | 12:b:225:HIS:HB2  | 1.76                     | 0.50              |
| 1:L:127:THR:HG22  | 1:L:228:LEU:HD21  | 1.92                     | 0.50              |
| 3:N:14:ASN:HA     | 3:N:18:ILE:HG12   | 1.94                     | 0.50              |
| 11:a:122:SER:OG   | 11:a:149:ALA:O    | 2.23                     | 0.50              |
| 20:j:66:PRO:O     | 20:j:67:MET:HG2   | 2.12                     | 0.50              |
| 3:N:88:PHE:O      | 3:N:92:PHE:CD2    | 2.65                     | 0.50              |
| 4:O:197:THR:HG23  | 6:Q:202:ARG:HH12  | 1.76                     | 0.50              |
| 11:a:26:LEU:O     | 11:a:30:VAL:HG22  | 2.12                     | 0.50              |
| 32:a:601:HEA:HMA  | 32:a:601:HEA:HBA2 | 1.92                     | 0.50              |
| 3:C:178:ARG:NH2   | 5:P:95:TRP:O      | 2.40                     | 0.50              |
| 1:L:295:MET:HE1   | 1:L:301:LEU:HD11  | 1.94                     | 0.50              |
| 12:b:159:VAL:HG23 | 12:b:162:ARG:HG2  | 1.94                     | 0.50              |
| 25:A:502:CDL:H512 | 25:A:502:CDL:H712 | 1.94                     | 0.49              |
| 5:E:190:PHE:HD1   | 5:E:197:HIS:HD1   | 1.60                     | 0.49              |
| 10:J:20:ILE:HG22  | 10:J:20:ILE:O     | 2.12                     | 0.49              |
| 11:a:173:ALA:HA   | 11:a:176:ILE:HG22 | 1.93                     | 0.49              |
| 11:a:536:LYS:HD3  | 14:d:119:GLY:CA   | 2.41                     | 0.49              |
| 1:A:31:LEU:HD12   | 1:A:32:THR:H      | 1.77                     | 0.49              |
| 1:A:67:PHE:HE1    | 1:A:183:ILE:HG23  | 1.75                     | 0.49              |
| 29:C:403:U10:H402 | 5:E:92:LEU:HD11   | 1.93                     | 0.49              |
| 11:a:101:TYR:HB2  | 11:a:104:VAL:HG12 | 1.94                     | 0.49              |
| 3:C:30:TRP:HA     | 3:C:99:ARG:HH12   | 1.77                     | 0.49              |
| 5:E:174:HIS:CD2   | 5:E:208:PRO:HB2   | 2.47                     | 0.49              |
| 25:L:502:CDL:H511 | 26:L:503:PCF:H321 | 1.94                     | 0.49              |
| 11:a:296:HIS:HA   | 11:a:299:PHE:CE1  | 2.47                     | 0.49              |
| 5:E:194:HIS:CG    | 31:E:301:FES:S2   | 2.90                     | 0.49              |
| 10:U:5:PHE:HE1    | 10:U:7:ASN:HB2    | 1.77                     | 0.49              |
| 11:a:34:ILE:HD11  | 18:h:54:ILE:HB    | 1.93                     | 0.49              |
| 12:b:175:LEU:HB3  | 12:b:201:ASN:HB2  | 1.93                     | 0.49              |
| 14:d:111:SER:HB3  | 14:d:152:LEU:HD11 | 1.92                     | 0.49              |
| 16:f:89:ALA:O     | 16:f:93:VAL:HG23  | 2.12                     | 0.49              |
| 18:h:50:VAL:O     | 18:h:54:ILE:HG13  | 2.11                     | 0.49              |
| 5:E:110:ASP:OD1   | 5:E:112:SER:OG    | 2.28                     | 0.49              |
| 5:P:177:CYS:CB    | 31:P:301:FES:S2   | 2.92                     | 0.49              |
| 11:a:118:LEU:HD11 | 11:a:156:SER:HB2  | 1.95                     | 0.49              |
| 14:d:143:CYS:HB3  | 14:d:146:CYS:SG   | 2.51                     | 0.49              |
| 5:E:164:GLU:OE1   | 5:E:164:GLU:N     | 2.45                     | 0.49              |
| 1:L:447:ARG:NH1   | 3:N:19:ASP:OD1    | 2.43                     | 0.49              |
| 11:a:91:PRO:HA    | 11:a:94:ILE:HG12  | 1.93                     | 0.49              |
| 2:M:279:SER:OG    | 2:M:280:HIS:N     | 2.45                     | 0.49              |
| 12:b:79:PHE:O     | 12:b:83:LEU:HG    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:128:ASN:N     | 1:A:128:ASN:OD1   | 2.46                     | 0.49              |
| 3:N:311:SER:OG    | 3:N:313:ILE:O     | 2.28                     | 0.49              |
| 11:a:516:SER:N    | 14:d:132:TRP:CZ3  | 2.81                     | 0.49              |
| 2:B:67:LYS:HA     | 2:B:67:LYS:HD3    | 1.62                     | 0.49              |
| 5:E:156:ASP:OD1   | 5:E:201:SER:OG    | 2.27                     | 0.49              |
| 11:a:390:MET:HE1  | 11:a:428:VAL:HB   | 1.95                     | 0.49              |
| 12:b:107:GLN:C    | 12:b:170:ARG:NH2  | 2.71                     | 0.49              |
| 27:k:201:PEF:H172 | 27:k:201:PEF:H431 | 1.93                     | 0.49              |
| 2:B:279:SER:OG    | 2:B:280:HIS:N     | 2.46                     | 0.48              |
| 7:G:47:GLU:O      | 8:H:10:TYR:OH     | 2.25                     | 0.48              |
| 1:L:100:SER:OG    | 1:L:101:ARG:N     | 2.46                     | 0.48              |
| 11:a:155:LEU:HD21 | 13:c:32:CYS:HB3   | 1.95                     | 0.48              |
| 12:b:183:SER:N    | 12:b:217:CYS:SG   | 2.83                     | 0.48              |
| 21:k:109:TRP:CH2  | 21:k:116:LEU:CD2  | 2.96                     | 0.48              |
| 5:P:162:LYS:CG    | 5:P:165:TRP:CH2   | 2.96                     | 0.48              |
| 12:b:173:LEU:N    | 12:b:203:VAL:O    | 2.46                     | 0.48              |
| 4:D:213:ASN:HD22  | 4:D:226:ALA:HA    | 1.77                     | 0.48              |
| 10:J:5:PHE:HD2    | 10:J:8:LYS:H      | 1.58                     | 0.48              |
| 10:U:5:PHE:CE1    | 10:U:7:ASN:HB2    | 2.49                     | 0.48              |
| 12:b:79:PHE:O     | 12:b:82:THR:OG1   | 2.25                     | 0.48              |
| 13:c:108:PHE:CE2  | 13:c:112:LEU:HD21 | 2.39                     | 0.48              |
| 3:C:132:TYR:CD1   | 3:C:132:TYR:C     | 2.91                     | 0.48              |
| 5:E:104:MET:HE2   | 5:E:104:MET:HA    | 1.96                     | 0.48              |
| 1:L:188:ARG:HG3   | 1:L:192:LEU:HD23  | 1.94                     | 0.48              |
| 5:P:172:CYS:HB2   | 5:P:177:CYS:H     | 1.79                     | 0.48              |
| 25:S:101:CDL:H541 | 25:S:101:CDL:H311 | 1.96                     | 0.48              |
| 11:a:423:ILE:HG22 | 11:a:471:SER:HB2  | 1.96                     | 0.48              |
| 7:G:46:GLU:OE1    | 7:G:52:GLN:NE2    | 2.47                     | 0.48              |
| 5:P:132:ARG:HE    | 5:P:200:ILE:HD11  | 1.77                     | 0.48              |
| 5:E:134:ARG:NH1   | 5:E:156:ASP:OD2   | 2.40                     | 0.48              |
| 1:L:66:HIS:NE2    | 1:L:70:HIS:CD2    | 2.82                     | 0.48              |
| 27:O:402:PEF:H431 | 27:O:402:PEF:H253 | 1.96                     | 0.48              |
| 5:P:139:ILE:HG12  | 5:P:163:PRO:HB2   | 1.96                     | 0.48              |
| 13:c:94:ILE:O     | 13:c:97:THR:OG1   | 2.24                     | 0.48              |
| 3:C:207:SER:OG    | 3:C:208:ASN:N     | 2.44                     | 0.48              |
| 9:T:12:ARG:O      | 9:T:12:ARG:HD3    | 2.14                     | 0.48              |
| 11:a:33:ILE:O     | 11:a:37:VAL:HG23  | 2.13                     | 0.48              |
| 11:a:452:GLU:HB3  | 15:e:139:MET:HE1  | 1.94                     | 0.48              |
| 3:N:274:TYR:CD1   | 3:N:275:LEU:HD23  | 2.48                     | 0.48              |
| 12:b:131:THR:HG22 | 12:b:132:ASN:N    | 2.23                     | 0.48              |
| 27:J:101:PEF:H431 | 27:J:101:PEF:H401 | 1.67                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:29:ASN:O      | 1:L:201:SER:OG    | 2.23                     | 0.48              |
| 15:e:47:ARG:HB3   | 15:e:48:LEU:HD12  | 1.95                     | 0.48              |
| 25:H:102:CDL:H802 | 25:H:102:CDL:H771 | 1.64                     | 0.47              |
| 11:a:479:MET:CG   | 11:a:483:PHE:CE2  | 2.93                     | 0.47              |
| 11:a:516:SER:CA   | 14:d:132:TRP:CE3  | 2.97                     | 0.47              |
| 3:N:274:TYR:CE1   | 3:N:275:LEU:HG    | 2.49                     | 0.47              |
| 3:N:274:TYR:CD1   | 3:N:275:LEU:HD21  | 2.46                     | 0.47              |
| 11:a:124:LEU:HD21 | 18:h:58:VAL:HG22  | 1.95                     | 0.47              |
| 11:a:481:ASP:O    | 11:a:485:SER:HB2  | 2.14                     | 0.47              |
| 13:c:184:GLY:O    | 13:c:188:GLU:HG2  | 2.14                     | 0.47              |
| 3:C:2:LYS:HG3     | 3:C:5:LYS:HG3     | 1.95                     | 0.47              |
| 5:E:116:GLU:HA    | 5:E:133:HIS:HB3   | 1.97                     | 0.47              |
| 5:E:181:GLY:HA2   | 5:E:189:TRP:HA    | 1.97                     | 0.47              |
| 13:c:100:PHE:CZ   | 13:c:260:LEU:CD2  | 2.77                     | 0.47              |
| 13:c:135:LEU:HD21 | 22:l:158:VAL:HG21 | 1.96                     | 0.47              |
| 13:c:241:ASN:N    | 27:c:301:PEF:O2P  | 2.47                     | 0.47              |
| 17:g:48:SER:O     | 17:g:52:ILE:HG22  | 2.15                     | 0.47              |
| 22:l:128:SER:HA   | 22:l:138:LYS:HD2  | 1.95                     | 0.47              |
| 9:T:54:PRO:HA     | 9:T:58:ASN:HB2    | 1.96                     | 0.47              |
| 11:a:155:LEU:HD11 | 13:c:32:CYS:SG    | 2.55                     | 0.47              |
| 25:H:102:CDL:H782 | 25:H:102:CDL:H752 | 1.55                     | 0.47              |
| 12:b:120:TRP:CE2  | 12:b:224:LEU:HB2  | 2.50                     | 0.47              |
| 13:c:215:HIS:CG   | 13:c:249:TYR:HH   | 2.29                     | 0.47              |
| 11:a:400:TYR:OH   | 11:a:482:GLN:NE2  | 2.45                     | 0.47              |
| 27:b:302:PEF:H142 | 27:b:302:PEF:H111 | 1.53                     | 0.47              |
| 15:e:75:LYS:HA    | 16:f:94:ASN:ND2   | 2.28                     | 0.47              |
| 5:E:86:ALA:HB2    | 9:I:29:LYS:NZ     | 2.29                     | 0.47              |
| 5:E:177:CYS:HB3   | 31:E:301:FES:S1   | 2.55                     | 0.47              |
| 5:E:199:ASP:OD1   | 5:E:203:ARG:N     | 2.47                     | 0.47              |
| 25:H:101:CDL:H152 | 25:H:101:CDL:H122 | 1.48                     | 0.47              |
| 2:M:195:VAL:HB    | 2:M:225:GLY:H     | 1.78                     | 0.47              |
| 11:a:103:ARG:HB3  | 13:c:63:TRP:HZ2   | 1.79                     | 0.47              |
| 11:a:114:PRO:HB2  | 13:c:29:PHE:CD1   | 2.50                     | 0.47              |
| 11:a:248:PRO:O    | 11:a:252:ILE:HG23 | 2.15                     | 0.47              |
| 11:a:440:LEU:O    | 12:b:19:PHE:HD1   | 1.97                     | 0.47              |
| 11:a:536:LYS:NZ   | 14:d:132:TRP:NE1  | 2.63                     | 0.47              |
| 13:c:97:THR:HG22  | 13:c:252:PHE:CE1  | 2.39                     | 0.47              |
| 14:d:80:LEU:O     | 14:d:83:GLU:HG3   | 2.14                     | 0.47              |
| 14:d:139:LYS:HE3  | 14:d:139:LYS:HA   | 1.97                     | 0.47              |
| 3:C:346:ASN:OD1   | 3:C:346:ASN:N     | 2.47                     | 0.47              |
| 1:L:48:VAL:HG22   | 1:L:206:ILE:HG22  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:110:ALA:HB1   | 1:L:114:ALA:HB3   | 1.97                     | 0.47              |
| 3:N:89:PHE:CE2    | 3:N:93:LEU:HD22   | 2.50                     | 0.47              |
| 11:a:171:LEU:O    | 11:a:175:MET:HG2  | 2.15                     | 0.47              |
| 5:P:50:MET:CE     | 8:S:28:TYR:CE1    | 2.92                     | 0.47              |
| 5:P:174:HIS:HE1   | 5:P:194:HIS:CG    | 2.33                     | 0.47              |
| 9:T:12:ARG:HG3    | 9:T:13:ARG:HG3    | 1.97                     | 0.47              |
| 11:a:212:GLY:O    | 11:a:215:MET:HG3  | 2.15                     | 0.47              |
| 2:B:68:PHE:HZ     | 2:B:133:LEU:HB2   | 1.79                     | 0.47              |
| 7:G:120:VAL:HG12  | 7:G:122:LYS:HG2   | 1.97                     | 0.47              |
| 11:a:403:TRP:O    | 11:a:407:MET:HG2  | 2.15                     | 0.47              |
| 12:b:20:GLN:NE2   | 12:b:187:PRO:HB2  | 2.30                     | 0.47              |
| 3:C:45:VAL:HG11   | 27:D:402:PEF:H232 | 1.96                     | 0.46              |
| 5:P:86:ALA:HB2    | 9:T:29:LYS:HE2    | 1.97                     | 0.46              |
| 16:f:43:SER:HB3   | 16:f:46:GLU:CD    | 2.39                     | 0.46              |
| 1:A:67:PHE:HZ     | 1:A:183:ILE:CB    | 2.29                     | 0.46              |
| 25:H:102:CDL:H312 | 25:H:102:CDL:H341 | 1.75                     | 0.46              |
| 3:N:274:TYR:CE1   | 3:N:275:LEU:CG    | 2.98                     | 0.46              |
| 11:a:8:VAL:HG12   | 11:a:12:ILE:HB    | 1.97                     | 0.46              |
| 11:a:466:VAL:HG21 | 15:e:125:PHE:HB2  | 1.97                     | 0.46              |
| 11:a:532:THR:CG2  | 14:d:116:ARG:CD   | 2.93                     | 0.46              |
| 13:c:140:LEU:O    | 13:c:143:VAL:HG12 | 2.15                     | 0.46              |
| 16:f:122:GLU:HG3  | 16:f:123:LEU:HD23 | 1.96                     | 0.46              |
| 21:k:88:LYS:O     | 21:k:124:HIS:NE2  | 2.47                     | 0.46              |
| 1:A:67:PHE:HZ     | 1:A:183:ILE:HA    | 1.78                     | 0.46              |
| 3:C:21:PRO:HB2    | 3:C:218:ARG:HD2   | 1.97                     | 0.46              |
| 29:C:403:U10:H72  | 29:C:403:U10:H1M3 | 1.66                     | 0.46              |
| 3:N:223:PRO:HB3   | 27:N:404:PEF:H11  | 1.96                     | 0.46              |
| 4:O:302:TYR:HB2   | 7:R:68:TYR:CE1    | 2.51                     | 0.46              |
| 14:d:46:LEU:HD23  | 14:d:46:LEU:HA    | 1.80                     | 0.46              |
| 19:i:11:LYS:HA    | 19:i:14:ILE:HG22  | 1.97                     | 0.46              |
| 5:P:96:SER:OG     | 5:P:97:ALA:N      | 2.49                     | 0.46              |
| 8:S:13:TRP:CD1    | 8:S:14:TRP:H      | 2.34                     | 0.46              |
| 10:U:59:GLN:NE2   | 10:U:69:LYS:HG2   | 2.30                     | 0.46              |
| 15:e:167:PHE:CZ   | 15:e:169:GLY:O    | 2.68                     | 0.46              |
| 22:l:152:VAL:O    | 22:l:155:LEU:HG   | 2.16                     | 0.46              |
| 27:J:101:PEF:H311 | 27:J:101:PEF:H341 | 1.64                     | 0.46              |
| 3:N:207:SER:OG    | 3:N:208:ASN:N     | 2.49                     | 0.46              |
| 5:P:172:CYS:HB2   | 5:P:177:CYS:N     | 2.30                     | 0.46              |
| 5:P:189:TRP:O     | 5:P:198:TYR:N     | 2.46                     | 0.46              |
| 5:P:190:PHE:HE1   | 5:P:195:GLY:HA2   | 1.80                     | 0.46              |
| 10:U:54:LYS:O     | 10:U:59:GLN:CG    | 2.47                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:197:SER:OG    | 2:M:224:ASP:OD1   | 2.27                     | 0.46              |
| 2:M:202:ILE:HD12  | 2:M:375:LEU:HD13  | 1.98                     | 0.46              |
| 3:N:121:PHE:HB2   | 28:N:402:HEM:HBB1 | 1.97                     | 0.46              |
| 14:d:60:GLY:H     | 14:d:71:GLN:HE21  | 1.63                     | 0.46              |
| 13:c:224:LEU:O    | 13:c:227:THR:HG22 | 2.16                     | 0.46              |
| 5:P:136:PRO:HA    | 5:P:139:ILE:HD12  | 1.98                     | 0.46              |
| 6:Q:190:CYS:O     | 6:Q:190:CYS:SG    | 2.73                     | 0.46              |
| 11:a:273:ILE:HD13 | 11:a:332:THR:HG21 | 1.98                     | 0.46              |
| 16:f:58:VAL:H     | 16:f:92:ARG:HH12  | 1.61                     | 0.46              |
| 18:h:29:THR:HG22  | 18:h:31:PRO:HD3   | 1.97                     | 0.46              |
| 7:G:39:ARG:HD3    | 7:G:93:GLU:O      | 2.16                     | 0.46              |
| 2:M:254:PHE:HB3   | 2:M:404:LEU:HD22  | 1.98                     | 0.46              |
| 3:N:23:PRO:HB2    | 3:N:26:ILE:HG23   | 1.98                     | 0.46              |
| 11:a:103:ARG:NH1  | 27:a:605:PEF:O1P  | 2.36                     | 0.46              |
| 12:b:164:VAL:HG22 | 12:b:233:GLN:NE2  | 2.30                     | 0.46              |
| 13:c:69:THR:O     | 13:c:73:ILE:HG22  | 2.16                     | 0.46              |
| 13:c:168:LEU:HD21 | 13:c:230:ILE:HG21 | 1.97                     | 0.46              |
| 29:N:403:U10:H102 | 27:N:404:PEF:H242 | 1.98                     | 0.45              |
| 11:a:162:ILE:HG22 | 27:a:605:PEF:H451 | 1.98                     | 0.45              |
| 11:a:443:MET:HG2  | 11:a:444:PRO:HD2  | 1.97                     | 0.45              |
| 12:b:140:ASP:OD1  | 12:b:140:ASP:N    | 2.49                     | 0.45              |
| 19:i:9:MET:HE3    | 19:i:9:MET:HB2    | 1.88                     | 0.45              |
| 3:C:172:SER:H     | 3:C:175:THR:HG22  | 1.81                     | 0.45              |
| 7:G:116:ASP:OD2   | 10:U:24:ARG:NH2   | 2.47                     | 0.45              |
| 3:N:240:ILE:HG23  | 3:N:241:ASN:HD22  | 1.81                     | 0.45              |
| 11:a:72:MET:SD    | 32:a:601:HEA:C1C  | 3.05                     | 0.45              |
| 11:a:357:ILE:HD11 | 12:b:45:PHE:CE1   | 2.51                     | 0.45              |
| 13:c:8:GLN:NE2    | 13:c:10:HIS:O     | 2.49                     | 0.45              |
| 3:C:70:ARG:NH2    | 4:D:110:LEU:CD1   | 2.51                     | 0.45              |
| 6:F:150:LEU:HG    | 6:F:209:VAL:HG11  | 1.98                     | 0.45              |
| 11:a:154:ILE:HD13 | 11:a:217:PHE:HB2  | 1.97                     | 0.45              |
| 18:h:56:PHE:N     | 18:h:56:PHE:CD1   | 2.84                     | 0.45              |
| 1:A:84:LEU:HD21   | 1:A:125:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:427:TRP:CD1   | 1:A:428:ASP:H     | 2.34                     | 0.45              |
| 29:C:403:U10:H151 | 29:C:403:U10:H171 | 1.70                     | 0.45              |
| 4:D:265:ILE:O     | 4:D:269:MET:HG3   | 2.17                     | 0.45              |
| 27:J:101:PEF:H381 | 27:J:101:PEF:H201 | 1.98                     | 0.45              |
| 4:O:286:TRP:HB2   | 25:S:102:CDL:H551 | 1.99                     | 0.45              |
| 11:a:251:TYR:O    | 11:a:255:MET:HG3  | 2.16                     | 0.45              |
| 11:a:266:PRO:O    | 11:a:270:HIS:N    | 2.49                     | 0.45              |
| 12:b:95:PRO:HA    | 12:b:98:LYS:NZ    | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:c:144:ILE:HD13 | 13:c:180:LEU:HD11 | 1.99                     | 0.45              |
| 29:C:403:U10:H453 | 3:N:182:LEU:HD13  | 1.99                     | 0.45              |
| 4:D:280:LEU:HD21  | 5:E:79:LEU:HB2    | 1.99                     | 0.45              |
| 5:E:135:THR:OG1   | 5:E:138:GLU:OE1   | 2.23                     | 0.45              |
| 10:J:5:PHE:HD2    | 10:J:8:LYS:CB     | 2.27                     | 0.45              |
| 1:L:88:PHE:HD1    | 1:L:93:ALA:HB3    | 1.81                     | 0.45              |
| 5:P:120:LEU:HB3   | 5:P:131:ILE:HG23  | 1.99                     | 0.45              |
| 11:a:209:LEU:HD12 | 11:a:245:PHE:CG   | 2.51                     | 0.45              |
| 12:b:175:LEU:HD12 | 12:b:175:LEU:HA   | 1.84                     | 0.45              |
| 13:c:142:THR:HG22 | 13:c:257:TRP:HE1  | 1.82                     | 0.45              |
| 2:B:293:SER:HB2   | 2:B:323:ALA:HB1   | 1.98                     | 0.45              |
| 7:G:75:GLN:HA     | 7:G:78:ILE:HD12   | 1.98                     | 0.45              |
| 11:a:42:ILE:HG13  | 11:a:43:ARG:N     | 2.30                     | 0.45              |
| 16:f:79:SER:O     | 16:f:83:ILE:HG22  | 2.17                     | 0.45              |
| 21:k:109:TRP:CZ3  | 21:k:116:LEU:HD23 | 2.52                     | 0.45              |
| 27:A:504:PEF:H222 | 29:C:403:U10:H121 | 1.99                     | 0.45              |
| 2:B:241:ARG:HH11  | 2:B:417:LEU:HD22  | 1.82                     | 0.45              |
| 3:N:59:ASP:OD1    | 3:N:59:ASP:N      | 2.48                     | 0.45              |
| 14:d:96:ASP:OD1   | 14:d:97:ALA:N     | 2.49                     | 0.45              |
| 15:e:73:ARG:HD2   | 15:e:81:LEU:HD22  | 1.99                     | 0.45              |
| 21:k:115:THR:HB   | 27:k:201:PEF:H12  | 1.99                     | 0.45              |
| 26:A:503:PCF:H232 | 26:A:503:PCF:H31  | 1.99                     | 0.45              |
| 2:B:98:ARG:HD3    | 2:B:169:ILE:O     | 2.17                     | 0.45              |
| 2:M:129:LEU:HD13  | 2:M:131:PHE:CZ    | 2.51                     | 0.45              |
| 2:M:163:LYS:HD2   | 2:M:163:LYS:HA    | 1.65                     | 0.45              |
| 3:C:132:TYR:HA    | 28:C:401:HEM:HAA1 | 1.99                     | 0.45              |
| 3:N:90:PHE:CZ     | 3:N:274:TYR:CD1   | 3.04                     | 0.45              |
| 11:a:37:VAL:CG2   | 18:h:52:PHE:CD1   | 3.00                     | 0.45              |
| 11:a:517:ILE:HG21 | 11:a:530:PHE:CZ   | 2.50                     | 0.45              |
| 5:P:50:MET:CE     | 8:S:28:TYR:OH     | 2.59                     | 0.45              |
| 9:T:41:LYS:HB3    | 9:T:41:LYS:HE2    | 1.90                     | 0.45              |
| 11:a:426:ILE:O    | 11:a:430:ILE:HG23 | 2.17                     | 0.45              |
| 13:c:189:TYR:HE1  | 13:c:209:THR:HG21 | 1.82                     | 0.45              |
| 14:d:108:MET:HE2  | 14:d:108:MET:HA   | 1.97                     | 0.45              |
| 5:E:47:SER:HB2    | 5:E:48:PRO:HD3    | 2.00                     | 0.44              |
| 5:P:139:ILE:HD11  | 5:P:164:GLU:HA    | 1.98                     | 0.44              |
| 11:a:32:GLY:HA3   | 11:a:76:PHE:CE1   | 2.52                     | 0.44              |
| 11:a:38:PHE:O     | 11:a:41:ILE:HG22  | 2.17                     | 0.44              |
| 11:a:374:PHE:HE1  | 12:b:19:PHE:HE1   | 1.65                     | 0.44              |
| 11:a:389:SER:C    | 11:a:390:MET:HE2  | 2.42                     | 0.44              |
| 12:b:79:PHE:CE1   | 12:b:83:LEU:HD21  | 2.53                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:b:122:TRP:HE1  | 12:b:228:MET:HG3  | 1.83                     | 0.44              |
| 1:A:32:THR:HB     | 1:A:205:ILE:HD12  | 1.97                     | 0.44              |
| 1:A:67:PHE:CZ     | 1:A:183:ILE:HG23  | 2.53                     | 0.44              |
| 1:A:71:LEU:HD13   | 1:A:131:ILE:HD12  | 1.97                     | 0.44              |
| 26:A:503:PCF:H132 | 26:A:503:PCF:H112 | 1.79                     | 0.44              |
| 2:B:404:LEU:HD23  | 2:B:404:LEU:HA    | 1.87                     | 0.44              |
| 3:C:228:LYS:HG3   | 4:D:288:LYS:HE3   | 2.00                     | 0.44              |
| 3:C:287:ASN:HB3   | 3:C:290:LEU:HB2   | 1.98                     | 0.44              |
| 1:L:352:GLN:NE2   | 1:L:454:MET:HG2   | 2.31                     | 0.44              |
| 4:O:277:LEU:HD23  | 4:O:277:LEU:HA    | 1.81                     | 0.44              |
| 11:a:52:GLN:HE22  | 15:e:129:ARG:HH22 | 1.65                     | 0.44              |
| 11:a:381:VAL:N    | 11:a:384:PHE:HE2  | 2.15                     | 0.44              |
| 12:b:84:ILE:HG21  | 27:b:302:PEF:H431 | 1.98                     | 0.44              |
| 15:e:178:PHE:C    | 15:e:180:PRO:HD3  | 2.42                     | 0.44              |
| 1:A:125:ILE:HG22  | 1:A:126:LEU:HD23  | 1.98                     | 0.44              |
| 26:A:503:PCF:H351 | 26:A:503:PCF:H382 | 1.62                     | 0.44              |
| 5:E:175:LEU:HB2   | 5:E:194:HIS:CE1   | 2.52                     | 0.44              |
| 1:L:154:ALA:HB1   | 1:L:263:ASN:ND2   | 2.26                     | 0.44              |
| 2:M:67:LYS:HD3    | 2:M:67:LYS:HA     | 1.71                     | 0.44              |
| 6:Q:190:CYS:HB2   | 6:Q:193:GLU:OE2   | 2.18                     | 0.44              |
| 18:h:51:ILE:HD12  | 18:h:54:ILE:HD12  | 1.99                     | 0.44              |
| 8:H:38:MET:HB3    | 8:H:38:MET:HE2    | 1.79                     | 0.44              |
| 27:J:101:PEF:H381 | 27:J:101:PEF:H171 | 1.99                     | 0.44              |
| 25:S:101:CDL:H511 | 25:S:101:CDL:HB4  | 1.85                     | 0.44              |
| 13:c:138:PRO:O    | 13:c:142:THR:HG23 | 2.17                     | 0.44              |
| 27:A:504:PEF:H312 | 27:A:504:PEF:H31  | 1.84                     | 0.44              |
| 8:H:55:THR:HB     | 8:H:56:GLU:OE2    | 2.18                     | 0.44              |
| 6:Q:180:LYS:HG2   | 6:Q:185:ASP:HB3   | 2.00                     | 0.44              |
| 13:c:185:GLN:O    | 13:c:189:TYR:CD2  | 2.70                     | 0.44              |
| 16:f:127:CYS:HB2  | 16:f:132:ILE:HB   | 2.00                     | 0.44              |
| 22:l:111:ILE:HG13 | 22:l:112:ILE:N    | 2.33                     | 0.44              |
| 1:A:35:THR:HB     | 1:A:208:SER:OG    | 2.18                     | 0.44              |
| 1:A:68:LEU:HD21   | 1:A:191:LEU:HB3   | 1.99                     | 0.44              |
| 2:B:284:LEU:HD11  | 2:B:338:LEU:HD13  | 1.99                     | 0.44              |
| 11:a:468:SER:HB3  | 32:a:601:HEA:H262 | 1.99                     | 0.44              |
| 14:d:110:THR:HG23 | 14:d:155:MET:HE3  | 1.95                     | 0.44              |
| 1:L:415:GLU:HG2   | 1:L:416:LYS:N     | 2.32                     | 0.44              |
| 11:a:338:ILE:CG2  | 11:a:345:MET:HE2  | 2.36                     | 0.44              |
| 12:b:24:SER:HB3   | 12:b:27:TYR:HB3   | 1.98                     | 0.44              |
| 1:A:456:ARG:N     | 25:A:502:CDL:OB3  | 2.51                     | 0.44              |
| 25:A:502:CDL:H542 | 26:A:503:PCF:H271 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:E:136:PRO:HA    | 5:E:139:ILE:HD12  | 1.99                     | 0.44              |
| 3:N:35:LEU:HD23   | 3:N:233:ILE:HD13  | 2.00                     | 0.44              |
| 11:a:323:GLY:C    | 11:a:327:PHE:HD2  | 2.17                     | 0.44              |
| 12:b:186:VAL:HG11 | 12:b:189:LEU:HD12 | 1.98                     | 0.44              |
| 12:b:241:LEU:O    | 12:b:245:GLU:HG2  | 2.18                     | 0.44              |
| 10:J:5:PHE:CE2    | 10:J:7:ASN:C      | 2.96                     | 0.44              |
| 26:L:503:PCF:H351 | 26:L:503:PCF:H292 | 1.99                     | 0.44              |
| 2:M:53:SER:HA     | 2:M:56:GLN:HE21   | 1.83                     | 0.44              |
| 11:a:419:ILE:HD13 | 15:e:113:GLY:HA3  | 2.00                     | 0.44              |
| 18:h:39:LEU:HB3   | 18:h:40:PRO:HD3   | 2.00                     | 0.44              |
| 1:L:397:THR:OG1   | 1:L:398:GLY:N     | 2.51                     | 0.43              |
| 4:O:246:GLN:NE2   | 6:Q:214:VAL:O     | 2.51                     | 0.43              |
| 11:a:381:VAL:CG2  | 11:a:384:PHE:CZ   | 3.00                     | 0.43              |
| 16:f:44:LEU:HB3   | 16:f:45:GLU:OE1   | 2.17                     | 0.43              |
| 1:L:147:GLN:O     | 1:L:150:VAL:HG12  | 2.18                     | 0.43              |
| 11:a:510:LYS:HZ1  | 14:d:144:PRO:HG3  | 1.83                     | 0.43              |
| 11:a:537:SER:OG   | 14:d:97:ALA:HB2   | 2.18                     | 0.43              |
| 12:b:54:LYS:HA    | 12:b:57:ILE:HG22  | 1.99                     | 0.43              |
| 13:c:169:LYS:HA   | 13:c:169:LYS:HD3  | 1.72                     | 0.43              |
| 15:e:167:PHE:CZ   | 15:e:170:ARG:O    | 2.57                     | 0.43              |
| 27:k:201:PEF:H141 | 27:k:201:PEF:H171 | 1.69                     | 0.43              |
| 10:J:11:TYR:HD1   | 7:R:118:LEU:HD23  | 1.84                     | 0.43              |
| 2:M:72:THR:HG21   | 2:M:129:LEU:HD12  | 1.99                     | 0.43              |
| 3:N:58:MET:HB3    | 3:N:173:ASN:OD1   | 2.19                     | 0.43              |
| 27:N:405:PEF:H351 | 27:N:405:PEF:H382 | 1.52                     | 0.43              |
| 5:P:152:ASP:O     | 5:P:212:ASN:ND2   | 2.49                     | 0.43              |
| 5:P:174:HIS:CE1   | 5:P:194:HIS:ND1   | 2.86                     | 0.43              |
| 13:c:190:TRP:HE1  | 21:k:119:ASN:ND2  | 2.16                     | 0.43              |
| 14:d:140:LEU:HD11 | 14:d:151:LYS:HD2  | 1.99                     | 0.43              |
| 16:f:110:LEU:HD13 | 16:f:115:GLN:HB3  | 1.99                     | 0.43              |
| 22:l:119:THR:O    | 22:l:123:SER:OG   | 2.30                     | 0.43              |
| 3:N:287:ASN:HB3   | 3:N:290:LEU:HB2   | 2.00                     | 0.43              |
| 11:a:5:TRP:CG     | 11:a:9:ASN:HD21   | 2.36                     | 0.43              |
| 13:c:141:ASN:ND2  | 13:c:185:GLN:HE21 | 2.10                     | 0.43              |
| 3:C:176:LEU:HD23  | 3:C:176:LEU:HA    | 1.84                     | 0.43              |
| 5:E:210:PRO:HG2   | 5:E:211:LEU:HD23  | 2.00                     | 0.43              |
| 7:G:104:GLU:HG3   | 7:G:108:GLU:OE2   | 2.19                     | 0.43              |
| 10:U:14:GLN:O     | 10:U:16:HIS:ND1   | 2.44                     | 0.43              |
| 11:a:222:LEU:HB3  | 11:a:224:THR:HG23 | 2.00                     | 0.43              |
| 14:d:77:ARG:O     | 14:d:81:LEU:HG    | 2.18                     | 0.43              |
| 1:A:250:SER:HB3   | 8:H:30:LEU:HD12   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:196:MET:HA    | 3:C:199:ILE:HG22  | 1.99                     | 0.43              |
| 11:a:24:TYR:HD2   | 11:a:84:ALA:HA    | 1.83                     | 0.43              |
| 11:a:37:VAL:HG22  | 18:h:52:PHE:CD1   | 2.54                     | 0.43              |
| 11:a:88:TYR:HD1   | 11:a:89:LEU:HG    | 1.82                     | 0.43              |
| 27:c:301:PEF:H142 | 27:c:301:PEF:H112 | 1.31                     | 0.43              |
| 26:A:505:PCF:H292 | 26:A:505:PCF:H481 | 1.74                     | 0.43              |
| 2:B:68:PHE:HE2    | 2:B:133:LEU:HD12  | 1.83                     | 0.43              |
| 1:L:57:GLU:OE1    | 1:L:62:ASN:ND2    | 2.52                     | 0.43              |
| 27:N:405:PEF:H161 | 27:N:405:PEF:H192 | 1.77                     | 0.43              |
| 9:T:46:GLY:N      | 9:T:51:GLU:OE1    | 2.51                     | 0.43              |
| 1:A:86:LEU:O      | 1:A:90:ASN:OD1    | 2.37                     | 0.43              |
| 25:L:502:CDL:H152 | 25:L:502:CDL:H182 | 1.60                     | 0.43              |
| 3:N:44:ILE:O      | 3:N:48:ILE:HG12   | 2.19                     | 0.43              |
| 29:N:403:U10:H422 | 29:N:403:U10:H401 | 1.73                     | 0.43              |
| 12:b:27:TYR:HD2   | 12:b:28:LEU:HD22  | 1.84                     | 0.43              |
| 12:b:183:SER:HG   | 12:b:218:SER:H    | 1.62                     | 0.43              |
| 13:c:50:GLY:O     | 13:c:54:LEU:HG    | 2.17                     | 0.43              |
| 1:A:79:ARG:HH21   | 1:A:121:VAL:HG22  | 1.80                     | 0.43              |
| 27:A:504:PEF:H372 | 27:A:504:PEF:H342 | 1.64                     | 0.43              |
| 5:E:120:LEU:HD22  | 5:E:122:VAL:HG13  | 2.01                     | 0.43              |
| 1:L:44:ALA:HB3    | 1:L:115:VAL:HG21  | 2.01                     | 0.43              |
| 9:T:7:TYR:HE2     | 9:T:12:ARG:HH21   | 1.67                     | 0.43              |
| 11:a:273:ILE:HD13 | 11:a:273:ILE:HA   | 1.93                     | 0.43              |
| 15:e:167:PHE:O    | 15:e:167:PHE:CD2  | 2.71                     | 0.43              |
| 4:D:119:VAL:HG12  | 4:D:120:THR:HG23  | 2.01                     | 0.43              |
| 4:D:228:PRO:HB2   | 30:D:401:HEC:HMC3 | 2.01                     | 0.43              |
| 9:I:8:ASN:OD1     | 9:I:12:ARG:NH2    | 2.33                     | 0.43              |
| 1:L:191:LEU:O     | 1:L:195:ILE:HG12  | 2.19                     | 0.43              |
| 2:M:222:ILE:H     | 2:M:222:ILE:HG13  | 1.62                     | 0.43              |
| 27:N:404:PEF:H221 | 27:N:404:PEF:H191 | 1.75                     | 0.43              |
| 9:T:12:ARG:HH11   | 9:T:12:ARG:HG2    | 1.84                     | 0.43              |
| 11:a:108:THR:HG21 | 11:a:167:GLY:HA3  | 2.01                     | 0.43              |
| 11:a:296:HIS:HD2  | 32:a:602:HEA:C3A  | 2.32                     | 0.43              |
| 12:b:163:LEU:HD23 | 12:b:232:VAL:HG22 | 2.00                     | 0.43              |
| 13:c:6:LYS:HD2    | 14:d:52:PRO:HD3   | 2.01                     | 0.43              |
| 15:e:141:ARG:O    | 15:e:141:ARG:HD3  | 2.18                     | 0.43              |
| 3:C:277:PRO:O     | 3:C:281:ILE:HG13  | 2.19                     | 0.42              |
| 12:b:174:ILE:HD13 | 12:b:174:ILE:HA   | 1.86                     | 0.42              |
| 13:c:242:GLY:HA3  | 27:c:301:PEF:H122 | 2.00                     | 0.42              |
| 14:d:143:CYS:HB3  | 14:d:147:GLY:H    | 1.84                     | 0.42              |
| 22:l:112:ILE:HA   | 22:l:115:THR:HG22 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:D:402:PEF:H453 | 27:D:402:PEF:H421 | 1.75                     | 0.42              |
| 7:G:115:PHE:H     | 7:G:115:PHE:HD1   | 1.68                     | 0.42              |
| 1:L:444:ASP:OD1   | 1:L:444:ASP:N     | 2.34                     | 0.42              |
| 1:L:456:ARG:HA    | 25:L:502:CDL:H512 | 2.01                     | 0.42              |
| 3:N:224:TYR:CE2   | 4:O:295:ILE:HG13  | 2.54                     | 0.42              |
| 8:S:81:LEU:HD23   | 8:S:81:LEU:HA     | 1.73                     | 0.42              |
| 26:T:101:PCF:H222 | 26:T:101:PCF:H251 | 1.70                     | 0.42              |
| 11:a:247:HIS:HB3  | 11:a:248:PRO:HD3  | 2.01                     | 0.42              |
| 11:a:536:LYS:NZ   | 14:d:132:TRP:HE1  | 2.17                     | 0.42              |
| 14:d:77:ARG:O     | 14:d:80:LEU:HG    | 2.19                     | 0.42              |
| 17:g:33:TYR:CE1   | 17:g:37:MET:HE3   | 2.53                     | 0.42              |
| 2:B:142:ARG:HA    | 2:B:142:ARG:HD3   | 1.83                     | 0.42              |
| 2:M:66:GLU:HB2    | 2:M:101:ILE:HD13  | 2.01                     | 0.42              |
| 27:N:404:PEF:H382 | 5:P:80:THR:HG21   | 2.00                     | 0.42              |
| 11:a:31:SER:O     | 11:a:34:ILE:HG22  | 2.19                     | 0.42              |
| 13:c:90:MET:HA    | 13:c:93:LEU:HG    | 2.01                     | 0.42              |
| 15:e:179:SER:N    | 15:e:180:PRO:HD3  | 2.35                     | 0.42              |
| 3:C:17:MET:HE2    | 3:C:17:MET:HB3    | 1.82                     | 0.42              |
| 8:H:81:LEU:HD23   | 8:H:81:LEU:HA     | 1.92                     | 0.42              |
| 2:M:217:LYS:HG2   | 2:M:218:TYR:HD1   | 1.83                     | 0.42              |
| 4:O:237:GLU:O     | 9:T:59:LYS:NZ     | 2.41                     | 0.42              |
| 9:T:36:THR:HA     | 9:T:39:VAL:HG12   | 2.02                     | 0.42              |
| 11:a:431:VAL:HG12 | 11:a:432:PHE:CD1  | 2.54                     | 0.42              |
| 29:C:403:U10:H471 | 29:C:403:U10:H451 | 1.85                     | 0.42              |
| 4:D:185:ARG:NH1   | 30:D:401:HEC:O1D  | 2.53                     | 0.42              |
| 29:N:403:U10:H3M3 | 29:N:403:U10:H4M2 | 2.01                     | 0.42              |
| 5:P:182:GLU:N     | 5:P:188:GLY:O     | 2.52                     | 0.42              |
| 9:T:49:TRP:HA     | 9:T:52:VAL:HG22   | 2.00                     | 0.42              |
| 11:a:357:ILE:O    | 11:a:361:THR:HG23 | 2.19                     | 0.42              |
| 1:A:393:GLN:O     | 1:A:397:THR:OG1   | 2.38                     | 0.42              |
| 4:D:102:CYS:SG    | 4:D:106:HIS:HB2   | 2.60                     | 0.42              |
| 7:G:118:LEU:HD11  | 10:U:4:PHE:HE2    | 1.83                     | 0.42              |
| 16:f:56:SER:OG    | 16:f:57:ASN:ND2   | 2.48                     | 0.42              |
| 4:D:86:PHE:HZ     | 4:D:263:LEU:CD2   | 2.26                     | 0.42              |
| 5:E:123:LYS:HA    | 5:E:123:LYS:HD2   | 1.85                     | 0.42              |
| 27:J:101:PEF:H201 | 27:J:101:PEF:H171 | 1.81                     | 0.42              |
| 6:Q:181:VAL:O     | 6:Q:186:LYS:NZ    | 2.52                     | 0.42              |
| 7:R:76:LEU:HD11   | 7:R:83:LEU:HG     | 2.01                     | 0.42              |
| 8:S:38:MET:H      | 8:S:38:MET:HE2    | 1.85                     | 0.42              |
| 12:b:217:CYS:SG   | 12:b:218:SER:N    | 2.92                     | 0.42              |
| 21:k:108:PRO:HG2  | 21:k:109:TRP:CE3  | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:28:LYS:HE2    | 1:A:28:LYS:HB3    | 1.85                     | 0.42              |
| 27:A:504:PEF:H362 | 5:E:76:MET:HG2    | 2.02                     | 0.42              |
| 25:H:102:CDL:H211 | 25:H:102:CDL:H181 | 1.81                     | 0.42              |
| 6:Q:159:ASP:OD1   | 6:Q:159:ASP:C     | 2.63                     | 0.42              |
| 11:a:72:MET:HG2   | 32:a:601:HEA:HBC1 | 2.02                     | 0.42              |
| 11:a:354:LEU:O    | 11:a:386:TYR:CE2  | 2.72                     | 0.42              |
| 11:a:389:SER:O    | 11:a:393:LEU:HB3  | 2.20                     | 0.42              |
| 12:b:133:GLU:HG2  | 12:b:135:GLU:H    | 1.84                     | 0.42              |
| 12:b:183:SER:HB3  | 12:b:219:GLU:HG3  | 2.02                     | 0.42              |
| 3:C:382:LEU:HD23  | 3:C:382:LEU:HA    | 1.83                     | 0.42              |
| 3:N:31:ASN:HD21   | 3:N:228:LYS:HG2   | 1.84                     | 0.42              |
| 11:a:3:SER:O      | 11:a:7:TYR:N      | 2.44                     | 0.42              |
| 18:h:36:LYS:O     | 18:h:40:PRO:HD2   | 2.20                     | 0.42              |
| 4:D:185:ARG:HA    | 4:D:185:ARG:HD3   | 1.68                     | 0.41              |
| 1:L:66:HIS:HE1    | 1:L:146:GLU:OE1   | 2.02                     | 0.41              |
| 26:T:101:PCF:H143 | 26:T:101:PCF:H111 | 1.80                     | 0.41              |
| 2:B:114:TYR:HB2   | 10:J:7:ASN:HD21   | 1.85                     | 0.41              |
| 4:O:304:ARG:NH2   | 7:R:61:MET:HE3    | 2.30                     | 0.41              |
| 11:a:158:GLN:O    | 11:a:162:ILE:HG23 | 2.20                     | 0.41              |
| 11:a:257:ALA:HA   | 11:a:260:VAL:HG12 | 2.01                     | 0.41              |
| 11:a:337:ALA:HB1  | 12:b:61:TYR:HD1   | 1.84                     | 0.41              |
| 11:a:510:LYS:HD2  | 11:a:510:LYS:HA   | 1.88                     | 0.41              |
| 5:E:70:TYR:HE2    | 9:I:7:TYR:HE2     | 1.68                     | 0.41              |
| 5:E:169:ILE:HB    | 5:E:214:ALA:HB3   | 2.02                     | 0.41              |
| 10:J:5:PHE:HD2    | 10:J:8:LYS:CA     | 2.32                     | 0.41              |
| 2:M:241:ARG:HB3   | 2:M:417:LEU:HD22  | 2.03                     | 0.41              |
| 3:N:66:GLU:O      | 3:N:70:ARG:HG2    | 2.20                     | 0.41              |
| 4:O:193:TYR:O     | 4:O:197:THR:HG22  | 2.19                     | 0.41              |
| 11:a:377:THR:O    | 11:a:380:VAL:HG22 | 2.20                     | 0.41              |
| 11:a:535:THR:CG2  | 14:d:116:ARG:HH22 | 2.28                     | 0.41              |
| 14:d:133:MET:HE2  | 14:d:144:PRO:HD2  | 2.02                     | 0.41              |
| 26:A:505:PCF:H111 | 26:A:505:PCF:H143 | 1.77                     | 0.41              |
| 7:G:109:ARG:HG2   | 7:G:113:GLU:OE2   | 2.20                     | 0.41              |
| 25:H:101:CDL:H341 | 25:H:101:CDL:H612 | 2.02                     | 0.41              |
| 5:P:125:GLN:HB3   | 5:P:127:LYS:NZ    | 2.36                     | 0.41              |
| 13:c:218:VAL:O    | 13:c:221:ILE:HG22 | 2.21                     | 0.41              |
| 21:k:119:ASN:OD1  | 21:k:122:VAL:N    | 2.42                     | 0.41              |
| 1:A:427:TRP:CG    | 1:A:428:ASP:H     | 2.39                     | 0.41              |
| 2:B:127:LYS:HD3   | 2:B:129:LEU:HD21  | 2.01                     | 0.41              |
| 3:C:49:LEU:HD23   | 3:C:49:LEU:HA     | 1.84                     | 0.41              |
| 3:C:277:PRO:HG3   | 3:C:337:ALA:HB2   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:M:84:GLU:HB2    | 10:U:5:PHE:CE2    | 2.55                     | 0.41              |
| 4:O:83:LEU:HD12   | 4:O:83:LEU:HA     | 1.90                     | 0.41              |
| 11:a:277:GLU:HG3  | 11:a:278:GLY:N    | 2.36                     | 0.41              |
| 11:a:381:VAL:HG13 | 11:a:385:HIS:HD1  | 1.85                     | 0.41              |
| 13:c:89:PHE:HZ    | 13:c:249:TYR:HB2  | 1.85                     | 0.41              |
| 14:d:138:ASP:O    | 14:d:151:LYS:NZ   | 2.53                     | 0.41              |
| 14:d:144:PRO:HG2  | 14:d:145:GLU:OE1  | 2.21                     | 0.41              |
| 15:e:78:TRP:HA    | 15:e:81:LEU:HG    | 2.01                     | 0.41              |
| 11:a:61:TYR:O     | 11:a:65:ILE:HG22  | 2.21                     | 0.41              |
| 13:c:56:LEU:HA    | 13:c:59:THR:HG22  | 2.02                     | 0.41              |
| 13:c:164:ARG:HG2  | 14:d:65:VAL:HG23  | 2.03                     | 0.41              |
| 20:j:75:GLU:O     | 20:j:79:ASN:ND2   | 2.53                     | 0.41              |
| 29:C:403:U10:H251 | 29:C:403:U10:H271 | 1.70                     | 0.41              |
| 5:E:118:LYS:HD2   | 5:E:118:LYS:HA    | 1.92                     | 0.41              |
| 25:H:101:CDL:H332 | 25:H:101:CDL:H362 | 1.86                     | 0.41              |
| 1:L:246:ARG:NH2   | 8:S:34:GLN:OE1    | 2.53                     | 0.41              |
| 11:a:107:PHE:HB2  | 13:c:21:PRO:HB3   | 2.03                     | 0.41              |
| 11:a:237:LEU:HD13 | 13:c:109:HIS:CG   | 2.55                     | 0.41              |
| 14:d:131:ILE:HD12 | 14:d:131:ILE:HA   | 1.94                     | 0.41              |
| 21:k:38:ASN:HB3   | 21:k:39:TRP:H     | 1.60                     | 0.41              |
| 11:a:81:LEU:HD13  | 11:a:396:LEU:HB2  | 2.02                     | 0.41              |
| 11:a:239:GLN:HB2  | 11:a:298:LEU:HD21 | 2.03                     | 0.41              |
| 12:b:212:LEU:HG   | 12:b:233:GLN:HB3  | 2.02                     | 0.41              |
| 18:h:54:ILE:O     | 18:h:57:ILE:HG22  | 2.20                     | 0.41              |
| 1:A:446:ASN:ND2   | 3:C:224:TYR:OH    | 2.53                     | 0.41              |
| 7:G:90:LYS:NZ     | 7:G:93:GLU:OE2    | 2.40                     | 0.41              |
| 3:N:50:LEU:HD12   | 3:N:50:LEU:HA     | 1.90                     | 0.41              |
| 4:O:93:ARG:O      | 4:O:97:VAL:HG23   | 2.21                     | 0.41              |
| 11:a:168:SER:O    | 11:a:172:ILE:HG13 | 2.21                     | 0.41              |
| 11:a:360:LEU:O    | 11:a:363:VAL:HG12 | 2.21                     | 0.41              |
| 11:a:498:SER:HB2  | 16:f:69:ASN:HD21  | 1.85                     | 0.41              |
| 5:E:132:ARG:HH22  | 5:E:182:GLU:HG3   | 1.85                     | 0.41              |
| 1:L:94:HIS:HB2    | 1:L:109:HIS:NE2   | 2.34                     | 0.41              |
| 12:b:120:TRP:NE1  | 12:b:224:LEU:HB2  | 2.36                     | 0.41              |
| 13:c:171:LEU:HD21 | 13:c:223:LEU:HD22 | 2.03                     | 0.41              |
| 15:e:70:LEU:HD23  | 15:e:70:LEU:HA    | 1.82                     | 0.41              |
| 26:A:505:PCF:H432 | 26:A:505:PCF:H402 | 1.87                     | 0.40              |
| 2:B:288:ALA:HB1   | 2:B:330:GLU:HG3   | 2.03                     | 0.40              |
| 6:Q:173:CYS:O     | 6:Q:174:THR:C     | 2.64                     | 0.40              |
| 8:S:54:MET:HE3    | 8:S:54:MET:HB3    | 1.79                     | 0.40              |
| 11:a:93:MET:HE1   | 11:a:191:PHE:CD2  | 2.55                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:a:138:PRO:HB2  | 12:b:180:VAL:HG12 | 2.03                     | 0.40              |
| 18:h:33:TYR:CE1   | 18:h:35:ASN:OD1   | 2.74                     | 0.40              |
| 2:B:308:ASP:OD1   | 2:B:308:ASP:N     | 2.54                     | 0.40              |
| 3:C:7:ASN:HB3     | 3:C:10:LEU:HD12   | 2.03                     | 0.40              |
| 3:C:93:LEU:HD12   | 3:C:93:LEU:HA     | 1.89                     | 0.40              |
| 5:E:102:LEU:HD23  | 5:E:102:LEU:HA    | 1.92                     | 0.40              |
| 5:E:111:LEU:H     | 5:E:111:LEU:HD12  | 1.85                     | 0.40              |
| 1:L:401:MET:HE2   | 1:L:401:MET:HB3   | 1.92                     | 0.40              |
| 11:a:265:ILE:HD13 | 11:a:265:ILE:HA   | 1.88                     | 0.40              |
| 16:f:59:GLN:OE1   | 16:f:92:ARG:NH1   | 2.55                     | 0.40              |
| 1:A:19:LEU:HD12   | 1:A:20:PRO:HD2    | 2.03                     | 0.40              |
| 4:D:141:ASP:O     | 4:O:164:GLU:HB3   | 2.21                     | 0.40              |
| 25:L:502:CDL:H712 | 26:L:503:PCF:H291 | 2.03                     | 0.40              |
| 2:M:100:HIS:NE2   | 2:M:376:VAL:HG21  | 2.37                     | 0.40              |
| 2:M:265:VAL:HG11  | 2:M:392:VAL:HG11  | 2.04                     | 0.40              |
| 3:N:300:LEU:HD23  | 3:N:300:LEU:HA    | 1.86                     | 0.40              |
| 3:N:381:ASN:HB2   | 7:R:24:SER:HB2    | 2.03                     | 0.40              |
| 4:O:274:ILE:HD13  | 4:O:274:ILE:HA    | 1.89                     | 0.40              |
| 7:R:102:LEU:O     | 7:R:106:ILE:HG12  | 2.22                     | 0.40              |
| 11:a:323:GLY:C    | 11:a:327:PHE:CD2  | 2.92                     | 0.40              |
| 13:c:221:ILE:HA   | 13:c:224:LEU:HG   | 2.03                     | 0.40              |
| 17:g:36:VAL:HG12  | 17:g:37:MET:HE2   | 2.03                     | 0.40              |
| 4:D:277:LEU:HD23  | 4:D:277:LEU:HA    | 1.86                     | 0.40              |
| 2:M:157:MET:HE1   | 2:M:315:VAL:HG21  | 2.02                     | 0.40              |
| 11:a:371:ASP:O    | 11:a:375:HIS:N    | 2.52                     | 0.40              |
| 11:a:420:GLN:NE2  | 11:a:475:PHE:N    | 2.69                     | 0.40              |
| 11:a:445:ARG:HE   | 11:a:446:ARG:HG3  | 1.87                     | 0.40              |
| 15:e:90:TYR:CE1   | 15:e:94:PHE:HB2   | 2.57                     | 0.40              |
| 16:f:77:VAL:HG11  | 16:f:110:LEU:HD21 | 2.02                     | 0.40              |
| 2:B:92:LEU:HD21   | 2:B:115:TYR:HE1   | 1.87                     | 0.40              |
| 5:E:175:LEU:HD13  | 3:N:264:LYS:HZ1   | 1.87                     | 0.40              |
| 7:G:41:ASP:OD2    | 7:G:96:HIS:HA     | 2.21                     | 0.40              |
| 9:T:6:ILE:HD13    | 9:T:6:ILE:HA      | 1.95                     | 0.40              |
| 9:T:11:PHE:HD1    | 9:T:17:PHE:HD1    | 1.70                     | 0.40              |
| 12:b:120:TRP:CD1  | 12:b:224:LEU:HB2  | 2.56                     | 0.40              |
| 13:c:89:PHE:CZ    | 13:c:249:TYR:HB2  | 2.57                     | 0.40              |
| 13:c:123:PRO:HA   | 13:c:124:PRO:HD3  | 1.99                     | 0.40              |
| 13:c:181:PHE:O    | 13:c:185:GLN:HG2  | 2.20                     | 0.40              |
| 14:d:93:LYS:HE2   | 14:d:93:LYS:HB2   | 1.95                     | 0.40              |
| 15:e:59:SER:OG    | 15:e:60:GLN:N     | 2.54                     | 0.40              |
| 16:f:48:ASN:OD1   | 16:f:48:ASN:C     | 2.64                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:k:201:PEF:H361 | 27:k:201:PEF:H391 | 1.85                     | 0.40              |
| 22:l:108:LYS:O    | 22:l:112:ILE:HB   | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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     | 441/457 (96%)  | 424 (96%) | 17 (4%) | 0        | 100         | 100 |
| 1   | L     | 441/457 (96%)  | 425 (96%) | 16 (4%) | 0        | 100         | 100 |
| 2   | B     | 404/426 (95%)  | 393 (97%) | 11 (3%) | 0        | 100         | 100 |
| 2   | M     | 404/426 (95%)  | 386 (96%) | 18 (4%) | 0        | 100         | 100 |
| 3   | C     | 385/387 (100%) | 367 (95%) | 18 (5%) | 0        | 100         | 100 |
| 3   | N     | 385/387 (100%) | 370 (96%) | 15 (4%) | 0        | 100         | 100 |
| 4   | D     | 243/307 (79%)  | 232 (96%) | 11 (4%) | 0        | 100         | 100 |
| 4   | O     | 243/307 (79%)  | 231 (95%) | 12 (5%) | 0        | 100         | 100 |
| 5   | E     | 180/228 (79%)  | 172 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 5   | P     | 180/228 (79%)  | 172 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 6   | F     | 64/214 (30%)   | 63 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | Q     | 64/214 (30%)   | 60 (94%)  | 4 (6%)  | 0        | 100         | 100 |
| 7   | G     | 120/137 (88%)  | 115 (96%) | 3 (2%)  | 2 (2%)   | 7           | 28  |
| 7   | R     | 120/137 (88%)  | 118 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 8   | H     | 84/92 (91%)    | 79 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 8   | S     | 85/92 (92%)    | 79 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 9   | I     | 58/67 (87%)    | 54 (93%)  | 4 (7%)  | 0        | 100         | 100 |
| 9   | T     | 58/67 (87%)    | 55 (95%)  | 2 (3%)  | 1 (2%)   | 7           | 28  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10  | J     | 75/79 (95%)     | 67 (89%)   | 8 (11%)  | 0        | 100         | 100 |
| 10  | U     | 75/79 (95%)     | 66 (88%)   | 9 (12%)  | 0        | 100         | 100 |
| 11  | a     | 535/538 (99%)   | 514 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 12  | b     | 236/248 (95%)   | 221 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 13  | c     | 266/269 (99%)   | 257 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 14  | d     | 119/159 (75%)   | 114 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 15  | e     | 143/228 (63%)   | 131 (92%)  | 12 (8%)  | 0        | 100         | 100 |
| 16  | f     | 98/140 (70%)    | 91 (93%)   | 7 (7%)   | 0        | 100         | 100 |
| 17  | g     | 55/59 (93%)     | 54 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 18  | h     | 43/66 (65%)     | 37 (86%)   | 6 (14%)  | 0        | 100         | 100 |
| 19  | i     | 53/58 (91%)     | 53 (100%)  | 0        | 0        | 100         | 100 |
| 20  | j     | 73/86 (85%)     | 69 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 21  | k     | 86/130 (66%)    | 81 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 22  | l     | 67/242 (28%)    | 64 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| All | All   | 5883/7011 (84%) | 5614 (95%) | 266 (4%) | 3 (0%)   | 49          | 78  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 114 | ALA  |
| 7   | G     | 113 | GLU  |
| 9   | T     | 9   | ILE  |

### 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     | 368/382 (96%) | 368 (100%) | 0        | 100         | 100 |
| 1   | L     | 368/382 (96%) | 368 (100%) | 0        | 100         | 100 |
| 2   | B     | 333/352 (95%) | 332 (100%) | 1 (0%)   | 86          | 84  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 2   | M     | 333/352 (95%)   | 333 (100%)  | 0        | 100         | 100 |
| 3   | C     | 335/335 (100%)  | 334 (100%)  | 1 (0%)   | 86          | 84  |
| 3   | N     | 335/335 (100%)  | 335 (100%)  | 0        | 100         | 100 |
| 4   | D     | 206/258 (80%)   | 206 (100%)  | 0        | 100         | 100 |
| 4   | O     | 206/258 (80%)   | 206 (100%)  | 0        | 100         | 100 |
| 5   | E     | 148/190 (78%)   | 148 (100%)  | 0        | 100         | 100 |
| 5   | P     | 148/190 (78%)   | 148 (100%)  | 0        | 100         | 100 |
| 6   | F     | 61/191 (32%)    | 61 (100%)   | 0        | 100         | 100 |
| 6   | Q     | 61/191 (32%)    | 61 (100%)   | 0        | 100         | 100 |
| 7   | G     | 112/123 (91%)   | 112 (100%)  | 0        | 100         | 100 |
| 7   | R     | 112/123 (91%)   | 111 (99%)   | 1 (1%)   | 70          | 76  |
| 8   | H     | 67/73 (92%)     | 67 (100%)   | 0        | 100         | 100 |
| 8   | S     | 68/73 (93%)     | 68 (100%)   | 0        | 100         | 100 |
| 9   | I     | 52/58 (90%)     | 51 (98%)    | 1 (2%)   | 50          | 66  |
| 9   | T     | 52/58 (90%)     | 52 (100%)   | 0        | 100         | 100 |
| 10  | J     | 68/70 (97%)     | 68 (100%)   | 0        | 100         | 100 |
| 10  | U     | 68/70 (97%)     | 68 (100%)   | 0        | 100         | 100 |
| 11  | a     | 452/453 (100%)  | 449 (99%)   | 3 (1%)   | 76          | 78  |
| 12  | b     | 213/223 (96%)   | 213 (100%)  | 0        | 100         | 100 |
| 13  | c     | 226/227 (100%)  | 225 (100%)  | 1 (0%)   | 84          | 83  |
| 14  | d     | 101/135 (75%)   | 101 (100%)  | 0        | 100         | 100 |
| 15  | e     | 119/180 (66%)   | 119 (100%)  | 0        | 100         | 100 |
| 16  | f     | 90/121 (74%)    | 90 (100%)   | 0        | 100         | 100 |
| 17  | g     | 47/49 (96%)     | 47 (100%)   | 0        | 100         | 100 |
| 18  | h     | 41/59 (70%)     | 41 (100%)   | 0        | 100         | 100 |
| 19  | i     | 44/46 (96%)     | 44 (100%)   | 0        | 100         | 100 |
| 20  | j     | 67/77 (87%)     | 67 (100%)   | 0        | 100         | 100 |
| 21  | k     | 76/113 (67%)    | 76 (100%)   | 0        | 100         | 100 |
| 22  | l     | 57/203 (28%)    | 57 (100%)   | 0        | 100         | 100 |
| All | All   | 5034/5950 (85%) | 5026 (100%) | 8 (0%)   | 85          | 85  |

All (8) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 77  | SER  |
| 3   | C     | 132 | TYR  |
| 9   | I     | 5   | THR  |
| 7   | R     | 118 | LEU  |
| 11  | a     | 34  | ILE  |
| 11  | a     | 176 | ILE  |
| 11  | a     | 178 | MET  |
| 13  | c     | 235 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 62  | ASN  |
| 1   | A     | 81  | GLN  |
| 1   | A     | 168 | GLN  |
| 1   | A     | 263 | ASN  |
| 1   | A     | 300 | HIS  |
| 3   | C     | 31  | ASN  |
| 3   | C     | 202 | HIS  |
| 4   | D     | 189 | GLN  |
| 4   | D     | 256 | HIS  |
| 7   | G     | 11  | GLN  |
| 7   | G     | 80  | ASN  |
| 8   | H     | 85  | HIS  |
| 8   | H     | 88  | HIS  |
| 1   | L     | 263 | ASN  |
| 2   | M     | 280 | HIS  |
| 3   | N     | 7   | ASN  |
| 3   | N     | 138 | GLN  |
| 3   | N     | 149 | ASN  |
| 3   | N     | 247 | ASN  |
| 3   | N     | 343 | HIS  |
| 4   | O     | 189 | GLN  |
| 5   | P     | 89  | HIS  |
| 5   | P     | 197 | HIS  |
| 7   | R     | 11  | GLN  |
| 7   | R     | 25  | ASN  |
| 7   | R     | 75  | GLN  |
| 9   | T     | 14  | ASN  |
| 11  | a     | 9   | ASN  |
| 11  | a     | 105 | ASN  |
| 11  | a     | 503 | ASN  |
| 12  | b     | 247 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | c     | 185 | GLN  |
| 14  | d     | 44  | GLN  |
| 14  | d     | 48  | ASN  |
| 15  | e     | 97  | HIS  |
| 16  | f     | 57  | ASN  |
| 16  | f     | 115 | GLN  |
| 16  | f     | 128 | ASN  |
| 18  | h     | 35  | ASN  |
| 20  | j     | 12  | GLN  |

### 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 39 ligands modelled in this entry, 6 are monoatomic - leaving 33 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 | $\# Z  > 2$ |
| 31  | FES  | P     | 301 | 5    | 0,4,4        | -    | -           | -           |      |             |
| 31  | FES  | E     | 301 | 5    | 0,4,4        | -    | -           | -           |      |             |
| 26  | PCF  | L     | 503 | -    | 49,49,49     | 1.12 | 3 (6%)      | 55,57,57    | 1.08 | 2 (3%)      |
| 28  | HEM  | N     | 402 | 3    | 50,50,50     | 1.36 | 8 (16%)     | 67,82,82    | 1.13 | 4 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 25  | CDL  | S     | 101 | -    | 76,76,99     | 0.34 | 0        | 82,88,111   | 0.23 | 0        |
| 27  | PEF  | a     | 605 | -    | 46,46,46     | 0.92 | 4 (8%)   | 49,51,51    | 1.10 | 2 (4%)   |
| 36  | CUA  | b     | 303 | 12   | 0,1,1        | -    | -        | -           | -    | -        |
| 28  | HEM  | C     | 402 | 3    | 50,50,50     | 1.37 | 8 (16%)  | 67,82,82    | 1.07 | 3 (4%)   |
| 26  | PCF  | T     | 101 | -    | 49,49,49     | 1.12 | 4 (8%)   | 55,57,57    | 1.07 | 2 (3%)   |
| 27  | PEF  | k     | 201 | -    | 46,46,46     | 0.93 | 4 (8%)   | 49,51,51    | 1.09 | 2 (4%)   |
| 27  | PEF  | c     | 301 | -    | 46,46,46     | 0.92 | 4 (8%)   | 49,51,51    | 1.06 | 2 (4%)   |
| 32  | HEA  | a     | 601 | 11   | 67,67,67     | 1.17 | 6 (8%)   | 81,103,103  | 1.40 | 13 (16%) |
| 25  | CDL  | H     | 102 | -    | 77,77,99     | 0.34 | 0        | 83,89,111   | 0.22 | 0        |
| 25  | CDL  | L     | 502 | -    | 56,56,99     | 0.39 | 0        | 62,68,111   | 0.27 | 0        |
| 32  | HEA  | a     | 602 | 11   | 67,67,67     | 1.17 | 6 (8%)   | 81,103,103  | 1.36 | 13 (16%) |
| 25  | CDL  | H     | 101 | -    | 78,78,99     | 0.34 | 0        | 84,90,111   | 0.22 | 0        |
| 25  | CDL  | A     | 502 | -    | 56,56,99     | 0.39 | 0        | 62,68,111   | 0.27 | 0        |
| 27  | PEF  | O     | 402 | -    | 46,46,46     | 0.91 | 4 (8%)   | 49,51,51    | 1.13 | 2 (4%)   |
| 30  | HEC  | O     | 401 | 4    | 46,50,50     | 1.84 | 7 (15%)  | 58,82,82    | 1.90 | 4 (6%)   |
| 25  | CDL  | S     | 102 | -    | 72,72,99     | 0.35 | 0        | 78,84,111   | 0.23 | 0        |
| 27  | PEF  | b     | 302 | -    | 46,46,46     | 0.91 | 4 (8%)   | 49,51,51    | 1.08 | 2 (4%)   |
| 29  | U10  | N     | 403 | -    | 63,63,63     | 2.77 | 17 (26%) | 78,79,79    | 1.79 | 24 (30%) |
| 26  | PCF  | A     | 505 | -    | 49,49,49     | 1.12 | 4 (8%)   | 55,57,57    | 1.09 | 2 (3%)   |
| 29  | U10  | C     | 403 | -    | 63,63,63     | 2.78 | 17 (26%) | 78,79,79    | 1.78 | 21 (26%) |
| 27  | PEF  | N     | 405 | -    | 46,46,46     | 0.92 | 4 (8%)   | 49,51,51    | 1.13 | 2 (4%)   |
| 28  | HEM  | C     | 401 | 3    | 50,50,50     | 1.37 | 8 (16%)  | 67,82,82    | 1.09 | 4 (5%)   |
| 27  | PEF  | N     | 404 | -    | 46,46,46     | 0.91 | 4 (8%)   | 49,51,51    | 1.14 | 2 (4%)   |
| 27  | PEF  | A     | 504 | -    | 46,46,46     | 0.92 | 4 (8%)   | 49,51,51    | 1.13 | 2 (4%)   |
| 28  | HEM  | N     | 401 | 3    | 50,50,50     | 1.36 | 8 (16%)  | 67,82,82    | 1.06 | 4 (5%)   |
| 27  | PEF  | J     | 101 | -    | 46,46,46     | 0.92 | 4 (8%)   | 49,51,51    | 1.13 | 2 (4%)   |
| 30  | HEC  | D     | 401 | 4    | 46,50,50     | 1.83 | 6 (13%)  | 58,82,82    | 1.93 | 4 (6%)   |
| 26  | PCF  | A     | 503 | -    | 49,49,49     | 1.13 | 4 (8%)   | 55,57,57    | 1.02 | 2 (3%)   |
| 27  | PEF  | D     | 402 | -    | 46,46,46     | 0.91 | 4 (8%)   | 49,51,51    | 1.06 | 2 (4%)   |

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   |
|-----|------|-------|-----|------|---------|----------|---------|
| 31  | FES  | P     | 301 | 5    | -       | -        | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 31  | FES  | E     | 301 | 5    | -       | -            | 0/1/1/1 |
| 26  | PCF  | L     | 503 | -    | -       | 18/53/53/53  | -       |
| 28  | HEM  | N     | 402 | 3    | -       | 3/14/54/54   | -       |
| 25  | CDL  | S     | 101 | -    | -       | 57/87/87/110 | -       |
| 27  | PEF  | a     | 605 | -    | -       | 22/50/50/50  | -       |
| 28  | HEM  | C     | 402 | 3    | -       | 1/14/54/54   | -       |
| 26  | PCF  | T     | 101 | -    | -       | 13/53/53/53  | -       |
| 27  | PEF  | k     | 201 | -    | -       | 20/50/50/50  | -       |
| 27  | PEF  | c     | 301 | -    | -       | 15/50/50/50  | -       |
| 32  | HEA  | a     | 601 | 11   | -       | 9/36/76/76   | -       |
| 25  | CDL  | H     | 102 | -    | -       | 54/88/88/110 | -       |
| 25  | CDL  | L     | 502 | -    | -       | 42/67/67/110 | -       |
| 32  | HEA  | a     | 602 | 11   | -       | 9/36/76/76   | -       |
| 25  | CDL  | H     | 101 | -    | -       | 58/89/89/110 | -       |
| 25  | CDL  | A     | 502 | -    | -       | 39/67/67/110 | -       |
| 27  | PEF  | O     | 402 | -    | -       | 18/50/50/50  | -       |
| 30  | HEC  | O     | 401 | 4    | -       | 4/14/54/54   | -       |
| 25  | CDL  | S     | 102 | -    | -       | 46/83/83/110 | -       |
| 27  | PEF  | b     | 302 | -    | -       | 21/50/50/50  | -       |
| 29  | U10  | N     | 403 | -    | -       | 27/63/87/87  | 0/1/1/1 |
| 26  | PCF  | A     | 505 | -    | -       | 17/53/53/53  | -       |
| 29  | U10  | C     | 403 | -    | -       | 26/63/87/87  | 0/1/1/1 |
| 27  | PEF  | N     | 405 | -    | -       | 16/50/50/50  | -       |
| 28  | HEM  | C     | 401 | 3    | -       | 1/14/54/54   | -       |
| 27  | PEF  | N     | 404 | -    | -       | 18/50/50/50  | -       |
| 27  | PEF  | A     | 504 | -    | -       | 15/50/50/50  | -       |
| 28  | HEM  | N     | 401 | 3    | -       | 3/14/54/54   | -       |
| 27  | PEF  | J     | 101 | -    | -       | 22/50/50/50  | -       |
| 30  | HEC  | D     | 401 | 4    | -       | 4/14/54/54   | -       |
| 26  | PCF  | A     | 503 | -    | -       | 16/53/53/53  | -       |
| 27  | PEF  | D     | 402 | -    | -       | 25/50/50/50  | -       |

All (146) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 29  | N     | 403 | U10  | C13-C14 | 6.34 | 1.47        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 29  | C     | 403 | U10  | C38-C39 | 6.33  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C18-C19 | 6.31  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C33-C34 | 6.31  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C13-C14 | 6.30  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C43-C44 | 6.30  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C23-C24 | 6.29  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C38-C39 | 6.27  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C18-C19 | 6.27  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C28-C29 | 6.25  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C33-C34 | 6.25  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C28-C29 | 6.24  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C23-C24 | 6.24  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C43-C44 | 6.24  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C48-C49 | 6.24  | 1.47        | 1.33     |
| 29  | C     | 403 | U10  | C48-C49 | 6.23  | 1.47        | 1.33     |
| 29  | N     | 403 | U10  | C8-C9   | 6.22  | 1.47        | 1.33     |
| 30  | O     | 401 | HEC  | CAB-C3B | 6.22  | 1.55        | 1.35     |
| 29  | C     | 403 | U10  | C8-C9   | 6.21  | 1.47        | 1.33     |
| 30  | D     | 401 | HEC  | CAC-C3C | 6.19  | 1.55        | 1.35     |
| 30  | O     | 401 | HEC  | CAC-C3C | 6.11  | 1.54        | 1.35     |
| 30  | D     | 401 | HEC  | CAB-C3B | 6.09  | 1.54        | 1.35     |
| 30  | O     | 401 | HEC  | C3D-C2D | 5.75  | 1.53        | 1.38     |
| 30  | D     | 401 | HEC  | C3D-C2D | 5.70  | 1.53        | 1.38     |
| 29  | C     | 403 | U10  | O3-C3   | -5.47 | 1.23        | 1.36     |
| 29  | N     | 403 | U10  | O4-C4   | -5.45 | 1.23        | 1.36     |
| 29  | C     | 403 | U10  | O4-C4   | -5.40 | 1.23        | 1.36     |
| 29  | N     | 403 | U10  | O3-C3   | -5.33 | 1.24        | 1.36     |
| 29  | N     | 403 | U10  | C53-C54 | 5.09  | 1.47        | 1.32     |
| 29  | C     | 403 | U10  | C53-C54 | 5.06  | 1.47        | 1.32     |
| 32  | a     | 601 | HEA  | CMA-C3A | -3.71 | 1.37        | 1.45     |
| 32  | a     | 602 | HEA  | CMA-C3A | -3.64 | 1.37        | 1.45     |
| 29  | C     | 403 | U10  | C3-C2   | -3.27 | 1.39        | 1.48     |
| 26  | A     | 503 | PCF  | O21-C21 | 3.24  | 1.43        | 1.34     |
| 26  | L     | 503 | PCF  | O21-C21 | 3.23  | 1.43        | 1.34     |
| 29  | N     | 403 | U10  | C4-C5   | -3.21 | 1.39        | 1.48     |
| 28  | N     | 402 | HEM  | FE-NB   | 3.20  | 2.04        | 1.94     |
| 29  | N     | 403 | U10  | C3-C2   | -3.18 | 1.39        | 1.48     |
| 29  | C     | 403 | U10  | C4-C5   | -3.18 | 1.39        | 1.48     |
| 26  | A     | 505 | PCF  | O21-C21 | 3.15  | 1.43        | 1.34     |
| 28  | C     | 401 | HEM  | FE-NB   | 3.12  | 2.04        | 1.94     |
| 28  | C     | 402 | HEM  | FE-NB   | 3.10  | 2.04        | 1.94     |
| 28  | C     | 401 | HEM  | CAB-C3B | 3.09  | 1.55        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 26  | T     | 101 | PCF  | O21-C21 | 3.08  | 1.43        | 1.34     |
| 28  | C     | 402 | HEM  | CAC-C3C | 3.06  | 1.55        | 1.47     |
| 28  | N     | 402 | HEM  | CAC-C3C | 3.05  | 1.55        | 1.47     |
| 28  | N     | 401 | HEM  | CAB-C3B | 3.04  | 1.55        | 1.47     |
| 28  | C     | 402 | HEM  | CAB-C3B | 3.04  | 1.55        | 1.47     |
| 26  | A     | 503 | PCF  | O31-C31 | 3.04  | 1.42        | 1.33     |
| 28  | N     | 401 | HEM  | CAC-C3C | 3.03  | 1.55        | 1.47     |
| 26  | L     | 503 | PCF  | O31-C31 | 3.03  | 1.42        | 1.33     |
| 26  | T     | 101 | PCF  | O31-C31 | 3.02  | 1.42        | 1.33     |
| 28  | N     | 402 | HEM  | CAB-C3B | 2.97  | 1.55        | 1.47     |
| 28  | C     | 402 | HEM  | FE-NA   | 2.95  | 2.04        | 1.95     |
| 28  | C     | 401 | HEM  | CAC-C3C | 2.95  | 1.55        | 1.47     |
| 26  | A     | 505 | PCF  | O31-C31 | 2.95  | 1.41        | 1.33     |
| 28  | N     | 401 | HEM  | FE-NB   | 2.94  | 2.04        | 1.94     |
| 28  | C     | 401 | HEM  | FE-ND   | 2.93  | 2.03        | 1.94     |
| 28  | N     | 402 | HEM  | FE-ND   | 2.88  | 2.03        | 1.94     |
| 28  | N     | 401 | HEM  | FE-NA   | 2.84  | 2.04        | 1.95     |
| 28  | C     | 401 | HEM  | FE-NA   | 2.77  | 2.04        | 1.95     |
| 28  | N     | 401 | HEM  | FE-NC   | 2.76  | 2.04        | 1.95     |
| 27  | A     | 504 | PEF  | O2-C2   | -2.75 | 1.40        | 1.46     |
| 27  | J     | 101 | PEF  | O2-C2   | -2.74 | 1.40        | 1.46     |
| 27  | a     | 605 | PEF  | O2-C2   | -2.73 | 1.40        | 1.46     |
| 27  | k     | 201 | PEF  | O2-C2   | -2.73 | 1.40        | 1.46     |
| 27  | N     | 405 | PEF  | O2-C2   | -2.73 | 1.40        | 1.46     |
| 28  | C     | 402 | HEM  | FE-NC   | 2.72  | 2.04        | 1.95     |
| 27  | D     | 402 | PEF  | O2-C2   | -2.71 | 1.40        | 1.46     |
| 27  | O     | 402 | PEF  | O2-C2   | -2.70 | 1.40        | 1.46     |
| 27  | N     | 404 | PEF  | O2-C2   | -2.69 | 1.40        | 1.46     |
| 28  | N     | 401 | HEM  | FE-ND   | 2.66  | 2.03        | 1.94     |
| 28  | C     | 401 | HEM  | FE-NC   | 2.66  | 2.03        | 1.95     |
| 28  | C     | 402 | HEM  | FE-ND   | 2.66  | 2.03        | 1.94     |
| 27  | c     | 301 | PEF  | O2-C2   | -2.65 | 1.40        | 1.46     |
| 27  | b     | 302 | PEF  | O2-C2   | -2.64 | 1.40        | 1.46     |
| 27  | k     | 201 | PEF  | O3-C30  | 2.63  | 1.41        | 1.33     |
| 28  | N     | 402 | HEM  | FE-NC   | 2.61  | 2.03        | 1.95     |
| 29  | N     | 403 | U10  | C6-C5   | -2.56 | 1.39        | 1.46     |
| 27  | J     | 101 | PEF  | O3-C30  | 2.52  | 1.40        | 1.33     |
| 27  | N     | 405 | PEF  | O3-C30  | 2.50  | 1.40        | 1.33     |
| 27  | c     | 301 | PEF  | O3-C30  | 2.49  | 1.40        | 1.33     |
| 32  | a     | 602 | HEA  | FE-NC   | 2.49  | 2.03        | 1.95     |
| 29  | C     | 403 | U10  | C6-C5   | -2.47 | 1.39        | 1.46     |
| 32  | a     | 602 | HEA  | C1D-C2D | 2.46  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | N     | 402 | HEM  | FE-NA   | 2.45  | 2.03        | 1.95     |
| 27  | a     | 605 | PEF  | O3-C30  | 2.44  | 1.40        | 1.33     |
| 27  | b     | 302 | PEF  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 27  | A     | 504 | PEF  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 32  | a     | 601 | HEA  | FE-NC   | 2.42  | 2.03        | 1.95     |
| 32  | a     | 602 | HEA  | CHC-C1C | -2.41 | 1.34        | 1.39     |
| 32  | a     | 601 | HEA  | C1D-C2D | 2.41  | 1.49        | 1.44     |
| 29  | N     | 403 | U10  | C6-C1   | 2.40  | 1.39        | 1.35     |
| 27  | O     | 402 | PEF  | O3-C30  | 2.36  | 1.40        | 1.33     |
| 27  | D     | 402 | PEF  | O3-C30  | 2.35  | 1.40        | 1.33     |
| 29  | C     | 403 | U10  | C1-C2   | -2.35 | 1.39        | 1.47     |
| 32  | a     | 601 | HEA  | C4C-NC  | -2.35 | 1.35        | 1.39     |
| 29  | C     | 403 | U10  | C6-C1   | 2.34  | 1.39        | 1.35     |
| 27  | N     | 404 | PEF  | O3-C30  | 2.34  | 1.40        | 1.33     |
| 29  | N     | 403 | U10  | C1-C2   | -2.33 | 1.39        | 1.47     |
| 32  | a     | 602 | HEA  | CMD-C2D | 2.29  | 1.55        | 1.50     |
| 32  | a     | 601 | HEA  | CMD-C2D | 2.22  | 1.55        | 1.50     |
| 32  | a     | 602 | HEA  | C4C-NC  | -2.22 | 1.35        | 1.39     |
| 26  | T     | 101 | PCF  | O21-C2  | -2.20 | 1.41        | 1.46     |
| 27  | D     | 402 | PEF  | O3-C3   | -2.20 | 1.40        | 1.45     |
| 27  | N     | 404 | PEF  | O3-C3   | -2.19 | 1.40        | 1.45     |
| 27  | A     | 504 | PEF  | O3-C3   | -2.19 | 1.40        | 1.45     |
| 26  | A     | 505 | PCF  | O21-C2  | -2.18 | 1.41        | 1.46     |
| 27  | c     | 301 | PEF  | O2-C10  | 2.18  | 1.40        | 1.34     |
| 27  | a     | 605 | PEF  | O3-C3   | -2.16 | 1.40        | 1.45     |
| 27  | k     | 201 | PEF  | O2-C10  | 2.16  | 1.40        | 1.34     |
| 27  | N     | 405 | PEF  | O3-C3   | -2.16 | 1.40        | 1.45     |
| 27  | O     | 402 | PEF  | O3-C3   | -2.15 | 1.40        | 1.45     |
| 27  | b     | 302 | PEF  | O2-C10  | 2.14  | 1.40        | 1.34     |
| 30  | D     | 401 | HEC  | C3B-C2B | -2.14 | 1.33        | 1.41     |
| 27  | J     | 101 | PEF  | O2-C10  | 2.14  | 1.40        | 1.34     |
| 26  | L     | 503 | PCF  | C22-C21 | 2.14  | 1.56        | 1.50     |
| 27  | D     | 402 | PEF  | O2-C10  | 2.13  | 1.40        | 1.34     |
| 27  | a     | 605 | PEF  | O2-C10  | 2.12  | 1.40        | 1.34     |
| 27  | N     | 405 | PEF  | O2-C10  | 2.12  | 1.40        | 1.34     |
| 27  | b     | 302 | PEF  | O3-C3   | -2.11 | 1.40        | 1.45     |
| 27  | c     | 301 | PEF  | O3-C3   | -2.11 | 1.40        | 1.45     |
| 26  | A     | 503 | PCF  | O21-C2  | -2.11 | 1.41        | 1.46     |
| 27  | A     | 504 | PEF  | O2-C10  | 2.11  | 1.40        | 1.34     |
| 27  | N     | 404 | PEF  | O2-C10  | 2.10  | 1.40        | 1.34     |
| 26  | A     | 503 | PCF  | C22-C21 | 2.09  | 1.56        | 1.50     |
| 27  | J     | 101 | PEF  | O3-C3   | -2.09 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 28  | C     | 401 | HEM  | CMC-C2C | 2.08  | 1.55        | 1.50     |
| 27  | O     | 402 | PEF  | O2-C10  | 2.08  | 1.40        | 1.34     |
| 28  | C     | 402 | HEM  | CMB-C2B | 2.08  | 1.55        | 1.50     |
| 28  | N     | 402 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 26  | A     | 505 | PCF  | C22-C21 | 2.07  | 1.56        | 1.50     |
| 28  | N     | 401 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 26  | T     | 101 | PCF  | C22-C21 | 2.06  | 1.56        | 1.50     |
| 28  | C     | 401 | HEM  | CMB-C2B | 2.06  | 1.55        | 1.50     |
| 30  | D     | 401 | HEC  | CMC-C2C | 2.04  | 1.55        | 1.50     |
| 28  | N     | 401 | HEM  | CMB-C2B | 2.04  | 1.55        | 1.50     |
| 30  | D     | 401 | HEC  | C3C-C2C | -2.04 | 1.34        | 1.41     |
| 28  | C     | 402 | HEM  | CMC-C2C | 2.03  | 1.54        | 1.50     |
| 30  | O     | 401 | HEC  | C3C-C2C | -2.03 | 1.34        | 1.41     |
| 30  | O     | 401 | HEC  | C3B-C2B | -2.03 | 1.34        | 1.41     |
| 30  | O     | 401 | HEC  | CMC-C2C | 2.01  | 1.54        | 1.50     |
| 30  | O     | 401 | HEC  | CMB-C2B | 2.01  | 1.54        | 1.50     |
| 28  | N     | 402 | HEM  | CMD-C2D | 2.00  | 1.54        | 1.50     |
| 27  | k     | 201 | PEF  | O3-C3   | -2.00 | 1.40        | 1.45     |
| 32  | a     | 601 | HEA  | CHC-C1C | -2.00 | 1.34        | 1.39     |

All (122) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 30  | D     | 401 | HEC  | CBB-CAB-C3B | -8.93 | 109.59      | 127.43   |
| 30  | O     | 401 | HEC  | CBC-CAC-C3C | -8.76 | 109.93      | 127.43   |
| 30  | D     | 401 | HEC  | CBC-CAC-C3C | -8.15 | 111.14      | 127.43   |
| 30  | O     | 401 | HEC  | CBB-CAB-C3B | -8.13 | 111.17      | 127.43   |
| 29  | C     | 403 | U10  | C7-C6-C1    | -4.98 | 116.35      | 124.89   |
| 26  | L     | 503 | PCF  | O21-C21-C22 | 4.19  | 120.55      | 111.48   |
| 27  | N     | 404 | PEF  | O2-C10-C11  | 4.09  | 120.33      | 111.48   |
| 29  | N     | 403 | U10  | C7-C8-C9    | -4.05 | 119.85      | 126.83   |
| 26  | A     | 505 | PCF  | O21-C21-C22 | 3.99  | 120.12      | 111.48   |
| 27  | O     | 402 | PEF  | O2-C10-C11  | 3.99  | 120.11      | 111.48   |
| 27  | N     | 405 | PEF  | O2-C10-C11  | 3.98  | 120.10      | 111.48   |
| 27  | J     | 101 | PEF  | O2-C10-C11  | 3.96  | 120.04      | 111.48   |
| 27  | A     | 504 | PEF  | O2-C10-C11  | 3.95  | 120.03      | 111.48   |
| 26  | T     | 101 | PCF  | O21-C21-C22 | 3.94  | 120.00      | 111.48   |
| 27  | b     | 302 | PEF  | O2-C10-C11  | 3.93  | 119.99      | 111.48   |
| 29  | N     | 403 | U10  | C7-C6-C1    | -3.89 | 118.21      | 124.89   |
| 27  | D     | 402 | PEF  | O2-C10-C11  | 3.84  | 119.79      | 111.48   |
| 32  | a     | 601 | HEA  | C12-C11-C3B | 3.83  | 118.10      | 112.12   |
| 27  | k     | 201 | PEF  | O2-C10-C11  | 3.80  | 119.71      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 27  | a     | 605 | PEF  | O2-C10-C11  | 3.80  | 119.70      | 111.48   |
| 27  | c     | 301 | PEF  | O2-C10-C11  | 3.77  | 119.63      | 111.48   |
| 30  | O     | 401 | HEC  | C4D-ND-C1D  | 3.67  | 111.80      | 105.82   |
| 26  | A     | 503 | PCF  | O21-C21-C22 | 3.65  | 119.37      | 111.48   |
| 30  | D     | 401 | HEC  | C4D-ND-C1D  | 3.53  | 111.57      | 105.82   |
| 32  | a     | 602 | HEA  | CMD-C2D-C1D | 3.49  | 130.49      | 125.03   |
| 32  | a     | 601 | HEA  | CMD-C2D-C1D | 3.43  | 130.40      | 125.03   |
| 29  | C     | 403 | U10  | C7-C8-C9    | -3.38 | 121.01      | 126.83   |
| 32  | a     | 602 | HEA  | CHB-C4A-NA  | -3.35 | 120.80      | 124.45   |
| 29  | C     | 403 | U10  | C10-C9-C11  | 3.35  | 121.04      | 115.23   |
| 29  | N     | 403 | U10  | C47-C48-C49 | -3.33 | 120.00      | 127.62   |
| 29  | N     | 403 | U10  | C22-C23-C24 | -3.32 | 120.02      | 127.62   |
| 29  | N     | 403 | U10  | C45-C44-C46 | 3.26  | 120.89      | 115.23   |
| 29  | C     | 403 | U10  | C45-C44-C46 | 3.25  | 120.87      | 115.23   |
| 29  | N     | 403 | U10  | C10-C9-C11  | 3.25  | 120.86      | 115.23   |
| 29  | C     | 403 | U10  | C27-C28-C29 | -3.22 | 120.26      | 127.62   |
| 29  | C     | 403 | U10  | C17-C18-C19 | -3.21 | 120.27      | 127.62   |
| 27  | J     | 101 | PEF  | O3-C30-C31  | 3.18  | 121.53      | 111.83   |
| 29  | C     | 403 | U10  | C42-C43-C44 | -3.17 | 120.38      | 127.62   |
| 32  | a     | 601 | HEA  | CHB-C4A-NA  | -3.13 | 121.05      | 124.45   |
| 29  | N     | 403 | U10  | C27-C28-C29 | -3.10 | 120.54      | 127.62   |
| 27  | N     | 405 | PEF  | O3-C30-C31  | 3.06  | 121.16      | 111.83   |
| 29  | N     | 403 | U10  | C20-C19-C21 | 3.06  | 120.53      | 115.23   |
| 29  | N     | 403 | U10  | C42-C43-C44 | -3.04 | 120.66      | 127.62   |
| 29  | N     | 403 | U10  | C40-C39-C41 | 3.00  | 120.44      | 115.23   |
| 29  | N     | 403 | U10  | C12-C13-C14 | -3.00 | 120.77      | 127.62   |
| 29  | C     | 403 | U10  | C32-C33-C34 | -2.99 | 120.78      | 127.62   |
| 29  | C     | 403 | U10  | C12-C13-C14 | -2.99 | 120.78      | 127.62   |
| 29  | C     | 403 | U10  | C25-C24-C26 | 2.91  | 120.28      | 115.23   |
| 27  | A     | 504 | PEF  | O3-C30-C31  | 2.86  | 120.56      | 111.83   |
| 29  | N     | 403 | U10  | C32-C33-C34 | -2.83 | 121.14      | 127.62   |
| 29  | C     | 403 | U10  | C20-C19-C21 | 2.82  | 120.12      | 115.23   |
| 28  | N     | 402 | HEM  | C3B-C2B-C1B | 2.81  | 108.52      | 106.41   |
| 29  | C     | 403 | U10  | C1M-C1-C6   | -2.80 | 119.85      | 124.45   |
| 29  | C     | 403 | U10  | C22-C23-C24 | -2.79 | 121.25      | 127.62   |
| 26  | L     | 503 | PCF  | O31-C31-C32 | 2.78  | 120.32      | 111.83   |
| 27  | O     | 402 | PEF  | O3-C30-C31  | 2.77  | 120.28      | 111.83   |
| 29  | N     | 403 | U10  | C17-C18-C19 | -2.76 | 121.31      | 127.62   |
| 29  | C     | 403 | U10  | C35-C34-C36 | 2.76  | 120.02      | 115.23   |
| 26  | A     | 503 | PCF  | O31-C31-C32 | 2.75  | 120.23      | 111.83   |
| 29  | C     | 403 | U10  | C50-C49-C51 | 2.74  | 119.99      | 115.23   |
| 29  | C     | 403 | U10  | C15-C14-C16 | 2.71  | 119.93      | 115.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 29  | N     | 403 | U10  | C25-C24-C26 | 2.71  | 119.93      | 115.23   |
| 29  | C     | 403 | U10  | C47-C48-C49 | -2.70 | 121.44      | 127.62   |
| 27  | a     | 605 | PEF  | O3-C30-C31  | 2.70  | 120.06      | 111.83   |
| 27  | b     | 302 | PEF  | O3-C30-C31  | 2.69  | 120.03      | 111.83   |
| 26  | A     | 505 | PCF  | O31-C31-C32 | 2.67  | 119.97      | 111.83   |
| 29  | C     | 403 | U10  | C30-C29-C31 | 2.67  | 119.86      | 115.23   |
| 29  | N     | 403 | U10  | C35-C34-C36 | 2.65  | 119.82      | 115.23   |
| 32  | a     | 601 | HEA  | OMA-CMA-C3A | -2.64 | 119.65      | 125.62   |
| 29  | N     | 403 | U10  | C30-C29-C31 | 2.64  | 119.80      | 115.23   |
| 26  | T     | 101 | PCF  | O31-C31-C32 | 2.63  | 119.87      | 111.83   |
| 27  | k     | 201 | PEF  | O3-C30-C31  | 2.62  | 119.82      | 111.83   |
| 32  | a     | 601 | HEA  | C3C-C4C-NC  | 2.61  | 112.00      | 109.80   |
| 27  | N     | 404 | PEF  | O3-C30-C31  | 2.60  | 119.77      | 111.83   |
| 28  | N     | 402 | HEM  | C1B-NB-C4B  | 2.60  | 108.28      | 105.21   |
| 29  | C     | 403 | U10  | C40-C39-C41 | 2.59  | 119.72      | 115.23   |
| 27  | c     | 301 | PEF  | O3-C30-C31  | 2.57  | 119.68      | 111.83   |
| 29  | N     | 403 | U10  | C50-C49-C51 | 2.56  | 119.68      | 115.23   |
| 28  | N     | 402 | HEM  | C3B-C4B-NB  | -2.56 | 107.63      | 109.47   |
| 32  | a     | 601 | HEA  | CBA-CAA-C2A | 2.51  | 119.47      | 112.53   |
| 29  | C     | 403 | U10  | C37-C38-C39 | -2.51 | 121.88      | 127.62   |
| 29  | N     | 403 | U10  | C37-C38-C39 | -2.50 | 121.91      | 127.62   |
| 27  | D     | 402 | PEF  | O3-C30-C31  | 2.48  | 119.39      | 111.83   |
| 32  | a     | 602 | HEA  | CMB-C2B-C3B | -2.44 | 125.55      | 130.28   |
| 28  | N     | 402 | HEM  | C4D-ND-C1D  | 2.39  | 108.04      | 105.21   |
| 28  | C     | 402 | HEM  | C4D-ND-C1D  | 2.39  | 108.04      | 105.21   |
| 29  | N     | 403 | U10  | C1M-C1-C6   | -2.37 | 120.55      | 124.45   |
| 32  | a     | 601 | HEA  | C1D-C2D-C3D | -2.36 | 104.50      | 106.98   |
| 28  | C     | 401 | HEM  | C4D-ND-C1D  | 2.36  | 108.00      | 105.21   |
| 29  | N     | 403 | U10  | C15-C14-C16 | 2.35  | 119.31      | 115.23   |
| 28  | C     | 402 | HEM  | C1B-NB-C4B  | 2.34  | 107.98      | 105.21   |
| 32  | a     | 602 | HEA  | C1D-C2D-C3D | -2.33 | 104.53      | 106.98   |
| 30  | O     | 401 | HEC  | C2A-C1A-NA  | -2.31 | 108.09      | 110.32   |
| 30  | D     | 401 | HEC  | C2A-C1A-NA  | -2.31 | 108.10      | 110.32   |
| 29  | C     | 403 | U10  | C56-C54-C55 | 2.31  | 119.90      | 114.59   |
| 28  | N     | 401 | HEM  | C4D-ND-C1D  | 2.31  | 107.94      | 105.21   |
| 32  | a     | 602 | HEA  | C2A-C1A-NA  | 2.29  | 112.53      | 110.32   |
| 32  | a     | 602 | HEA  | OMA-CMA-C3A | -2.27 | 120.50      | 125.62   |
| 29  | N     | 403 | U10  | C56-C54-C55 | 2.25  | 119.77      | 114.59   |
| 32  | a     | 602 | HEA  | C3C-C4C-NC  | 2.25  | 111.69      | 109.80   |
| 32  | a     | 601 | HEA  | CHA-C1A-NA  | -2.24 | 122.01      | 124.45   |
| 32  | a     | 601 | HEA  | C2A-C1A-NA  | 2.21  | 112.46      | 110.32   |
| 32  | a     | 601 | HEA  | C20-C19-C18 | -2.21 | 116.22      | 121.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 32  | a     | 601 | HEA  | O1D-CGD-CBD | -2.18 | 116.17      | 123.09   |
| 32  | a     | 602 | HEA  | C13-C14-C15 | -2.17 | 122.65      | 127.62   |
| 28  | C     | 401 | HEM  | C2A-C1A-NA  | -2.17 | 107.74      | 110.15   |
| 28  | C     | 401 | HEM  | C3D-C4D-ND  | -2.15 | 107.81      | 110.17   |
| 32  | a     | 602 | HEA  | C20-C19-C18 | -2.13 | 116.39      | 121.17   |
| 28  | C     | 402 | HEM  | C3B-C2B-C1B | 2.12  | 108.01      | 106.41   |
| 32  | a     | 602 | HEA  | C3D-C4D-ND  | 2.11  | 112.39      | 110.35   |
| 28  | N     | 401 | HEM  | C3B-C2B-C1B | 2.10  | 107.99      | 106.41   |
| 28  | N     | 401 | HEM  | C2A-C1A-NA  | -2.09 | 107.84      | 110.15   |
| 32  | a     | 601 | HEA  | C3B-C4B-NB  | 2.06  | 112.20      | 109.84   |
| 28  | C     | 401 | HEM  | C1B-NB-C4B  | 2.05  | 107.64      | 105.21   |
| 29  | N     | 403 | U10  | O3-C3-C4    | -2.05 | 115.89      | 123.64   |
| 32  | a     | 601 | HEA  | C26-C15-C14 | -2.04 | 118.40      | 123.63   |
| 32  | a     | 602 | HEA  | C3B-C4B-NB  | 2.03  | 112.18      | 109.84   |
| 32  | a     | 602 | HEA  | O1D-CGD-CBD | -2.03 | 116.66      | 123.09   |
| 29  | N     | 403 | U10  | C6-C1-C2    | 2.03  | 120.77      | 119.17   |
| 28  | N     | 401 | HEM  | C1B-NB-C4B  | 2.02  | 107.60      | 105.21   |
| 29  | N     | 403 | U10  | C52-C53-C54 | -2.00 | 120.97      | 127.64   |
| 32  | a     | 602 | HEA  | C26-C15-C14 | -2.00 | 118.49      | 123.63   |

There are no chirality outliers.

All (639) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | A     | 502 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | A     | 502 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | A     | 502 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | A     | 502 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | H     | 101 | CDL  | O1-C1-CB2-OB2   |
| 25  | H     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | H     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | H     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | H     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | H     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 25  | H     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | H     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | H     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | H     | 101 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | H     | 102 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | H     | 102 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | H     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | L     | 502 | CDL  | O1-C1-CA2-OA2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | L     | 502 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | L     | 502 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | L     | 502 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | L     | 502 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | L     | 502 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | S     | 101 | CDL  | O1-C1-CA2-OA2   |
| 25  | S     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | S     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 25  | S     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | S     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | S     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 25  | S     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | S     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | S     | 101 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | S     | 101 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | S     | 101 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | S     | 101 | CDL  | C51-CB5-OB6-CB4 |
| 25  | S     | 102 | CDL  | O1-C1-CA2-OA2   |
| 25  | S     | 102 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | S     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 25  | S     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 25  | S     | 102 | CDL  | CB3-OB5-PB2-OB4 |
| 26  | A     | 503 | PCF  | C1-O11-P-O13    |
| 26  | A     | 503 | PCF  | O13-C11-C12-N   |
| 26  | A     | 503 | PCF  | C22-C21-O21-C2  |
| 26  | L     | 503 | PCF  | C1-O11-P-O13    |
| 26  | L     | 503 | PCF  | C1-O11-P-O14    |
| 26  | L     | 503 | PCF  | O13-C11-C12-N   |
| 26  | L     | 503 | PCF  | O21-C2-C3-O31   |
| 26  | L     | 503 | PCF  | C22-C21-O21-C2  |
| 27  | A     | 504 | PEF  | O4P-C4-C5-N     |
| 27  | A     | 504 | PEF  | C31-C30-O3-C3   |
| 27  | A     | 504 | PEF  | O5-C30-O3-C3    |
| 27  | D     | 402 | PEF  | O4P-C4-C5-N     |
| 27  | D     | 402 | PEF  | C1-O3P-P-O2P    |
| 27  | D     | 402 | PEF  | C1-O3P-P-O4P    |
| 27  | D     | 402 | PEF  | C4-O4P-P-O1P    |
| 27  | J     | 101 | PEF  | C31-C30-O3-C3   |
| 27  | J     | 101 | PEF  | O5-C30-O3-C3    |
| 27  | J     | 101 | PEF  | C4-O4P-P-O1P    |
| 27  | J     | 101 | PEF  | C4-O4P-P-O3P    |
| 27  | N     | 404 | PEF  | C1-O3P-P-O4P    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | N     | 405 | PEF  | C31-C30-O3-C3   |
| 27  | N     | 405 | PEF  | O5-C30-O3-C3    |
| 27  | N     | 405 | PEF  | C1-O3P-P-O4P    |
| 27  | O     | 402 | PEF  | C4-O4P-P-O1P    |
| 27  | a     | 605 | PEF  | O2-C2-C3-O3     |
| 27  | a     | 605 | PEF  | O4P-C4-C5-N     |
| 27  | b     | 302 | PEF  | O4P-C4-C5-N     |
| 27  | b     | 302 | PEF  | C4-O4P-P-O3P    |
| 27  | c     | 301 | PEF  | C11-C10-O2-C2   |
| 27  | k     | 201 | PEF  | O4P-C4-C5-N     |
| 29  | C     | 403 | U10  | C7-C8-C9-C10    |
| 29  | C     | 403 | U10  | C7-C8-C9-C11    |
| 29  | C     | 403 | U10  | C25-C24-C26-C27 |
| 29  | C     | 403 | U10  | C24-C26-C27-C28 |
| 29  | C     | 403 | U10  | C43-C44-C46-C47 |
| 29  | C     | 403 | U10  | C45-C44-C46-C47 |
| 29  | C     | 403 | U10  | C47-C48-C49-C50 |
| 29  | C     | 403 | U10  | C47-C48-C49-C51 |
| 29  | N     | 403 | U10  | C7-C8-C9-C10    |
| 29  | N     | 403 | U10  | C7-C8-C9-C11    |
| 29  | N     | 403 | U10  | C12-C13-C14-C15 |
| 29  | N     | 403 | U10  | C17-C18-C19-C20 |
| 29  | N     | 403 | U10  | C17-C18-C19-C21 |
| 29  | N     | 403 | U10  | C37-C38-C39-C40 |
| 29  | N     | 403 | U10  | C37-C38-C39-C41 |
| 29  | N     | 403 | U10  | C40-C39-C41-C42 |
| 29  | N     | 403 | U10  | C47-C48-C49-C50 |
| 29  | N     | 403 | U10  | C47-C48-C49-C51 |
| 30  | D     | 401 | HEC  | C2B-C3B-CAB-CBB |
| 30  | D     | 401 | HEC  | C4B-C3B-CAB-CBB |
| 30  | D     | 401 | HEC  | C2C-C3C-CAC-CBC |
| 30  | O     | 401 | HEC  | C2B-C3B-CAB-CBB |
| 30  | O     | 401 | HEC  | C4B-C3B-CAB-CBB |
| 30  | O     | 401 | HEC  | C2C-C3C-CAC-CBC |
| 32  | a     | 601 | HEA  | C3A-C2A-CAA-CBA |
| 32  | a     | 601 | HEA  | C2A-C3A-CMA-OMA |
| 32  | a     | 601 | HEA  | C4A-C3A-CMA-OMA |
| 32  | a     | 602 | HEA  | C2A-C3A-CMA-OMA |
| 25  | L     | 502 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | A     | 502 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | H     | 101 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | L     | 502 | CDL  | OA9-CA7-OA8-CA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 101 | CDL  | OB9-CB7-OB8-CB6 |
| 25  | S     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 26  | A     | 503 | PCF  | O22-C21-O21-C2  |
| 26  | L     | 503 | PCF  | O22-C21-O21-C2  |
| 27  | c     | 301 | PEF  | O4-C10-O2-C2    |
| 32  | a     | 601 | HEA  | C21-C22-C23-C25 |
| 25  | A     | 502 | CDL  | C71-CB7-OB8-CB6 |
| 25  | H     | 101 | CDL  | C71-CB7-OB8-CB6 |
| 25  | L     | 502 | CDL  | C31-CA7-OA8-CA6 |
| 25  | L     | 502 | CDL  | C71-CB7-OB8-CB6 |
| 25  | S     | 101 | CDL  | C71-CB7-OB8-CB6 |
| 25  | S     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 29  | C     | 403 | U10  | C20-C19-C21-C22 |
| 29  | C     | 403 | U10  | C23-C24-C26-C27 |
| 29  | N     | 403 | U10  | C38-C39-C41-C42 |
| 29  | N     | 403 | U10  | C32-C33-C34-C35 |
| 29  | N     | 403 | U10  | C12-C13-C14-C16 |
| 25  | H     | 101 | CDL  | OA9-CA7-OA8-CA6 |
| 32  | a     | 601 | HEA  | C1A-C2A-CAA-CBA |
| 32  | a     | 602 | HEA  | C21-C22-C23-C25 |
| 25  | A     | 502 | CDL  | O1-C1-CA2-OA2   |
| 25  | H     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 25  | H     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 32  | a     | 601 | HEA  | C21-C22-C23-C24 |
| 25  | H     | 101 | CDL  | C31-CA7-OA8-CA6 |
| 29  | C     | 403 | U10  | C14-C16-C17-C18 |
| 29  | N     | 403 | U10  | C19-C21-C22-C23 |
| 29  | N     | 403 | U10  | C29-C31-C32-C33 |
| 28  | N     | 401 | HEM  | C3D-CAD-CBD-CGD |
| 32  | a     | 601 | HEA  | C2A-CAA-CBA-CGA |
| 25  | S     | 102 | CDL  | C11-C12-C13-C14 |
| 25  | H     | 101 | CDL  | C12-C13-C14-C15 |
| 29  | C     | 403 | U10  | C12-C13-C14-C15 |
| 25  | A     | 502 | CDL  | C51-CB5-OB6-CB4 |
| 25  | A     | 502 | CDL  | CB2-C1-CA2-OA2  |
| 25  | H     | 102 | CDL  | CA2-C1-CB2-OB2  |
| 25  | L     | 502 | CDL  | CA2-C1-CB2-OB2  |
| 25  | H     | 102 | CDL  | C77-C78-C79-C80 |
| 27  | c     | 301 | PEF  | C11-C12-C13-C14 |
| 25  | A     | 502 | CDL  | C13-C14-C15-C16 |
| 25  | L     | 502 | CDL  | C32-C33-C34-C35 |
| 29  | C     | 403 | U10  | C15-C14-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 29  | C     | 403 | U10  | C18-C19-C21-C22 |
| 25  | L     | 502 | CDL  | O1-C1-CB2-OB2   |
| 25  | H     | 102 | CDL  | C18-C19-C20-C21 |
| 25  | A     | 502 | CDL  | OB7-CB5-OB6-CB4 |
| 27  | D     | 402 | PEF  | O2-C2-C3-O3     |
| 25  | A     | 502 | CDL  | CB7-C71-C72-C73 |
| 25  | S     | 101 | CDL  | C31-C32-C33-C34 |
| 25  | H     | 101 | CDL  | C72-C73-C74-C75 |
| 25  | L     | 502 | CDL  | C12-C13-C14-C15 |
| 27  | b     | 302 | PEF  | C10-C11-C12-C13 |
| 29  | C     | 403 | U10  | C39-C41-C42-C43 |
| 29  | N     | 403 | U10  | C24-C26-C27-C28 |
| 25  | H     | 102 | CDL  | C75-C76-C77-C78 |
| 25  | H     | 101 | CDL  | CA5-C11-C12-C13 |
| 25  | H     | 101 | CDL  | CB7-C71-C72-C73 |
| 25  | S     | 101 | CDL  | CA5-C11-C12-C13 |
| 26  | L     | 503 | PCF  | C21-C22-C23-C24 |
| 27  | a     | 605 | PEF  | C10-C11-C12-C13 |
| 27  | c     | 301 | PEF  | C30-C31-C32-C33 |
| 25  | H     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 28  | C     | 401 | HEM  | C3D-CAD-CBD-CGD |
| 25  | S     | 101 | CDL  | C19-C20-C21-C22 |
| 27  | b     | 302 | PEF  | C11-C12-C13-C14 |
| 25  | A     | 502 | CDL  | O1-C1-CB2-OB2   |
| 25  | H     | 102 | CDL  | O1-C1-CB2-OB2   |
| 27  | k     | 201 | PEF  | C30-C31-C32-C33 |
| 25  | H     | 102 | CDL  | C51-CB5-OB6-CB4 |
| 25  | L     | 502 | CDL  | C15-C16-C17-C18 |
| 25  | H     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | H     | 102 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | A     | 502 | CDL  | CA2-C1-CB2-OB2  |
| 25  | H     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 25  | L     | 502 | CDL  | CB2-C1-CA2-OA2  |
| 25  | S     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 25  | S     | 102 | CDL  | CB2-C1-CA2-OA2  |
| 25  | H     | 102 | CDL  | C15-C16-C17-C18 |
| 29  | N     | 403 | U10  | C45-C44-C46-C47 |
| 29  | C     | 403 | U10  | C13-C14-C16-C17 |
| 25  | S     | 102 | CDL  | O1-C1-CB2-OB2   |
| 25  | S     | 101 | CDL  | C1-CB2-OB2-PB2  |
| 25  | L     | 502 | CDL  | C52-C53-C54-C55 |
| 25  | S     | 102 | CDL  | C78-C79-C80-C81 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | b     | 302 | PEF  | C16-C17-C18-C19 |
| 25  | S     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 25  | H     | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 27  | a     | 605 | PEF  | C40-C41-C42-C43 |
| 25  | H     | 101 | CDL  | C52-C53-C54-C55 |
| 27  | O     | 402 | PEF  | C12-C13-C14-C15 |
| 27  | k     | 201 | PEF  | C34-C35-C36-C37 |
| 29  | C     | 403 | U10  | C52-C53-C54-C55 |
| 25  | H     | 102 | CDL  | C16-C17-C18-C19 |
| 27  | b     | 302 | PEF  | C31-C32-C33-C34 |
| 27  | k     | 201 | PEF  | C31-C32-C33-C34 |
| 26  | T     | 101 | PCF  | C47-C48-C49-C50 |
| 27  | N     | 404 | PEF  | C16-C17-C18-C19 |
| 27  | N     | 405 | PEF  | C37-C38-C39-C40 |
| 27  | O     | 402 | PEF  | C31-C32-C33-C34 |
| 32  | a     | 601 | HEA  | C4C-C3C-CAC-CBC |
| 29  | N     | 403 | U10  | C32-C33-C34-C36 |
| 25  | H     | 101 | CDL  | C20-C21-C22-C23 |
| 25  | H     | 101 | CDL  | C51-CB5-OB6-CB4 |
| 25  | L     | 502 | CDL  | C51-CB5-OB6-CB4 |
| 25  | H     | 102 | CDL  | C74-C75-C76-C77 |
| 27  | k     | 201 | PEF  | C13-C14-C15-C16 |
| 25  | H     | 101 | CDL  | C71-C72-C73-C74 |
| 27  | b     | 302 | PEF  | C18-C19-C20-C21 |
| 25  | H     | 102 | CDL  | C11-C12-C13-C14 |
| 27  | O     | 402 | PEF  | C40-C41-C42-C43 |
| 27  | N     | 404 | PEF  | C31-C32-C33-C34 |
| 27  | A     | 504 | PEF  | C40-C41-C42-C43 |
| 25  | H     | 101 | CDL  | CB5-C51-C52-C53 |
| 26  | A     | 505 | PCF  | C24-C25-C26-C27 |
| 27  | J     | 101 | PEF  | C32-C33-C34-C35 |
| 25  | H     | 101 | CDL  | C23-C24-C25-C26 |
| 25  | A     | 502 | CDL  | CA3-CA4-CA6-OA8 |
| 27  | b     | 302 | PEF  | C1-C2-C3-O3     |
| 25  | H     | 101 | CDL  | C13-C14-C15-C16 |
| 27  | b     | 302 | PEF  | C12-C13-C14-C15 |
| 25  | H     | 101 | CDL  | CA7-C31-C32-C33 |
| 27  | J     | 101 | PEF  | C10-C11-C12-C13 |
| 27  | O     | 402 | PEF  | C10-C11-C12-C13 |
| 25  | H     | 101 | CDL  | C77-C78-C79-C80 |
| 25  | H     | 101 | CDL  | C17-C18-C19-C20 |
| 25  | S     | 102 | CDL  | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 102 | CDL  | C57-C58-C59-C60 |
| 26  | T     | 101 | PCF  | C25-C26-C27-C28 |
| 27  | N     | 405 | PEF  | C35-C36-C37-C38 |
| 25  | S     | 101 | CDL  | CB7-C71-C72-C73 |
| 26  | A     | 503 | PCF  | C26-C27-C28-C29 |
| 25  | S     | 101 | CDL  | C73-C74-C75-C76 |
| 27  | c     | 301 | PEF  | C12-C13-C14-C15 |
| 25  | S     | 101 | CDL  | C80-C81-C82-C83 |
| 25  | S     | 101 | CDL  | C12-C13-C14-C15 |
| 27  | D     | 402 | PEF  | C16-C17-C18-C19 |
| 25  | L     | 502 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | S     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | H     | 102 | CDL  | C73-C74-C75-C76 |
| 29  | N     | 403 | U10  | C43-C44-C46-C47 |
| 25  | S     | 102 | CDL  | C71-C72-C73-C74 |
| 26  | A     | 505 | PCF  | C32-C31-O31-C3  |
| 25  | H     | 101 | CDL  | C14-C15-C16-C17 |
| 25  | S     | 101 | CDL  | C13-C14-C15-C16 |
| 26  | T     | 101 | PCF  | C22-C23-C24-C25 |
| 26  | A     | 505 | PCF  | C37-C38-C39-C40 |
| 27  | D     | 402 | PEF  | C13-C14-C15-C16 |
| 27  | c     | 301 | PEF  | C37-C38-C39-C40 |
| 25  | H     | 101 | CDL  | C32-C33-C34-C35 |
| 25  | H     | 101 | CDL  | C57-C58-C59-C60 |
| 25  | H     | 101 | CDL  | C75-C76-C77-C78 |
| 26  | T     | 101 | PCF  | C30-C47-C48-C49 |
| 27  | b     | 302 | PEF  | C39-C40-C41-C42 |
| 25  | A     | 502 | CDL  | C71-C72-C73-C74 |
| 25  | H     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 25  | S     | 101 | CDL  | C11-CA5-OA6-CA4 |
| 29  | C     | 403 | U10  | C6-C7-C8-C9     |
| 25  | L     | 502 | CDL  | CB7-C71-C72-C73 |
| 25  | H     | 101 | CDL  | OB7-CB5-OB6-CB4 |
| 25  | H     | 101 | CDL  | C19-C20-C21-C22 |
| 25  | S     | 101 | CDL  | C71-C72-C73-C74 |
| 25  | S     | 102 | CDL  | C51-C52-C53-C54 |
| 27  | J     | 101 | PEF  | C39-C40-C41-C42 |
| 25  | A     | 502 | CDL  | C16-C17-C18-C19 |
| 25  | S     | 102 | CDL  | C34-C35-C36-C37 |
| 27  | b     | 302 | PEF  | C36-C37-C38-C39 |
| 25  | S     | 101 | CDL  | C75-C76-C77-C78 |
| 27  | N     | 405 | PEF  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | c     | 301 | PEF  | C32-C33-C34-C35 |
| 27  | N     | 405 | PEF  | C11-C10-O2-C2   |
| 28  | N     | 402 | HEM  | C4B-C3B-CAB-CBB |
| 27  | b     | 302 | PEF  | C35-C36-C37-C38 |
| 26  | T     | 101 | PCF  | C23-C24-C25-C26 |
| 25  | S     | 102 | CDL  | C13-C14-C15-C16 |
| 26  | A     | 505 | PCF  | O21-C2-C3-O31   |
| 27  | N     | 404 | PEF  | O2-C2-C3-O3     |
| 27  | b     | 302 | PEF  | O2-C2-C3-O3     |
| 25  | S     | 102 | CDL  | C52-C53-C54-C55 |
| 25  | S     | 102 | CDL  | C32-C33-C34-C35 |
| 26  | A     | 505 | PCF  | C42-C43-C44-C45 |
| 25  | H     | 101 | CDL  | C55-C56-C57-C58 |
| 25  | H     | 102 | CDL  | C1-CB2-OB2-PB2  |
| 25  | H     | 101 | CDL  | C11-C12-C13-C14 |
| 25  | S     | 102 | CDL  | C14-C15-C16-C17 |
| 27  | A     | 504 | PEF  | C12-C13-C14-C15 |
| 25  | H     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 27  | J     | 101 | PEF  | C38-C39-C40-C41 |
| 27  | k     | 201 | PEF  | C12-C13-C14-C15 |
| 25  | S     | 101 | CDL  | C17-C18-C19-C20 |
| 27  | A     | 504 | PEF  | C11-C12-C13-C14 |
| 25  | H     | 102 | CDL  | C32-C33-C34-C35 |
| 27  | a     | 605 | PEF  | C14-C15-C16-C17 |
| 27  | b     | 302 | PEF  | C32-C33-C34-C35 |
| 25  | A     | 502 | CDL  | C33-C34-C35-C36 |
| 25  | S     | 102 | CDL  | C73-C74-C75-C76 |
| 27  | O     | 402 | PEF  | C34-C35-C36-C37 |
| 27  | b     | 302 | PEF  | C34-C35-C36-C37 |
| 25  | A     | 502 | CDL  | OB5-CB3-CB4-CB6 |
| 25  | H     | 102 | CDL  | OA5-CA3-CA4-CA6 |
| 25  | L     | 502 | CDL  | OB5-CB3-CB4-CB6 |
| 25  | S     | 102 | CDL  | OA5-CA3-CA4-CA6 |
| 27  | O     | 402 | PEF  | O3P-C1-C2-C3    |
| 25  | H     | 102 | CDL  | C34-C35-C36-C37 |
| 25  | S     | 101 | CDL  | C72-C73-C74-C75 |
| 26  | A     | 505 | PCF  | O32-C31-O31-C3  |
| 25  | H     | 101 | CDL  | C22-C23-C24-C25 |
| 25  | H     | 102 | CDL  | C20-C21-C22-C23 |
| 27  | N     | 404 | PEF  | C37-C38-C39-C40 |
| 25  | S     | 102 | CDL  | C55-C56-C57-C58 |
| 25  | H     | 102 | CDL  | CA3-CA4-CA6-OA8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 101 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | S     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 25  | S     | 102 | CDL  | C75-C76-C77-C78 |
| 27  | k     | 201 | PEF  | C35-C36-C37-C38 |
| 27  | N     | 404 | PEF  | C10-C11-C12-C13 |
| 27  | N     | 404 | PEF  | C13-C14-C15-C16 |
| 25  | H     | 102 | CDL  | CA5-C11-C12-C13 |
| 26  | L     | 503 | PCF  | C37-C38-C39-C40 |
| 27  | b     | 302 | PEF  | C2-C1-O3P-P     |
| 27  | N     | 405 | PEF  | C13-C14-C15-C16 |
| 25  | A     | 502 | CDL  | C32-C33-C34-C35 |
| 25  | A     | 502 | CDL  | C11-C12-C13-C14 |
| 25  | H     | 101 | CDL  | C15-C16-C17-C18 |
| 25  | H     | 101 | CDL  | C33-C34-C35-C36 |
| 25  | H     | 102 | CDL  | C23-C24-C25-C26 |
| 25  | S     | 101 | CDL  | C11-C12-C13-C14 |
| 25  | S     | 101 | CDL  | CA7-C31-C32-C33 |
| 27  | c     | 301 | PEF  | C10-C11-C12-C13 |
| 25  | H     | 102 | CDL  | C17-C18-C19-C20 |
| 27  | N     | 405 | PEF  | C31-C32-C33-C34 |
| 27  | k     | 201 | PEF  | C18-C19-C20-C21 |
| 25  | A     | 502 | CDL  | CB6-CB4-OB6-CB5 |
| 26  | L     | 503 | PCF  | C1-C2-O21-C21   |
| 27  | N     | 404 | PEF  | C33-C34-C35-C36 |
| 29  | C     | 403 | U10  | C52-C53-C54-C56 |
| 27  | c     | 301 | PEF  | C35-C36-C37-C38 |
| 25  | H     | 101 | CDL  | C74-C75-C76-C77 |
| 25  | L     | 502 | CDL  | C71-C72-C73-C74 |
| 27  | D     | 402 | PEF  | C12-C13-C14-C15 |
| 25  | S     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 27  | a     | 605 | PEF  | O3P-C1-C2-O2    |
| 25  | S     | 101 | CDL  | C32-C33-C34-C35 |
| 26  | A     | 505 | PCF  | C38-C39-C40-C41 |
| 27  | c     | 301 | PEF  | C34-C35-C36-C37 |
| 25  | A     | 502 | CDL  | C12-C13-C14-C15 |
| 27  | A     | 504 | PEF  | C32-C33-C34-C35 |
| 27  | A     | 504 | PEF  | C34-C35-C36-C37 |
| 25  | S     | 101 | CDL  | C52-C53-C54-C55 |
| 25  | S     | 101 | CDL  | C15-C16-C17-C18 |
| 27  | k     | 201 | PEF  | C11-C12-C13-C14 |
| 25  | A     | 502 | CDL  | OA6-CA4-CA6-OA8 |
| 27  | A     | 504 | PEF  | O2-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | a     | 602 | HEA  | C21-C22-C23-C24 |
| 29  | N     | 403 | U10  | C49-C51-C52-C53 |
| 25  | L     | 502 | CDL  | C33-C34-C35-C36 |
| 27  | A     | 504 | PEF  | C31-C32-C33-C34 |
| 25  | H     | 102 | CDL  | C31-CA7-OA8-CA6 |
| 25  | H     | 101 | CDL  | C59-C60-C61-C62 |
| 27  | k     | 201 | PEF  | C31-C30-O3-C3   |
| 27  | J     | 101 | PEF  | C33-C34-C35-C36 |
| 26  | A     | 505 | PCF  | C26-C27-C28-C29 |
| 27  | a     | 605 | PEF  | C12-C13-C14-C15 |
| 27  | k     | 201 | PEF  | C37-C38-C39-C40 |
| 25  | S     | 101 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | H     | 101 | CDL  | C76-C77-C78-C79 |
| 27  | J     | 101 | PEF  | C35-C36-C37-C38 |
| 27  | O     | 402 | PEF  | C37-C38-C39-C40 |
| 27  | a     | 605 | PEF  | C34-C35-C36-C37 |
| 26  | T     | 101 | PCF  | C32-C31-O31-C3  |
| 29  | C     | 403 | U10  | C12-C13-C14-C16 |
| 25  | S     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 27  | J     | 101 | PEF  | O3P-C1-C2-C3    |
| 27  | b     | 302 | PEF  | O3P-C1-C2-C3    |
| 25  | L     | 502 | CDL  | C11-C12-C13-C14 |
| 26  | A     | 505 | PCF  | C43-C44-C45-C46 |
| 27  | a     | 605 | PEF  | C42-C43-C44-C45 |
| 25  | H     | 102 | CDL  | C21-C22-C23-C24 |
| 27  | D     | 402 | PEF  | C34-C35-C36-C37 |
| 27  | J     | 101 | PEF  | C37-C38-C39-C40 |
| 25  | S     | 102 | CDL  | CA2-C1-CB2-OB2  |
| 25  | H     | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 25  | L     | 502 | CDL  | CA3-CA4-CA6-OA8 |
| 26  | A     | 503 | PCF  | C1-C2-C3-O31    |
| 26  | L     | 503 | PCF  | C1-C2-C3-O31    |
| 27  | A     | 504 | PEF  | C1-C2-C3-O3     |
| 27  | D     | 402 | PEF  | C1-C2-C3-O3     |
| 27  | N     | 404 | PEF  | C1-C2-C3-O3     |
| 27  | N     | 405 | PEF  | C1-C2-C3-O3     |
| 29  | C     | 403 | U10  | C9-C11-C12-C13  |
| 29  | C     | 403 | U10  | C29-C31-C32-C33 |
| 25  | H     | 102 | CDL  | C71-C72-C73-C74 |
| 27  | a     | 605 | PEF  | C37-C38-C39-C40 |
| 25  | S     | 102 | CDL  | C74-C75-C76-C77 |
| 27  | J     | 101 | PEF  | C40-C41-C42-C43 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | N     | 404 | PEF  | C35-C36-C37-C38 |
| 25  | S     | 102 | CDL  | C59-C60-C61-C62 |
| 25  | A     | 502 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | H     | 102 | CDL  | OA5-CA3-CA4-OA6 |
| 25  | S     | 102 | CDL  | OA5-CA3-CA4-OA6 |
| 27  | D     | 402 | PEF  | O3P-C1-C2-O2    |
| 27  | O     | 402 | PEF  | O3P-C1-C2-O2    |
| 27  | a     | 605 | PEF  | C2-C1-O3P-P     |
| 25  | S     | 101 | CDL  | C51-C52-C53-C54 |
| 27  | N     | 405 | PEF  | C41-C42-C43-C44 |
| 25  | S     | 102 | CDL  | C17-C18-C19-C20 |
| 25  | H     | 102 | CDL  | C12-C13-C14-C15 |
| 25  | A     | 502 | CDL  | OB6-CB4-CB6-OB8 |
| 25  | S     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 27  | N     | 405 | PEF  | O2-C2-C3-O3     |
| 25  | H     | 102 | CDL  | C24-C25-C26-C27 |
| 27  | N     | 405 | PEF  | C30-C31-C32-C33 |
| 26  | A     | 503 | PCF  | C22-C23-C24-C25 |
| 26  | A     | 503 | PCF  | C36-C37-C38-C39 |
| 27  | A     | 504 | PEF  | C35-C36-C37-C38 |
| 27  | J     | 101 | PEF  | C12-C13-C14-C15 |
| 25  | S     | 101 | CDL  | C23-C24-C25-C26 |
| 27  | a     | 605 | PEF  | C13-C14-C15-C16 |
| 25  | A     | 502 | CDL  | C14-C15-C16-C17 |
| 25  | S     | 102 | CDL  | C72-C73-C74-C75 |
| 27  | N     | 405 | PEF  | C34-C35-C36-C37 |
| 27  | O     | 402 | PEF  | C11-C10-O2-C2   |
| 25  | S     | 101 | CDL  | C21-C22-C23-C24 |
| 25  | H     | 101 | CDL  | C56-C57-C58-C59 |
| 27  | N     | 404 | PEF  | C15-C16-C17-C18 |
| 25  | S     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 27  | a     | 605 | PEF  | C39-C40-C41-C42 |
| 25  | S     | 102 | CDL  | C15-C16-C17-C18 |
| 26  | A     | 505 | PCF  | C25-C26-C27-C28 |
| 27  | D     | 402 | PEF  | C20-C21-C22-C23 |
| 27  | a     | 605 | PEF  | C18-C19-C20-C21 |
| 27  | D     | 402 | PEF  | O3P-C1-C2-C3    |
| 27  | a     | 605 | PEF  | O3P-C1-C2-C3    |
| 25  | S     | 102 | CDL  | C1-CB2-OB2-PB2  |
| 25  | S     | 101 | CDL  | C76-C77-C78-C79 |
| 25  | S     | 101 | CDL  | C16-C17-C18-C19 |
| 26  | A     | 503 | PCF  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 28  | C     | 402 | HEM  | C2A-CAA-CBA-CGA |
| 27  | k     | 201 | PEF  | O5-C30-O3-C3    |
| 25  | A     | 502 | CDL  | C72-C73-C74-C75 |
| 25  | H     | 102 | CDL  | C31-C32-C33-C34 |
| 27  | N     | 405 | PEF  | O4-C10-O2-C2    |
| 25  | L     | 502 | CDL  | C16-C17-C18-C19 |
| 25  | L     | 502 | CDL  | C31-C32-C33-C34 |
| 25  | H     | 102 | CDL  | OA9-CA7-OA8-CA6 |
| 26  | T     | 101 | PCF  | O32-C31-O31-C3  |
| 25  | H     | 102 | CDL  | C19-C20-C21-C22 |
| 27  | D     | 402 | PEF  | C38-C39-C40-C41 |
| 25  | A     | 502 | CDL  | CB3-CB4-CB6-OB8 |
| 27  | a     | 605 | PEF  | C1-C2-C3-O3     |
| 26  | L     | 503 | PCF  | C36-C37-C38-C39 |
| 29  | C     | 403 | U10  | C30-C29-C31-C32 |
| 29  | N     | 403 | U10  | C25-C24-C26-C27 |
| 25  | H     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 26  | A     | 503 | PCF  | O21-C2-C3-O31   |
| 27  | D     | 402 | PEF  | C39-C40-C41-C42 |
| 25  | S     | 102 | CDL  | C16-C17-C18-C19 |
| 27  | b     | 302 | PEF  | C20-C21-C22-C23 |
| 25  | H     | 102 | CDL  | C54-C55-C56-C57 |
| 25  | L     | 502 | CDL  | C14-C15-C16-C17 |
| 26  | A     | 505 | PCF  | O13-C11-C12-N   |
| 26  | T     | 101 | PCF  | O13-C11-C12-N   |
| 29  | N     | 403 | U10  | C23-C24-C26-C27 |
| 27  | k     | 201 | PEF  | C14-C15-C16-C17 |
| 27  | a     | 605 | PEF  | C19-C20-C21-C22 |
| 29  | N     | 403 | U10  | C5-C4-O4-C4M    |
| 25  | A     | 502 | CDL  | OA5-CA3-CA4-CA6 |
| 27  | c     | 301 | PEF  | O3P-C1-C2-C3    |
| 27  | k     | 201 | PEF  | O3P-C1-C2-C3    |
| 27  | J     | 101 | PEF  | C34-C35-C36-C37 |
| 27  | O     | 402 | PEF  | C11-C12-C13-C14 |
| 27  | O     | 402 | PEF  | C32-C33-C34-C35 |
| 26  | T     | 101 | PCF  | C48-C49-C50-C51 |
| 25  | S     | 101 | CDL  | C34-C35-C36-C37 |
| 30  | D     | 401 | HEC  | C4C-C3C-CAC-CBC |
| 30  | O     | 401 | HEC  | C4C-C3C-CAC-CBC |
| 25  | L     | 502 | CDL  | C13-C14-C15-C16 |
| 27  | O     | 402 | PEF  | O4-C10-O2-C2    |
| 25  | A     | 502 | CDL  | OB5-CB3-CB4-OB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | L     | 502 | CDL  | OB5-CB3-CB4-OB6 |
| 27  | J     | 101 | PEF  | O3P-C1-C2-O2    |
| 27  | N     | 404 | PEF  | O3P-C1-C2-O2    |
| 27  | b     | 302 | PEF  | O3P-C1-C2-O2    |
| 27  | c     | 301 | PEF  | O3P-C1-C2-O2    |
| 25  | S     | 102 | CDL  | C12-C13-C14-C15 |
| 25  | H     | 102 | CDL  | C76-C77-C78-C79 |
| 32  | a     | 602 | HEA  | C4A-C3A-CMA-OMA |
| 27  | a     | 605 | PEF  | C33-C34-C35-C36 |
| 25  | L     | 502 | CDL  | OA6-CA4-CA6-OA8 |
| 25  | S     | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 27  | b     | 302 | PEF  | C40-C41-C42-C43 |
| 27  | k     | 201 | PEF  | C15-C16-C17-C18 |
| 29  | C     | 403 | U10  | C28-C29-C31-C32 |
| 25  | A     | 502 | CDL  | CA3-OA5-PA1-OA2 |
| 25  | A     | 502 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | A     | 502 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | H     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 25  | H     | 101 | CDL  | CB3-OB5-PB2-OB4 |
| 25  | H     | 102 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | H     | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 25  | H     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 25  | L     | 502 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | S     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 25  | S     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 25  | S     | 102 | CDL  | CA2-OA2-PA1-OA4 |
| 26  | A     | 503 | PCF  | C1-O11-P-O12    |
| 26  | L     | 503 | PCF  | C1-O11-P-O12    |
| 26  | T     | 101 | PCF  | C1-O11-P-O12    |
| 27  | A     | 504 | PEF  | C4-O4P-P-O1P    |
| 27  | N     | 404 | PEF  | C4-O4P-P-O1P    |
| 27  | N     | 405 | PEF  | O4P-C4-C5-N     |
| 27  | O     | 402 | PEF  | C1-O3P-P-O1P    |
| 27  | a     | 605 | PEF  | C1-O3P-P-O4P    |
| 27  | a     | 605 | PEF  | C4-O4P-P-O1P    |
| 27  | k     | 201 | PEF  | C4-O4P-P-O1P    |
| 27  | D     | 402 | PEF  | C10-C11-C12-C13 |
| 32  | a     | 601 | HEA  | C2C-C3C-CAC-CBC |
| 26  | L     | 503 | PCF  | C39-C40-C41-C42 |
| 25  | A     | 502 | CDL  | CB4-CB3-OB5-PB2 |
| 25  | H     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 25  | L     | 502 | CDL  | CB4-CB3-OB5-PB2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 27  | k     | 201 | PEF  | C32-C33-C34-C35 |
| 25  | S     | 102 | CDL  | C53-C54-C55-C56 |
| 25  | L     | 502 | CDL  | CB3-CB4-OB6-CB5 |
| 27  | J     | 101 | PEF  | C13-C14-C15-C16 |
| 25  | H     | 102 | CDL  | C79-C80-C81-C82 |
| 27  | k     | 201 | PEF  | O3P-C1-C2-O2    |
| 26  | A     | 505 | PCF  | C39-C40-C41-C42 |
| 25  | L     | 502 | CDL  | C11-CA5-OA6-CA4 |
| 27  | O     | 402 | PEF  | C18-C19-C20-C21 |
| 27  | a     | 605 | PEF  | C11-C12-C13-C14 |
| 26  | A     | 505 | PCF  | C1-C2-C3-O31    |
| 25  | S     | 101 | CDL  | C54-C55-C56-C57 |
| 25  | A     | 502 | CDL  | CB4-CB6-OB8-CB7 |
| 29  | C     | 403 | U10  | C1-C6-C7-C8     |
| 26  | A     | 505 | PCF  | C40-C41-C42-C43 |
| 27  | b     | 302 | PEF  | C14-C15-C16-C17 |
| 25  | L     | 502 | CDL  | OA7-CA5-OA6-CA4 |
| 25  | S     | 102 | CDL  | C1-CA2-OA2-PA1  |
| 29  | C     | 403 | U10  | C5-C4-O4-C4M    |
| 25  | H     | 102 | CDL  | C52-C53-C54-C55 |
| 25  | L     | 502 | CDL  | CA5-C11-C12-C13 |
| 26  | A     | 503 | PCF  | C35-C36-C37-C38 |
| 27  | N     | 404 | PEF  | O3P-C1-C2-C3    |
| 25  | H     | 102 | CDL  | C72-C73-C74-C75 |
| 25  | H     | 101 | CDL  | C16-C17-C18-C19 |
| 27  | k     | 201 | PEF  | O3-C30-C31-C32  |
| 27  | J     | 101 | PEF  | C31-C32-C33-C34 |
| 27  | J     | 101 | PEF  | C22-C23-C24-C25 |
| 27  | A     | 504 | PEF  | C38-C39-C40-C41 |
| 29  | N     | 403 | U10  | C13-C14-C16-C17 |
| 27  | A     | 504 | PEF  | C18-C19-C20-C21 |
| 27  | J     | 101 | PEF  | C16-C17-C18-C19 |
| 27  | c     | 301 | PEF  | C13-C14-C15-C16 |
| 29  | N     | 403 | U10  | C15-C14-C16-C17 |
| 25  | L     | 502 | CDL  | C51-C52-C53-C54 |
| 26  | L     | 503 | PCF  | C33-C34-C35-C36 |
| 27  | O     | 402 | PEF  | C36-C37-C38-C39 |
| 25  | H     | 101 | CDL  | C73-C74-C75-C76 |
| 26  | A     | 503 | PCF  | C27-C28-C29-C30 |
| 25  | S     | 101 | CDL  | C55-C56-C57-C58 |
| 27  | D     | 402 | PEF  | C41-C42-C43-C44 |
| 25  | S     | 101 | CDL  | OB5-CB3-CB4-CB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 32  | a     | 602 | HEA  | CAD-CBD-CGD-O1D |
| 25  | H     | 101 | CDL  | C24-C25-C26-C27 |
| 32  | a     | 602 | HEA  | C26-C15-C16-C17 |
| 32  | a     | 602 | HEA  | CAA-CBA-CGA-O1A |
| 25  | H     | 101 | CDL  | CB4-CB3-OB5-PB2 |
| 25  | H     | 101 | CDL  | C31-C32-C33-C34 |
| 32  | a     | 602 | HEA  | CAA-CBA-CGA-O2A |
| 25  | S     | 102 | CDL  | CB3-CB4-CB6-OB8 |
| 27  | O     | 402 | PEF  | C42-C43-C44-C45 |
| 26  | L     | 503 | PCF  | C38-C39-C40-C41 |
| 28  | N     | 401 | HEM  | C1A-C2A-CAA-CBA |
| 26  | T     | 101 | PCF  | C36-C37-C38-C39 |
| 27  | a     | 605 | PEF  | C36-C37-C38-C39 |
| 29  | N     | 403 | U10  | C35-C34-C36-C37 |
| 32  | a     | 602 | HEA  | CAD-CBD-CGD-O2D |
| 27  | D     | 402 | PEF  | C32-C33-C34-C35 |
| 27  | N     | 404 | PEF  | C18-C19-C20-C21 |
| 29  | N     | 403 | U10  | C33-C34-C36-C37 |
| 27  | N     | 404 | PEF  | C42-C43-C44-C45 |
| 26  | T     | 101 | PCF  | C21-C22-C23-C24 |
| 25  | A     | 502 | CDL  | C31-C32-C33-C34 |
| 25  | S     | 101 | CDL  | C74-C75-C76-C77 |
| 27  | D     | 402 | PEF  | C11-C12-C13-C14 |
| 25  | A     | 502 | CDL  | C12-C11-CA5-OA6 |
| 25  | S     | 101 | CDL  | C12-C11-CA5-OA6 |
| 25  | H     | 102 | CDL  | C56-C57-C58-C59 |
| 25  | L     | 502 | CDL  | C52-C51-CB5-OB6 |
| 26  | L     | 503 | PCF  | O31-C31-C32-C33 |
| 25  | H     | 102 | CDL  | C52-C51-CB5-OB6 |
| 27  | N     | 404 | PEF  | C39-C40-C41-C42 |
| 25  | S     | 101 | CDL  | O1-C1-CB2-OB2   |
| 25  | H     | 102 | CDL  | C32-C31-CA7-OA8 |
| 27  | k     | 201 | PEF  | C16-C17-C18-C19 |
| 25  | H     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 25  | S     | 101 | CDL  | OB5-CB3-CB4-OB6 |
| 28  | N     | 402 | HEM  | CAD-CBD-CGD-O1D |
| 25  | H     | 102 | CDL  | C72-C71-CB7-OB8 |
| 25  | S     | 102 | CDL  | C72-C71-CB7-OB8 |
| 27  | D     | 402 | PEF  | O3-C30-C31-C32  |
| 25  | L     | 502 | CDL  | C12-C11-CA5-OA6 |
| 27  | J     | 101 | PEF  | O3-C30-C31-C32  |
| 26  | L     | 503 | PCF  | C22-C23-C24-C25 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 25  | S     | 102 | CDL  | C32-C31-CA7-OA8 |
| 27  | D     | 402 | PEF  | O2-C10-C11-C12  |
| 25  | H     | 102 | CDL  | C55-C56-C57-C58 |
| 28  | N     | 402 | HEM  | CAD-CBD-CGD-O2D |
| 26  | A     | 505 | PCF  | O31-C31-C32-C33 |
| 27  | O     | 402 | PEF  | C35-C36-C37-C38 |
| 26  | T     | 101 | PCF  | O31-C31-C32-C33 |
| 27  | c     | 301 | PEF  | C36-C37-C38-C39 |
| 25  | L     | 502 | CDL  | C52-C51-CB5-OB7 |
| 25  | H     | 102 | CDL  | C52-C51-CB5-OB7 |
| 27  | D     | 402 | PEF  | C42-C43-C44-C45 |
| 25  | H     | 102 | CDL  | C72-C71-CB7-OB9 |
| 26  | A     | 503 | PCF  | C37-C38-C39-C40 |
| 25  | S     | 101 | CDL  | C12-C11-CA5-OA7 |
| 26  | A     | 505 | PCF  | O32-C31-C32-C33 |
| 25  | S     | 101 | CDL  | C14-C15-C16-C17 |
| 26  | L     | 503 | PCF  | C23-C24-C25-C26 |
| 25  | A     | 502 | CDL  | C12-C11-CA5-OA7 |
| 25  | S     | 102 | CDL  | C72-C71-CB7-OB9 |
| 25  | H     | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 28  | N     | 401 | HEM  | CAD-CBD-CGD-O2D |
| 25  | H     | 102 | CDL  | C32-C31-CA7-OA9 |
| 26  | A     | 503 | PCF  | O21-C21-C22-C23 |
| 27  | D     | 402 | PEF  | O5-C30-C31-C32  |
| 27  | D     | 402 | PEF  | O4-C10-C11-C12  |
| 27  | J     | 101 | PEF  | O5-C30-C31-C32  |
| 25  | S     | 102 | CDL  | C32-C31-CA7-OA9 |
| 26  | A     | 503 | PCF  | C34-C35-C36-C37 |
| 26  | A     | 505 | PCF  | C28-C29-C30-C47 |
| 27  | D     | 402 | PEF  | C18-C19-C20-C21 |
| 27  | c     | 301 | PEF  | O3-C30-C31-C32  |
| 27  | N     | 404 | PEF  | O3-C30-C31-C32  |
| 25  | L     | 502 | CDL  | C12-C11-CA5-OA7 |

There are no ring outliers.

32 monomers are involved in 127 short contacts:

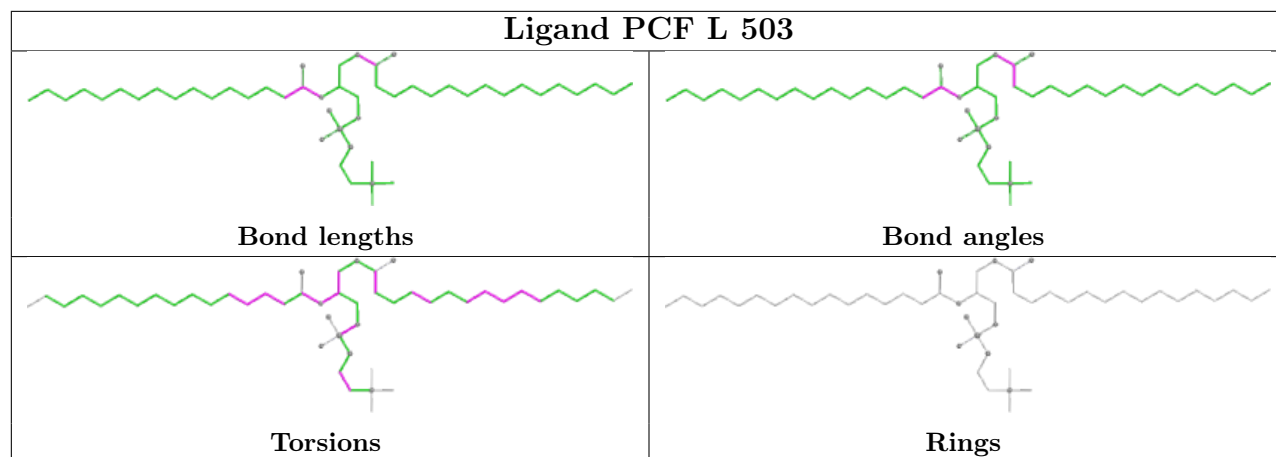
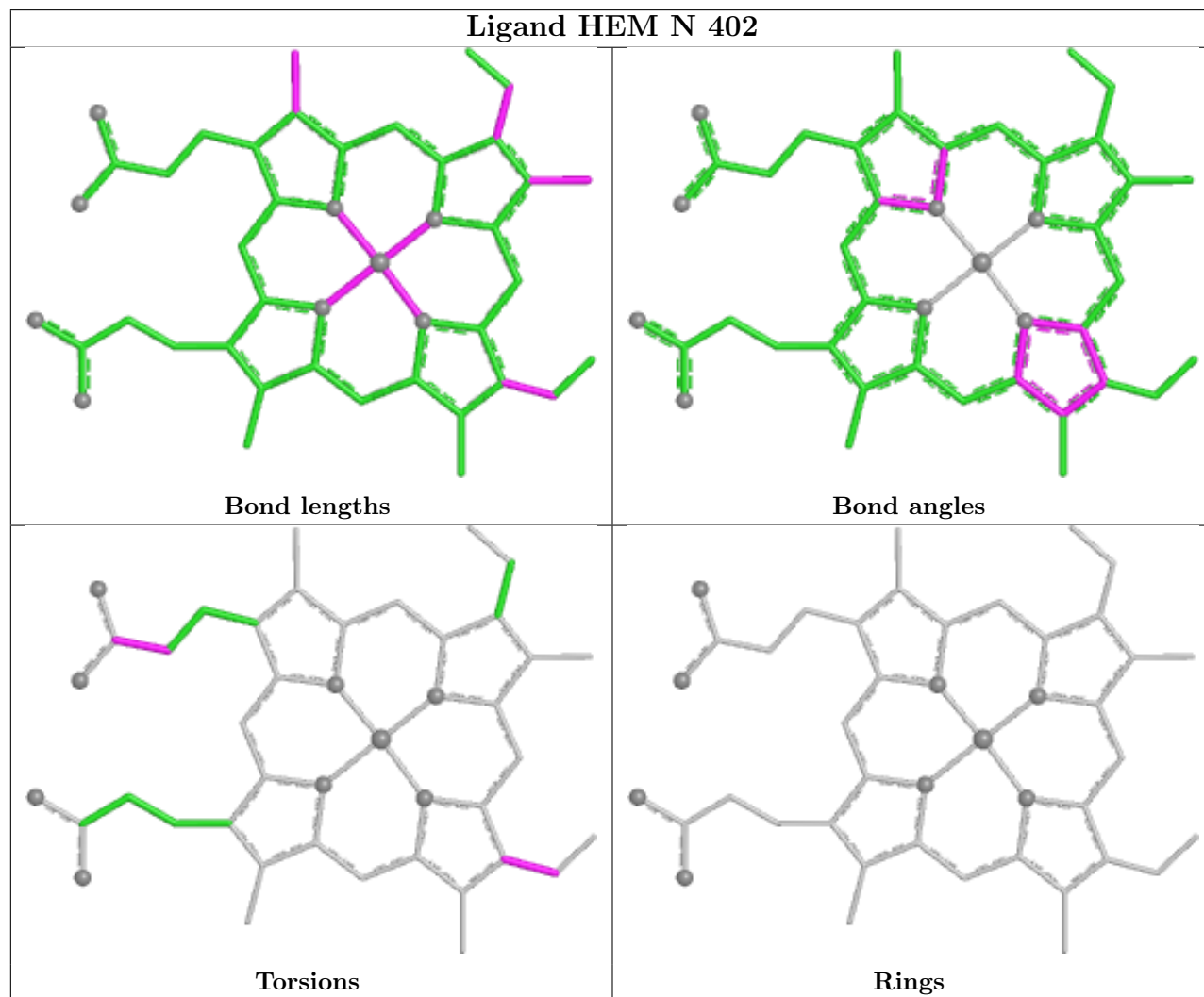
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 31  | P     | 301 | FES  | 2       | 0            |
| 31  | E     | 301 | FES  | 4       | 0            |
| 26  | L     | 503 | PCF  | 3       | 0            |
| 28  | N     | 402 | HEM  | 3       | 0            |

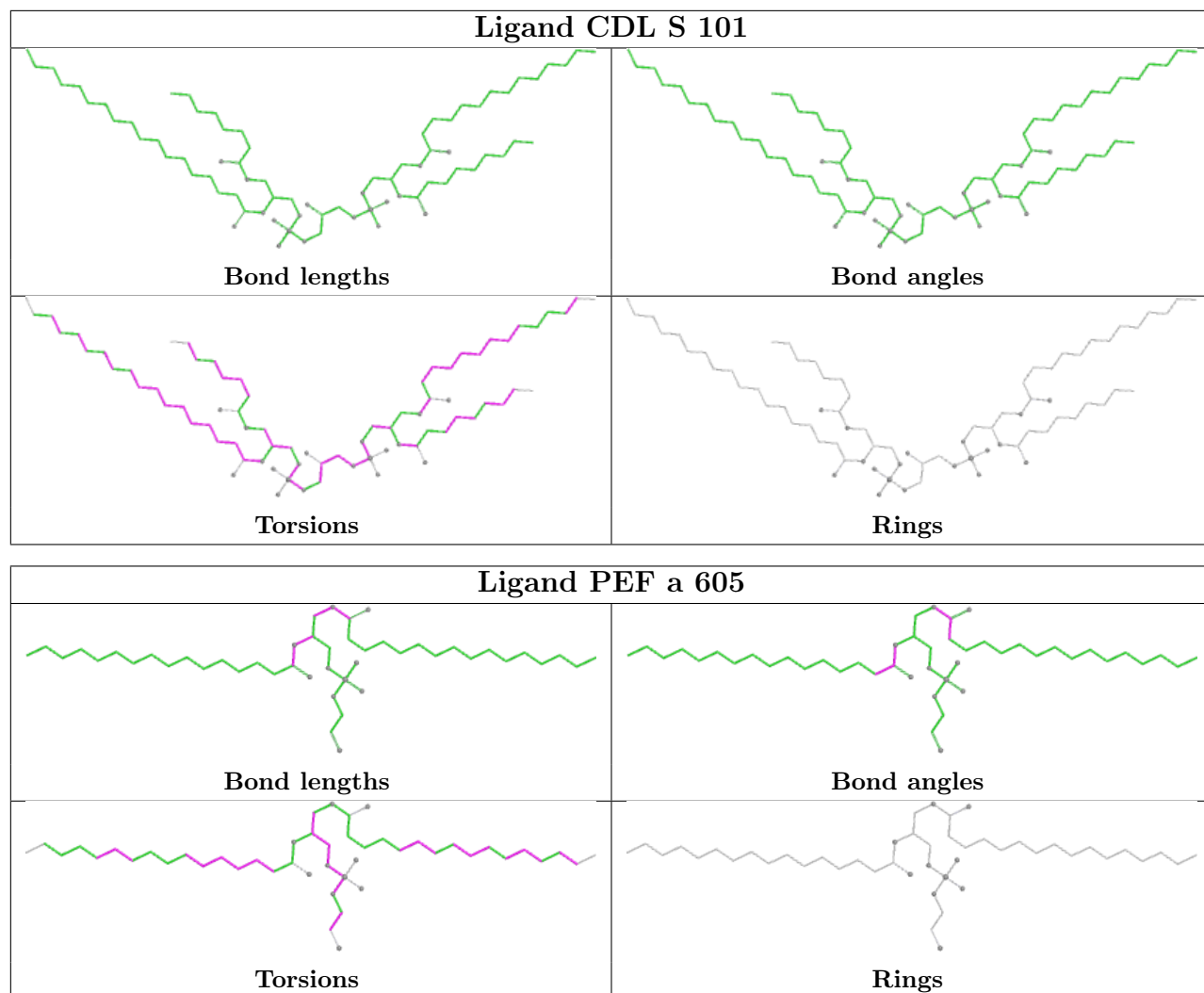
*Continued on next page...*

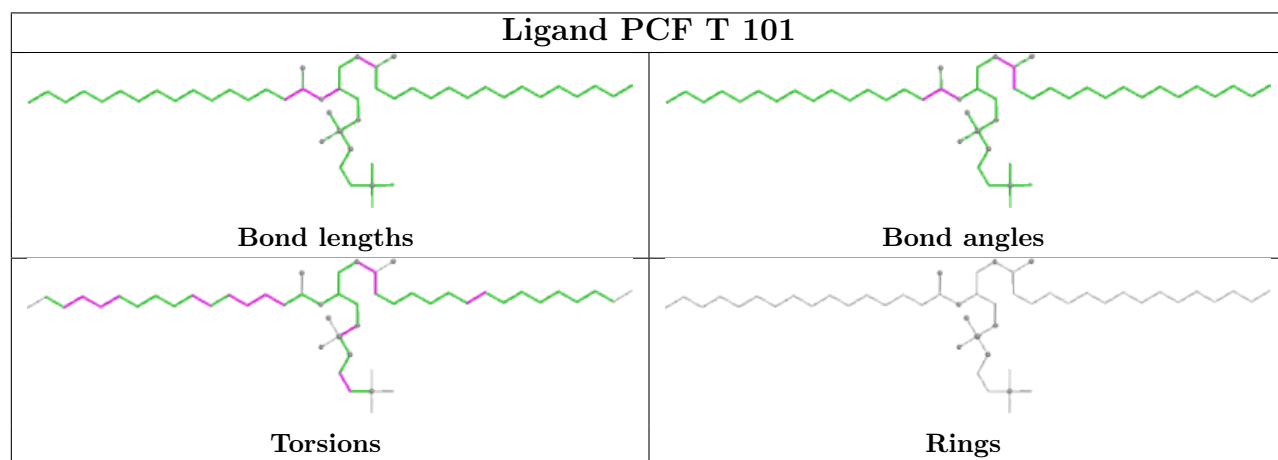
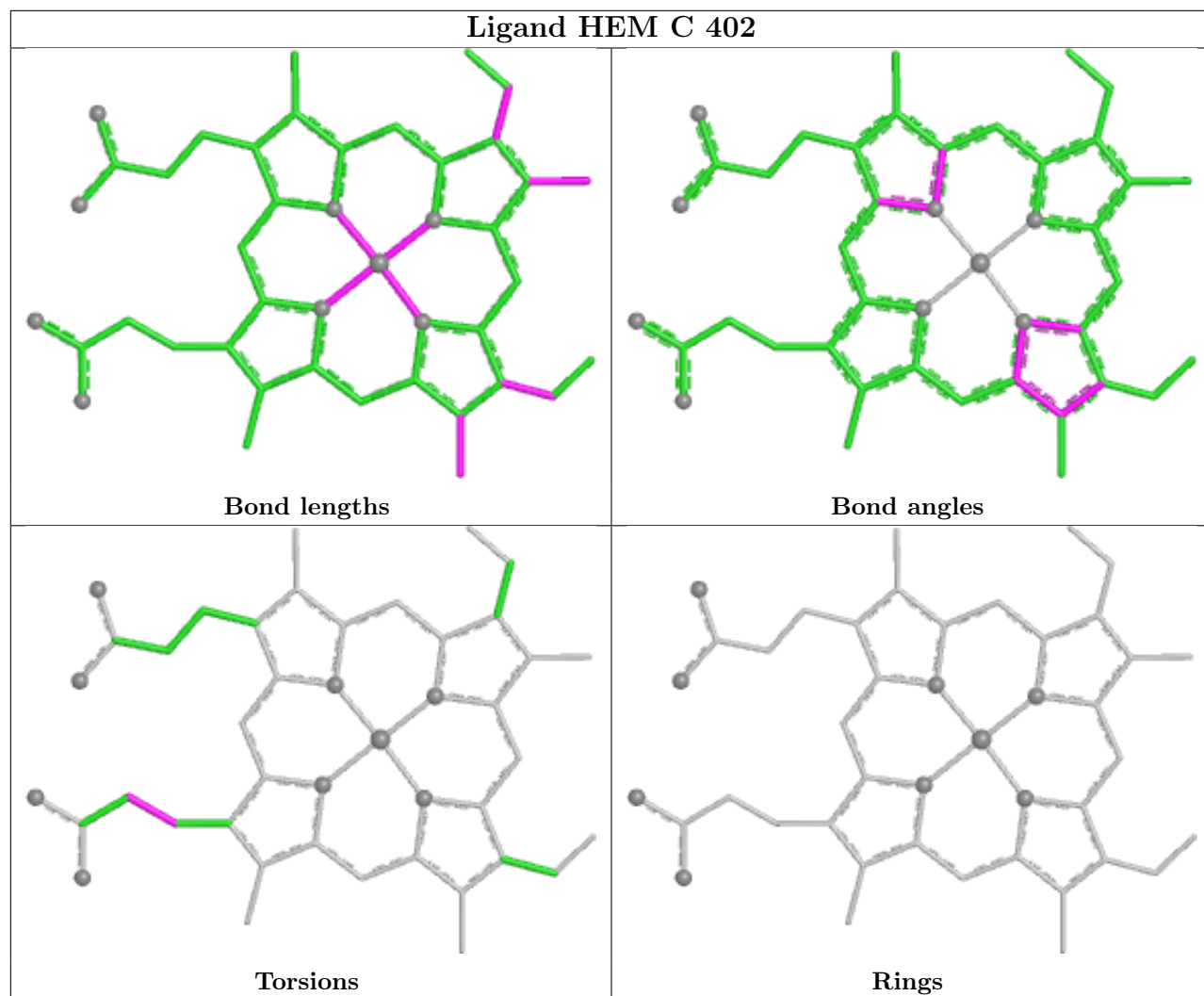
*Continued from previous page...*

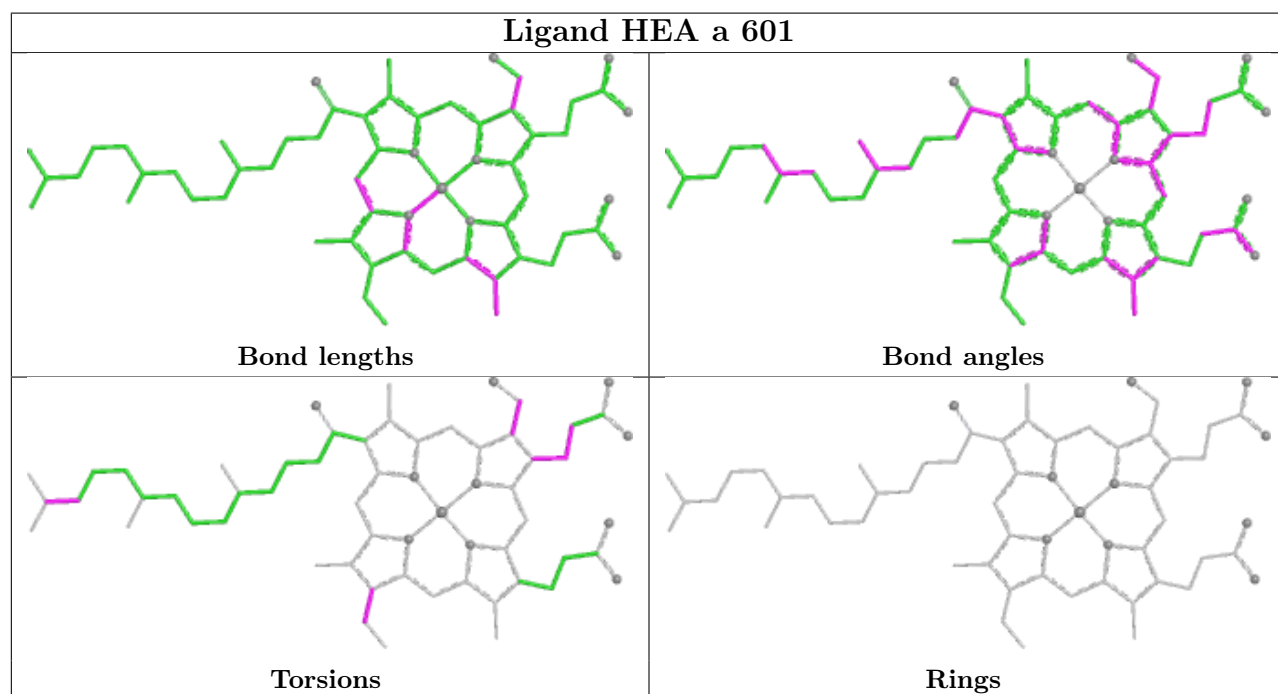
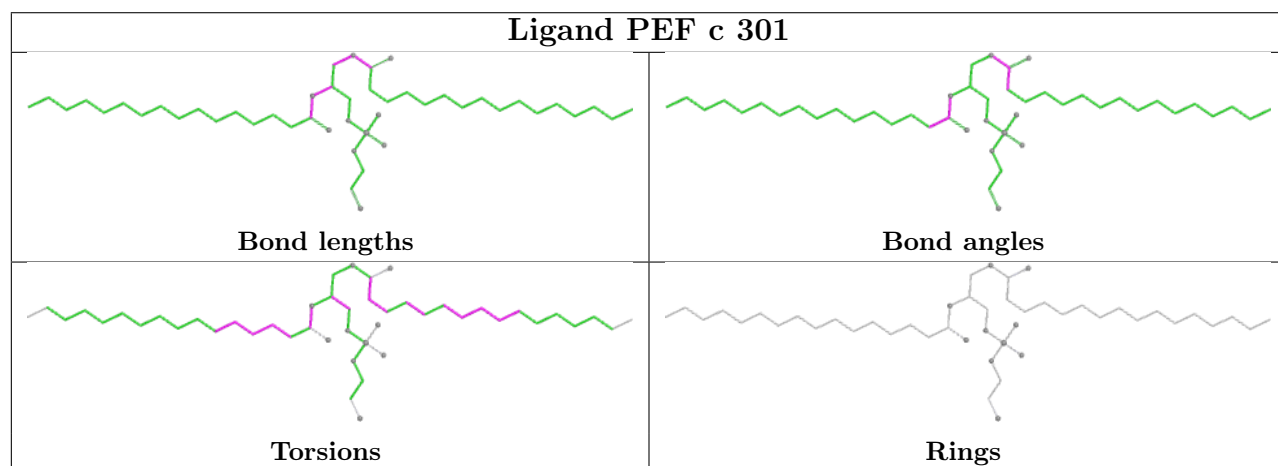
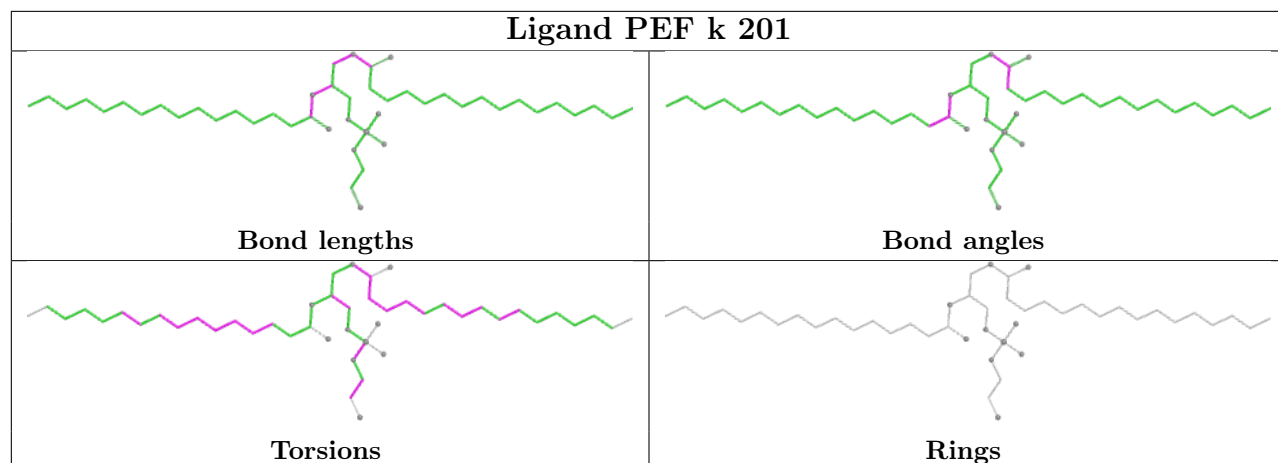
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 25  | S     | 101 | CDL  | 3       | 0            |
| 27  | a     | 605 | PEF  | 2       | 0            |
| 28  | C     | 402 | HEM  | 2       | 0            |
| 26  | T     | 101 | PCF  | 3       | 0            |
| 27  | k     | 201 | PEF  | 12      | 0            |
| 27  | c     | 301 | PEF  | 3       | 0            |
| 32  | a     | 601 | HEA  | 8       | 0            |
| 25  | H     | 102 | CDL  | 6       | 0            |
| 25  | L     | 502 | CDL  | 5       | 0            |
| 32  | a     | 602 | HEA  | 2       | 0            |
| 25  | H     | 101 | CDL  | 4       | 0            |
| 25  | A     | 502 | CDL  | 5       | 0            |
| 27  | O     | 402 | PEF  | 1       | 0            |
| 30  | O     | 401 | HEC  | 3       | 0            |
| 25  | S     | 102 | CDL  | 3       | 0            |
| 27  | b     | 302 | PEF  | 3       | 0            |
| 29  | N     | 403 | U10  | 5       | 0            |
| 26  | A     | 505 | PCF  | 6       | 0            |
| 29  | C     | 403 | U10  | 7       | 0            |
| 27  | N     | 405 | PEF  | 2       | 0            |
| 28  | C     | 401 | HEM  | 5       | 0            |
| 27  | N     | 404 | PEF  | 5       | 0            |
| 27  | A     | 504 | PEF  | 7       | 0            |
| 28  | N     | 401 | HEM  | 3       | 0            |
| 27  | J     | 101 | PEF  | 6       | 0            |
| 30  | D     | 401 | HEC  | 6       | 0            |
| 26  | A     | 503 | PCF  | 5       | 0            |
| 27  | D     | 402 | PEF  | 2       | 0            |

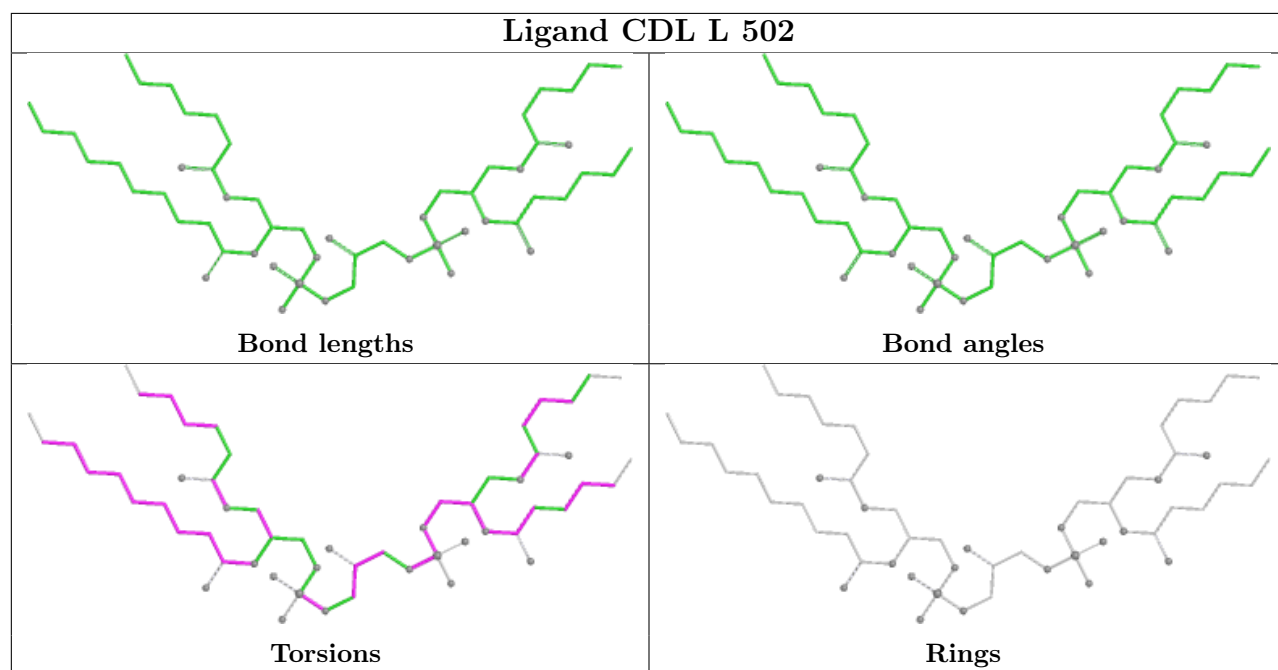
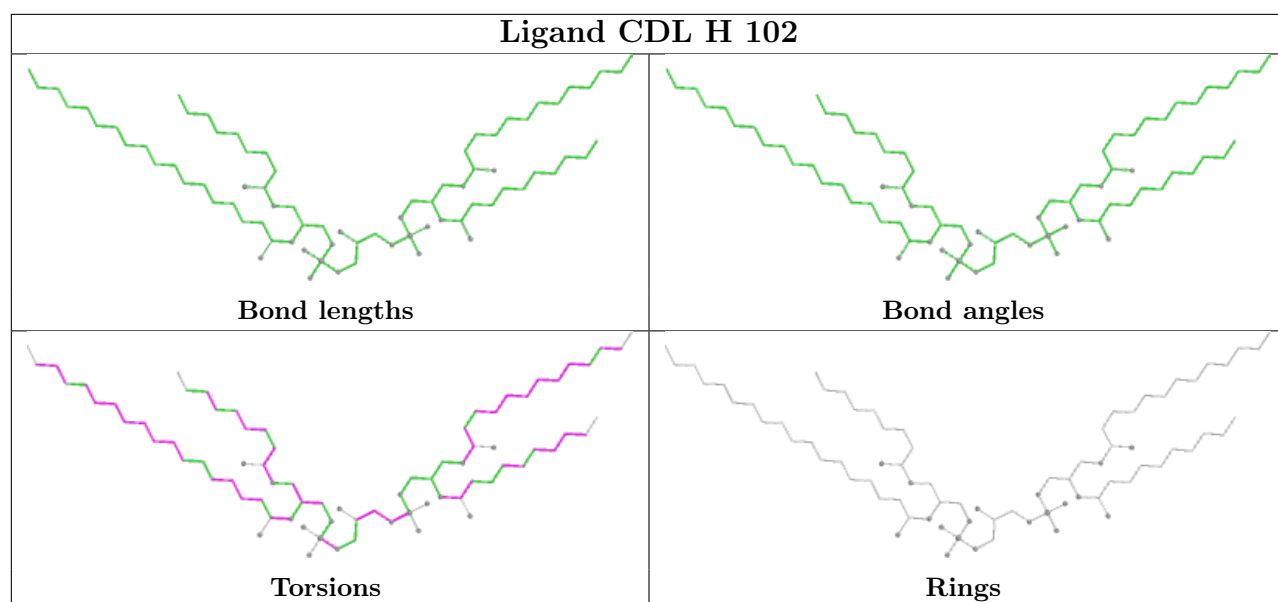
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

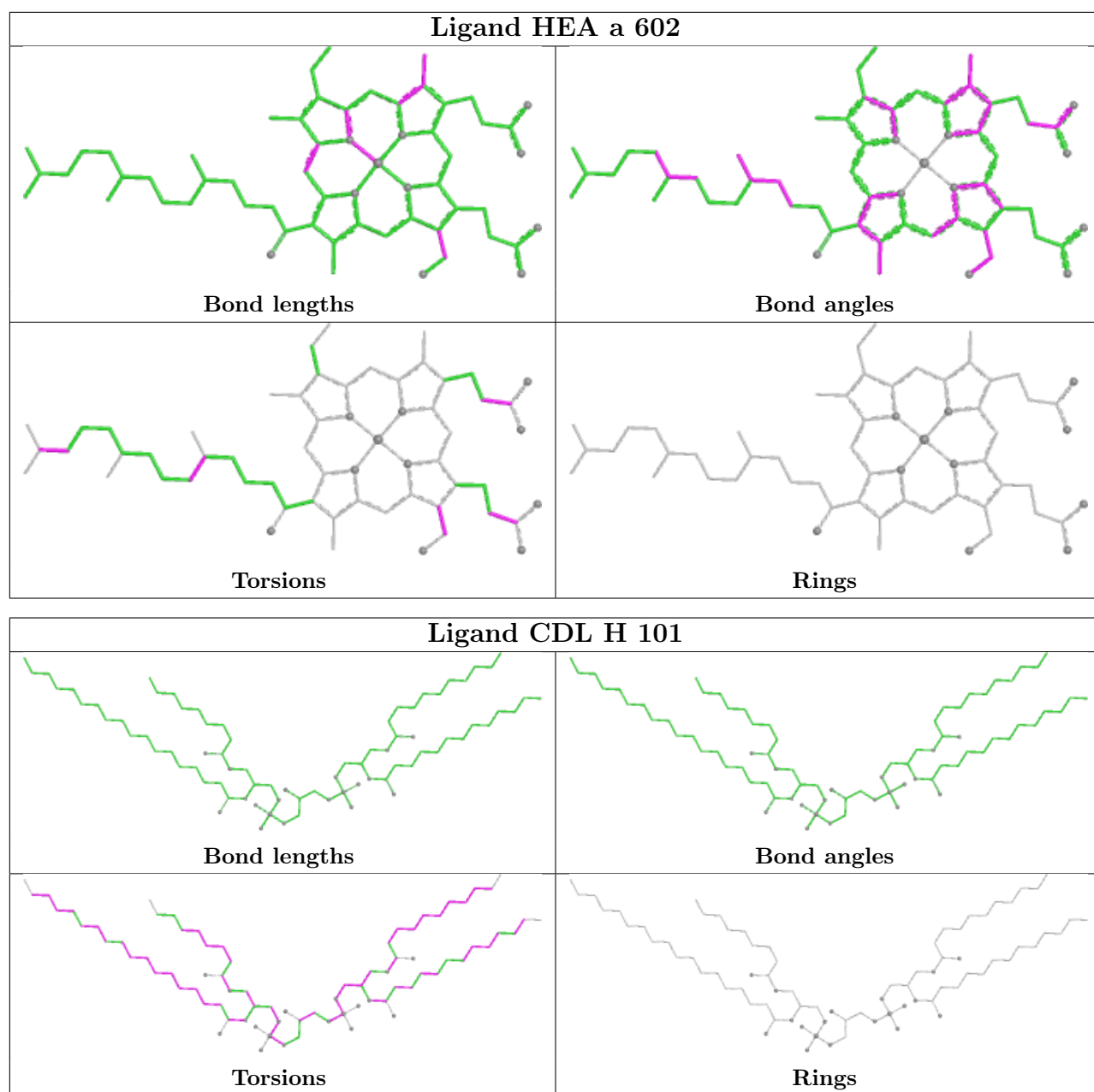
**Ligand PCF L 503****Ligand HEM N 402**

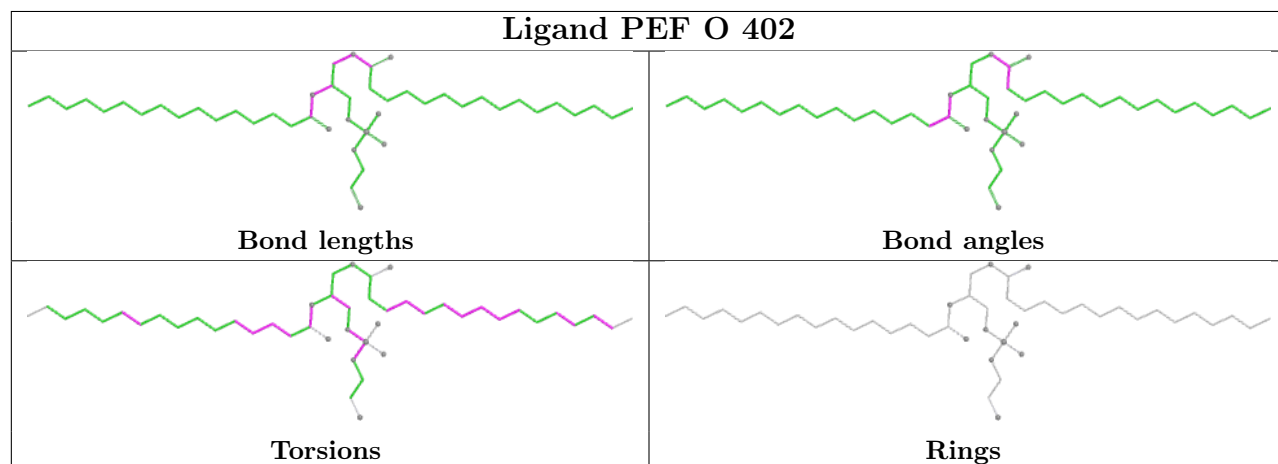
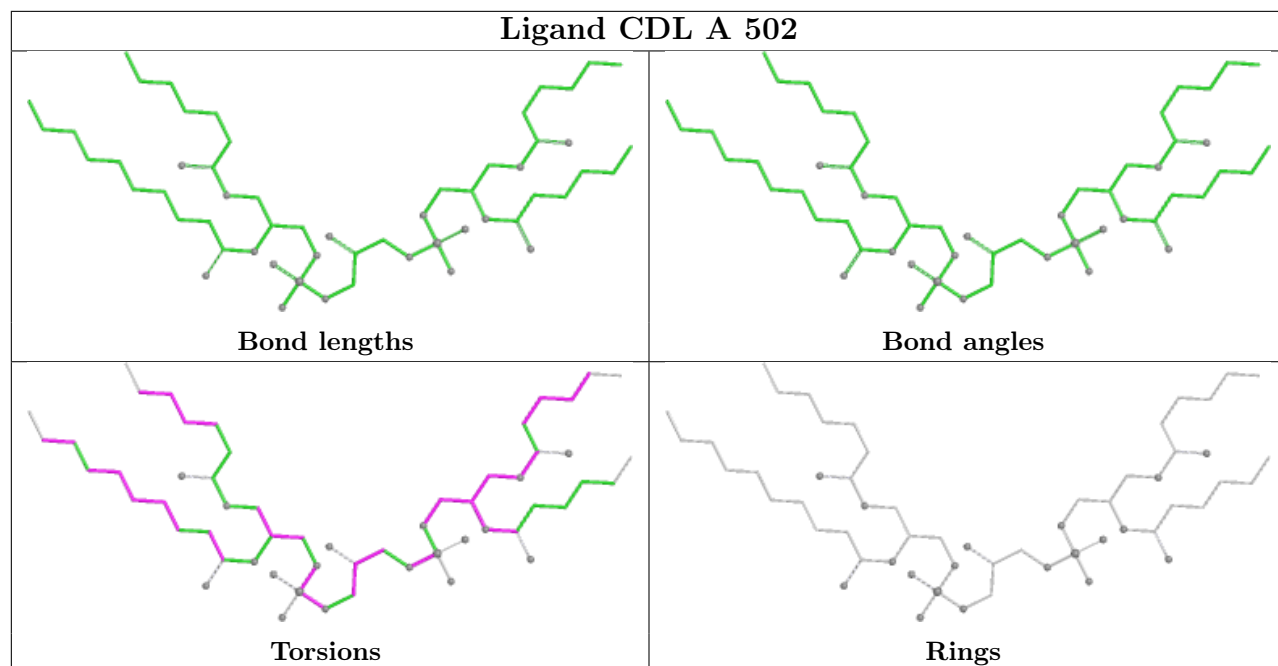


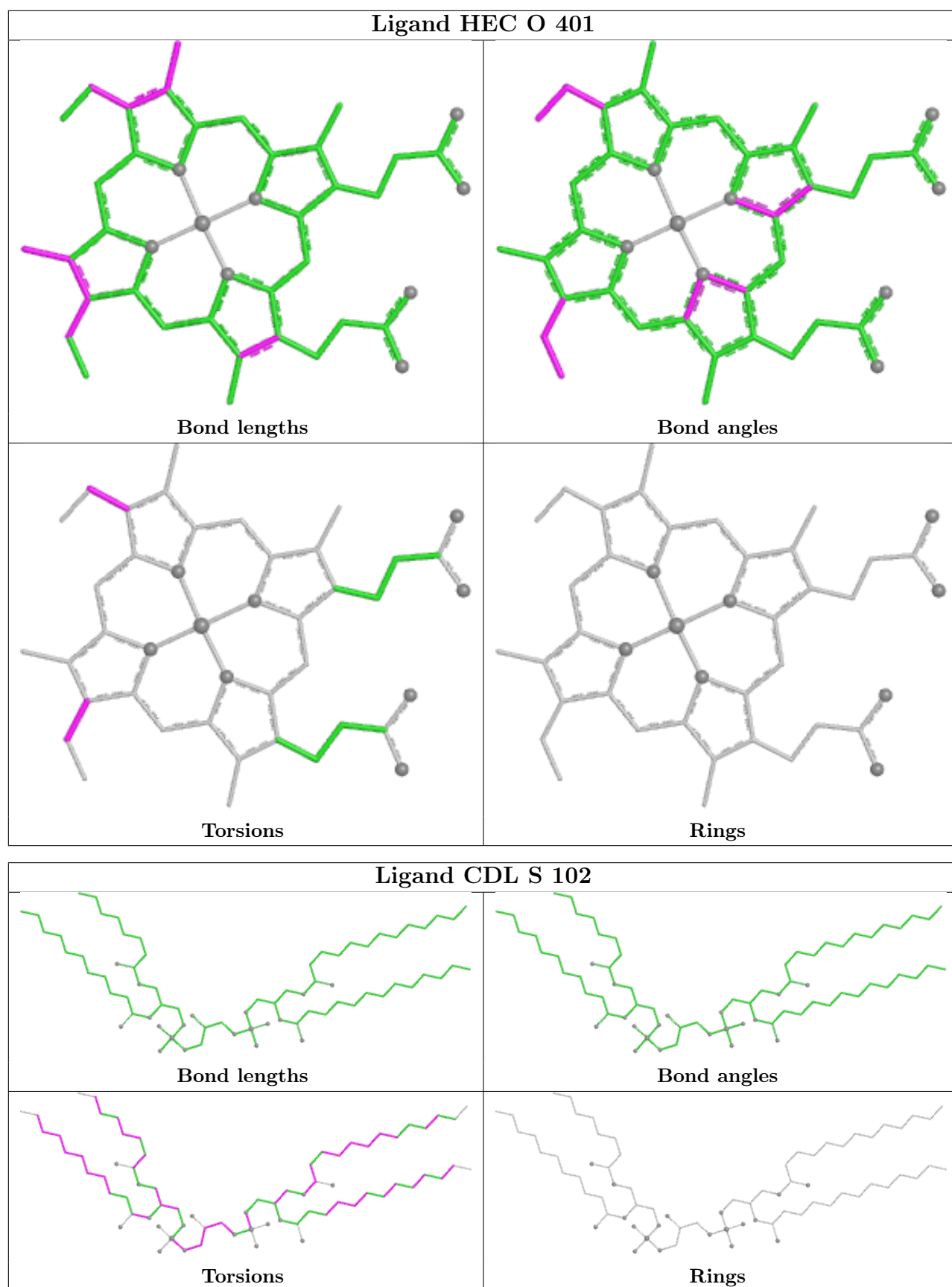


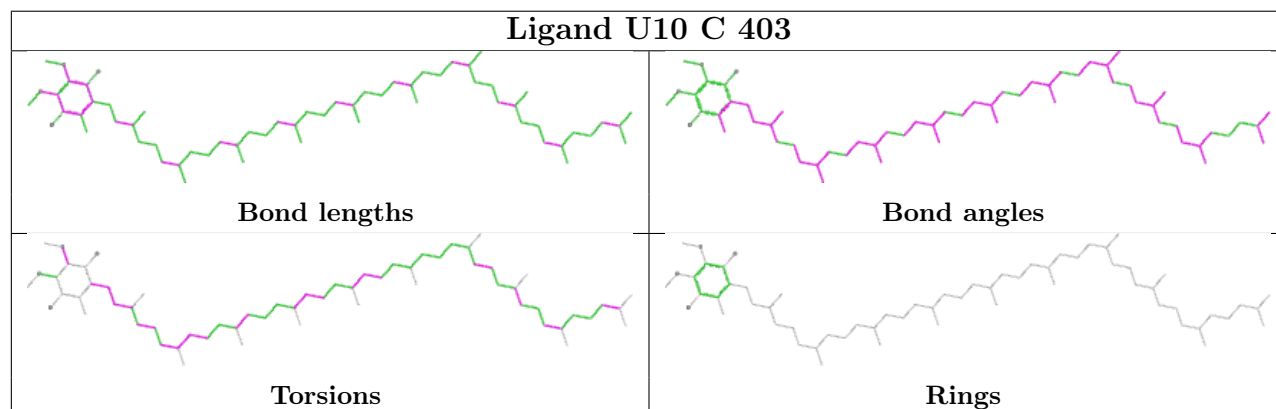
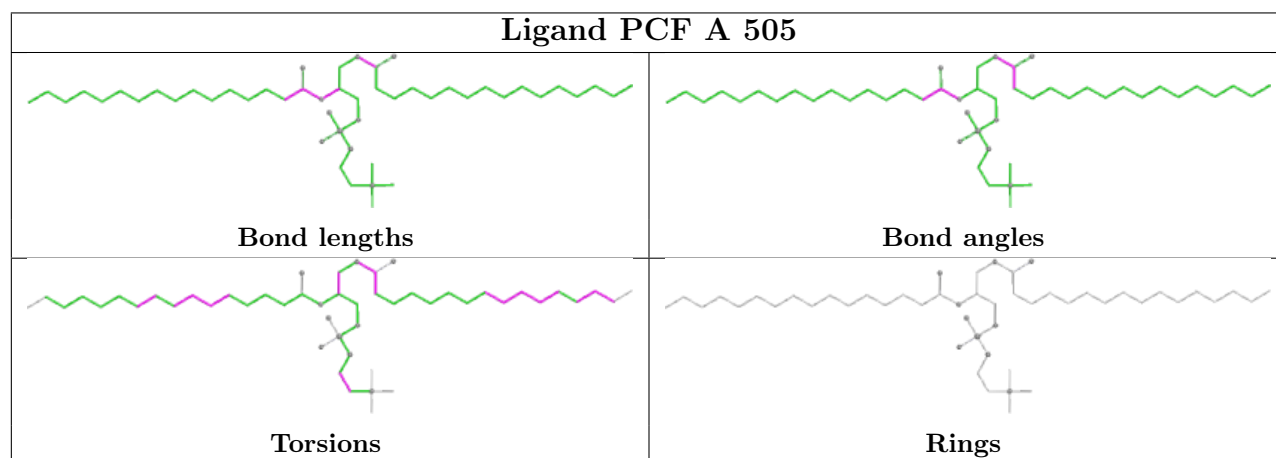
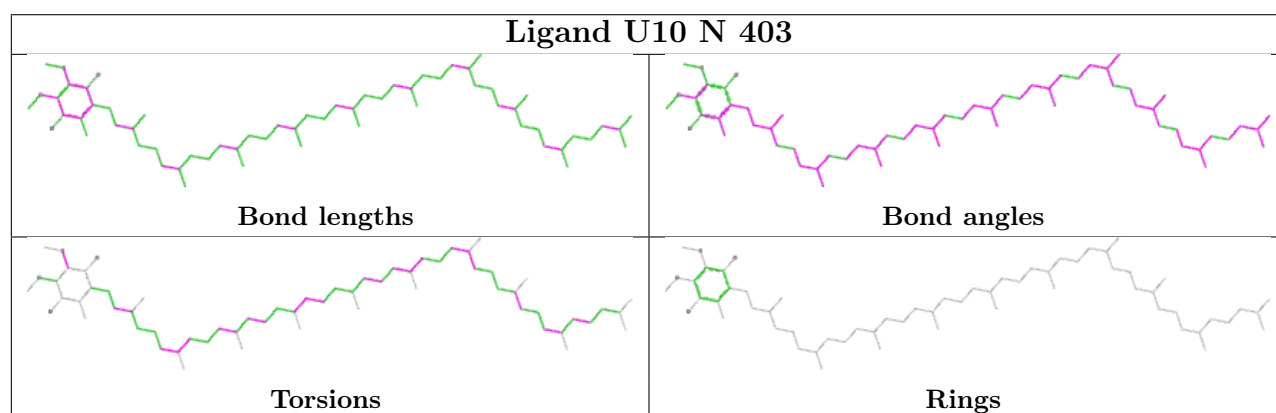
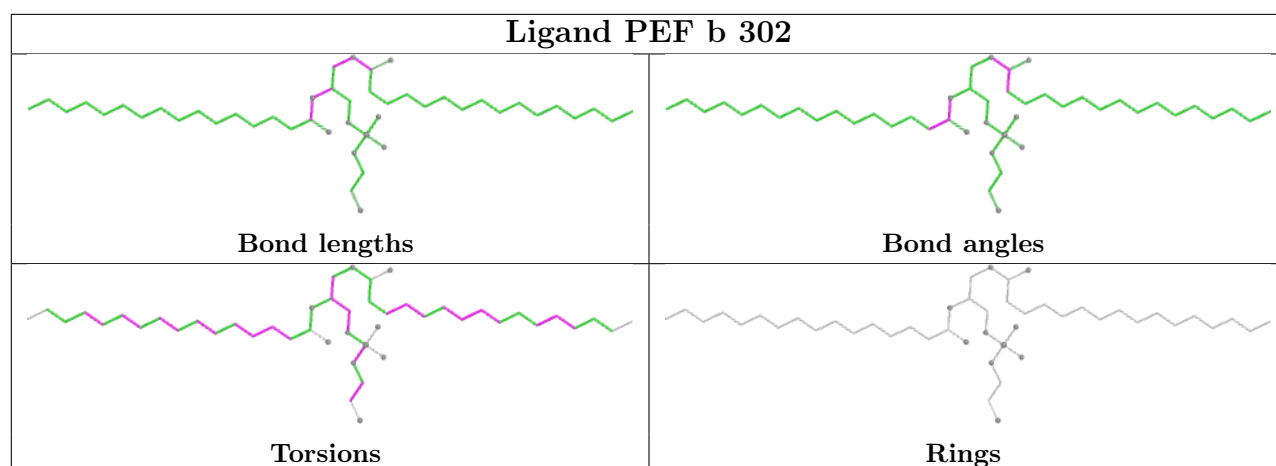


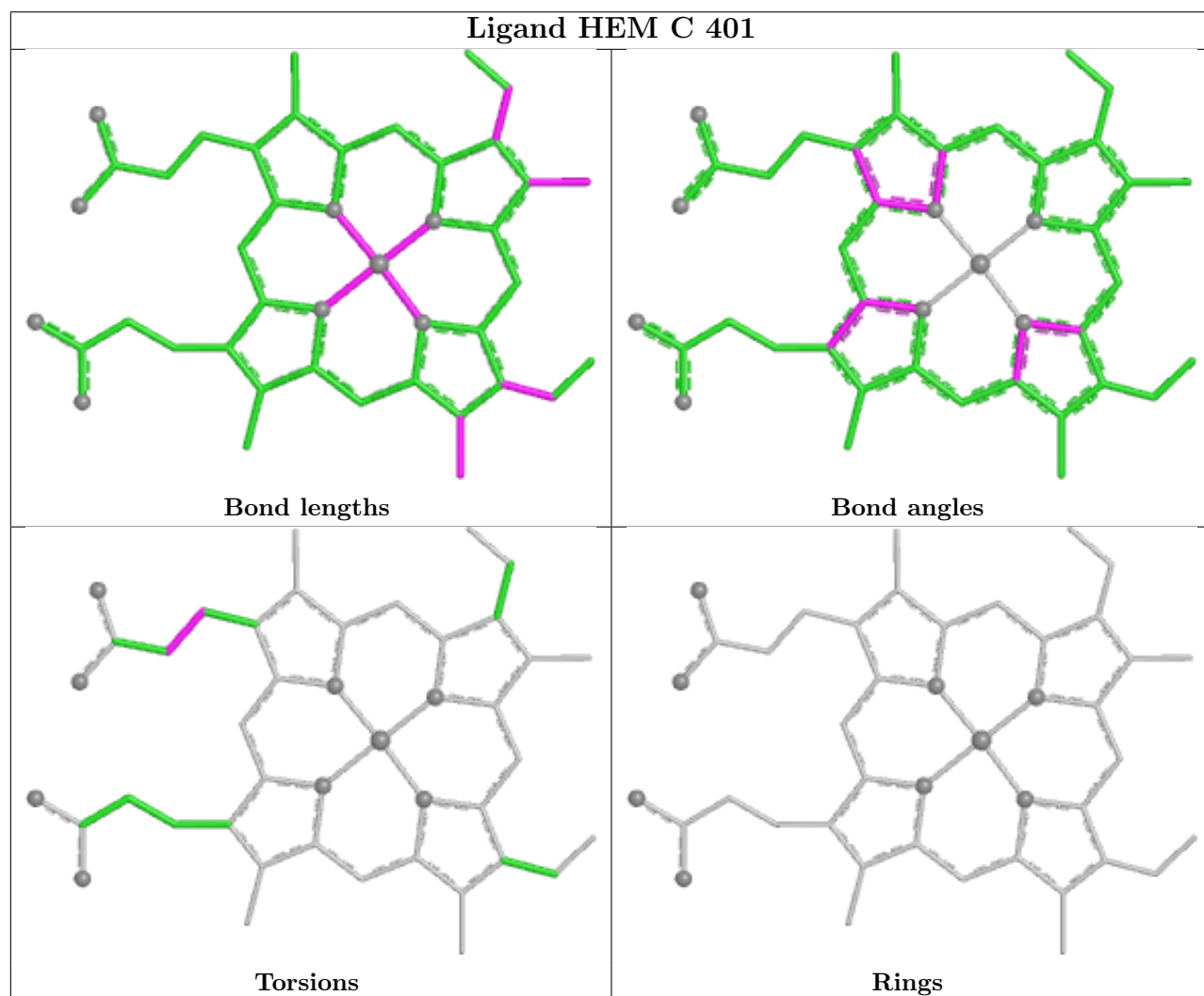
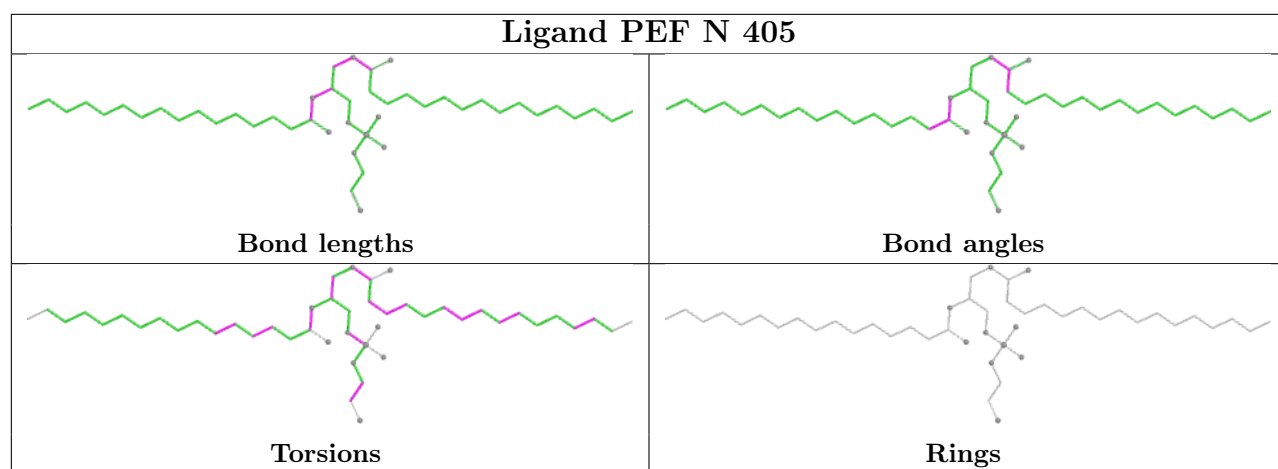


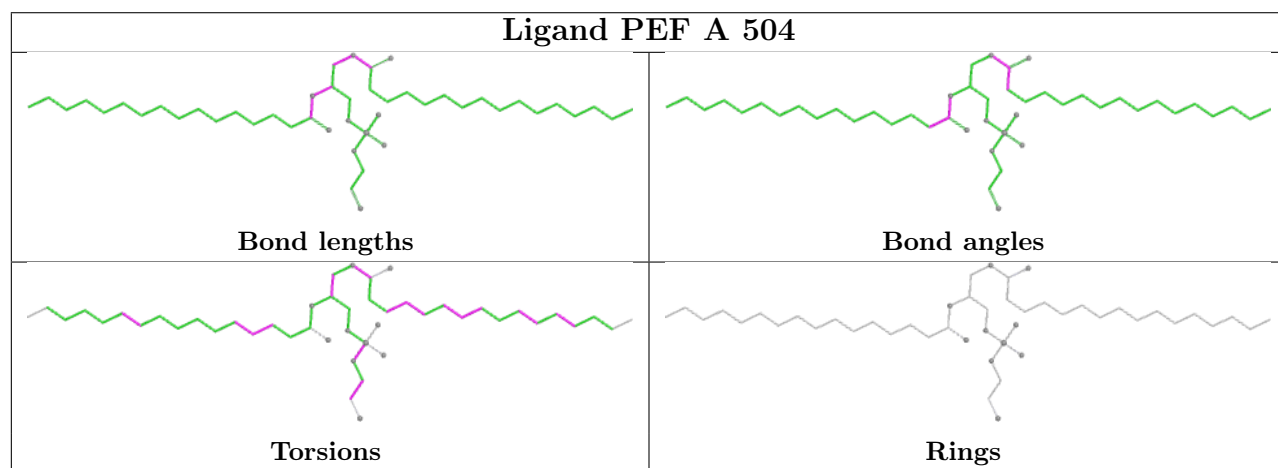
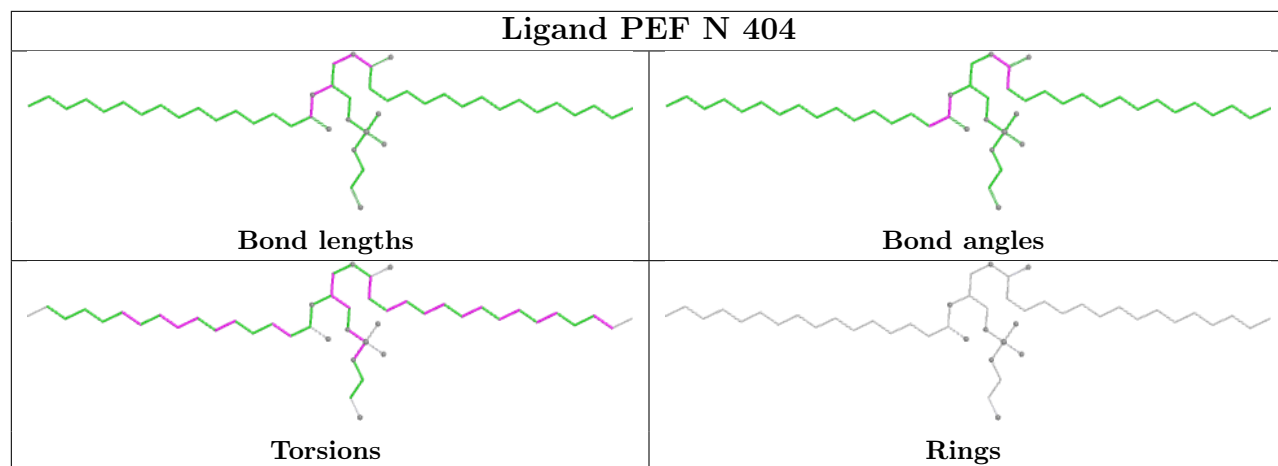


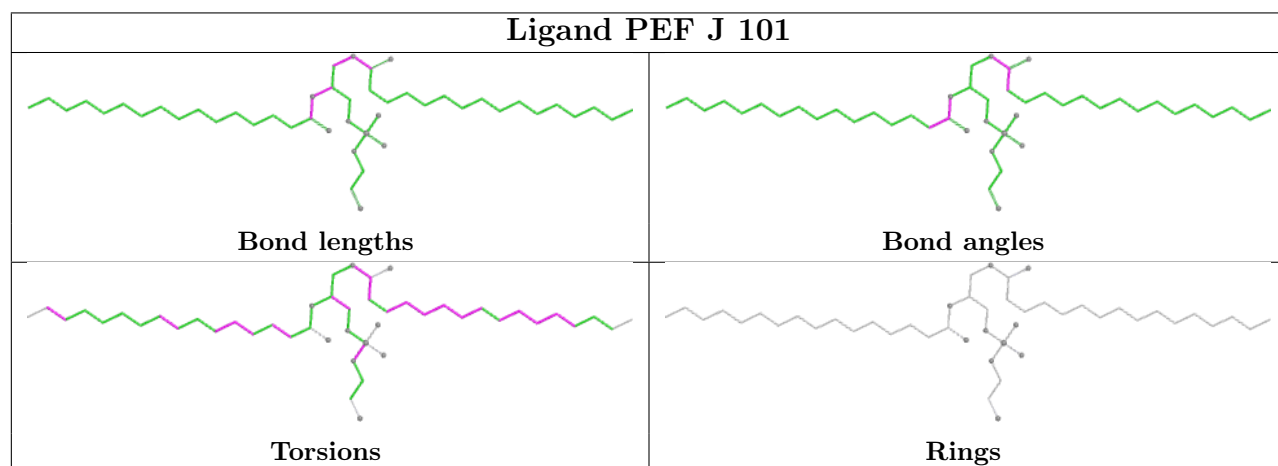
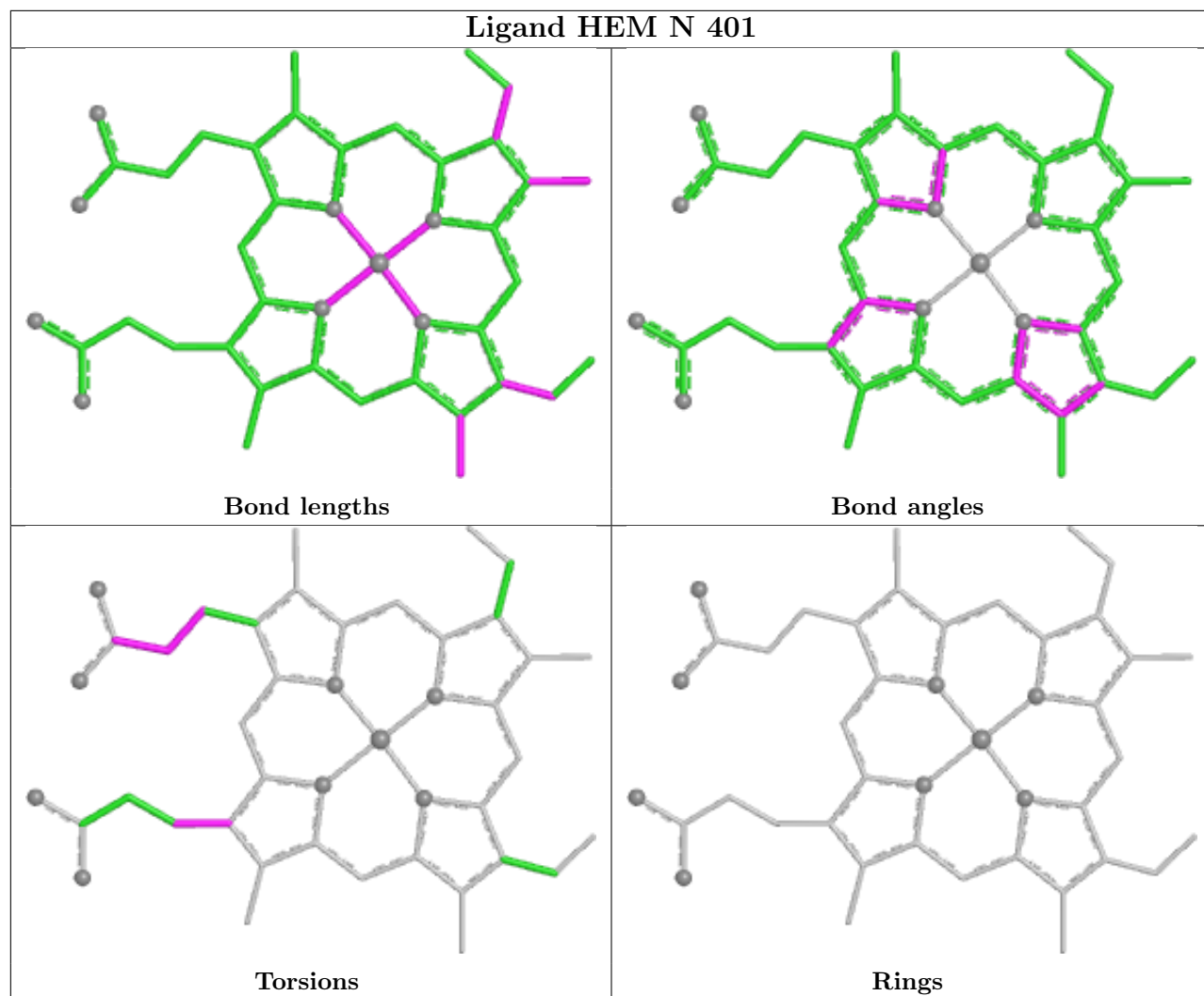




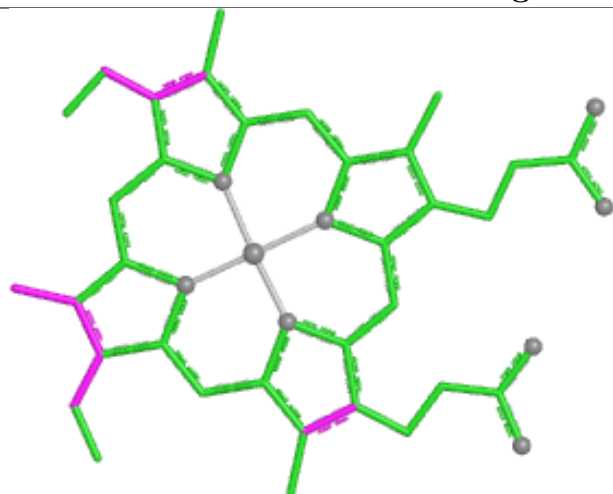




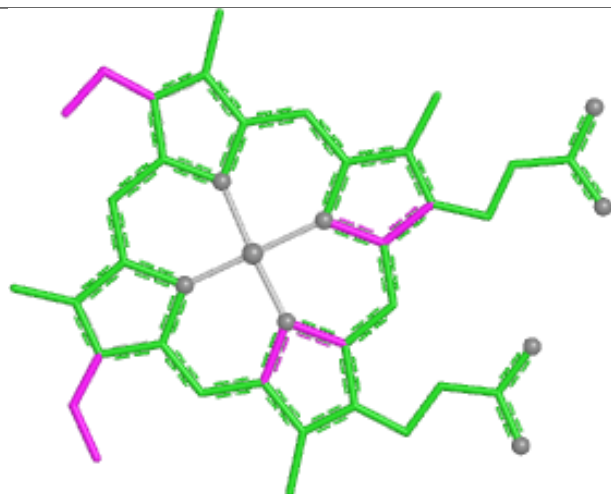




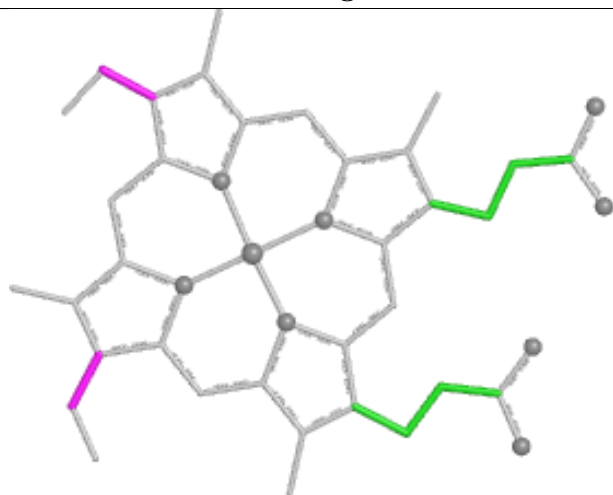
## Ligand HEC D 401



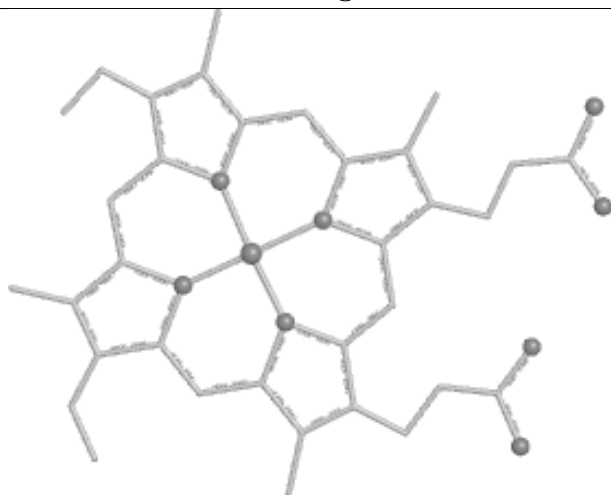
Bond lengths



Bond angles

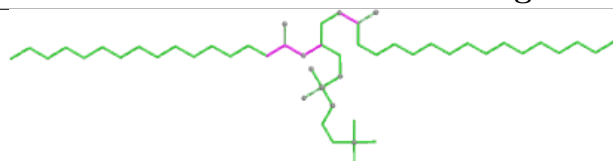


Torsions

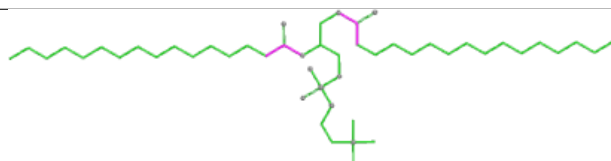


Rings

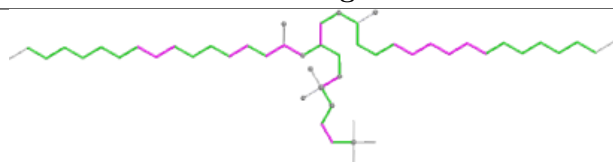
## Ligand PCF A 503



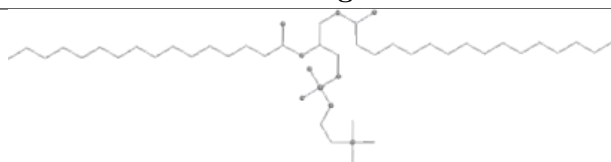
Bond lengths



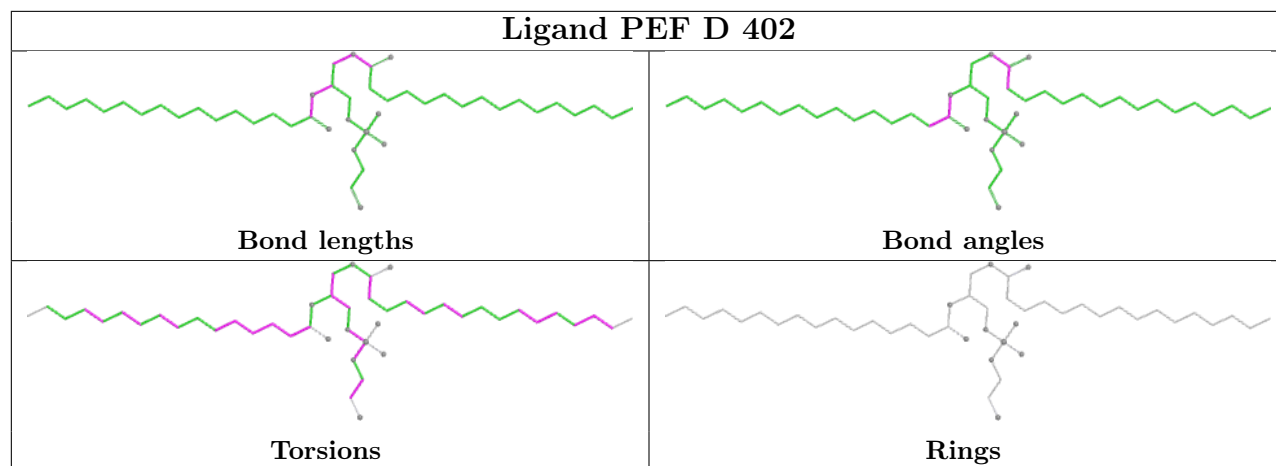
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

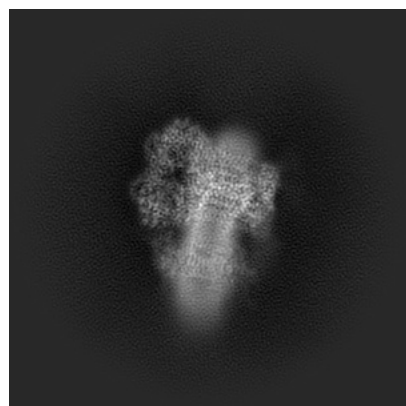
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18062. These allow visual inspection of the internal detail of the map and identification of artifacts.

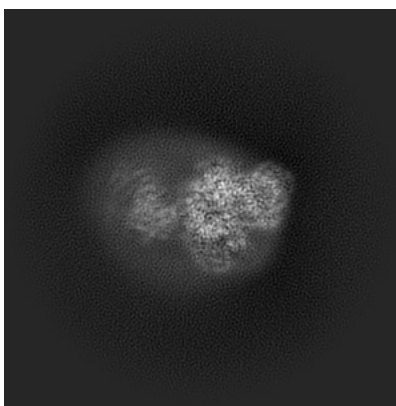
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

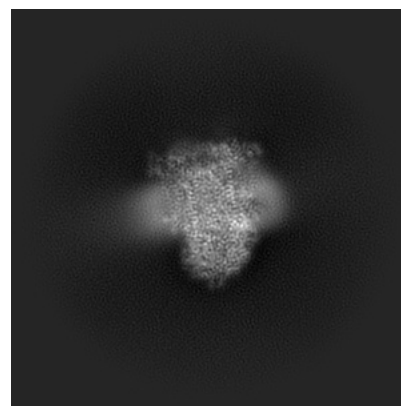
#### 6.1.1 Primary map



X

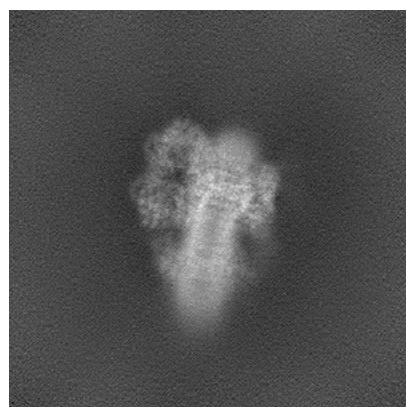


Y

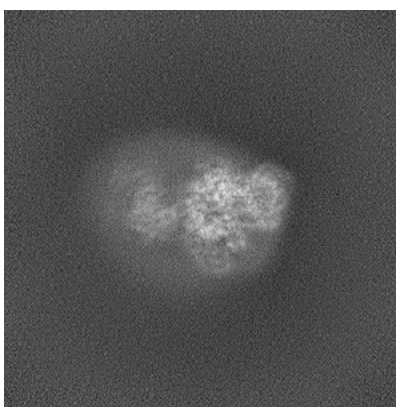


Z

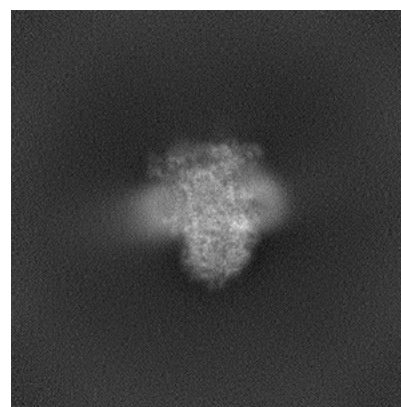
#### 6.1.2 Raw map



X



Y

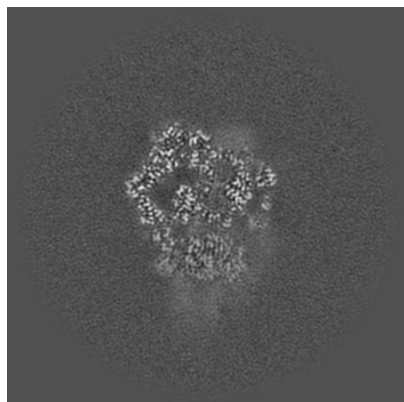


Z

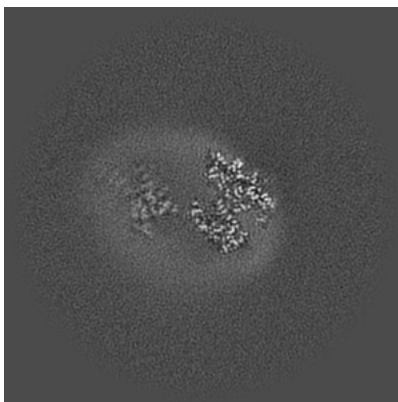
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

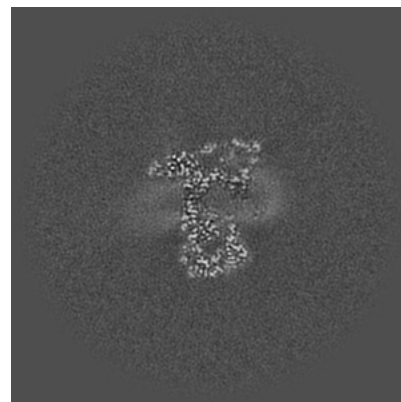
### 6.2.1 Primary map



X Index: 256

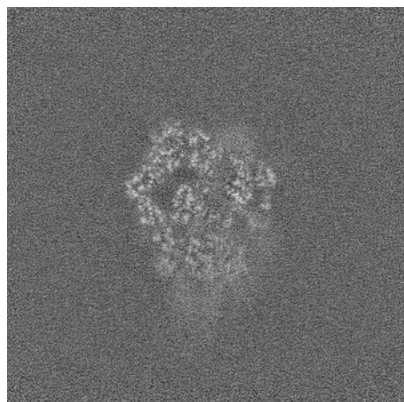


Y Index: 256

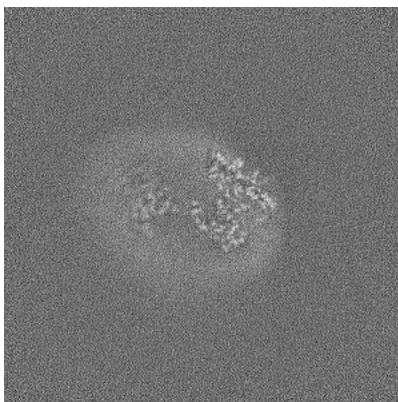


Z Index: 256

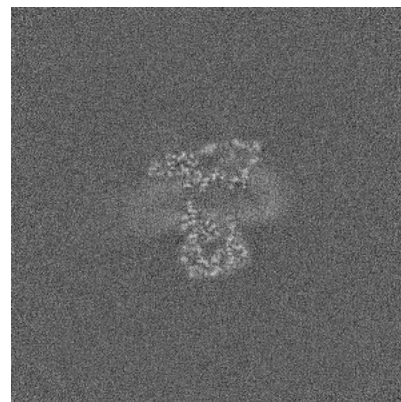
### 6.2.2 Raw map



X Index: 256



Y Index: 256

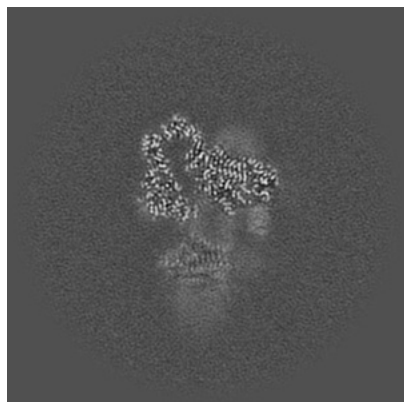


Z Index: 256

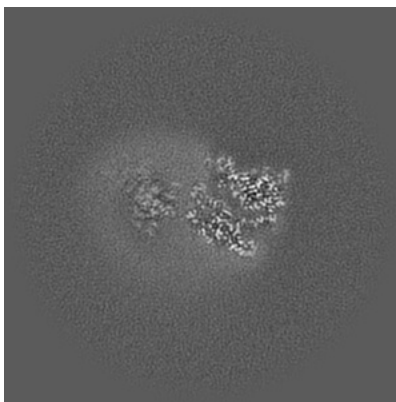
The images above show central slices of the map in three orthogonal directions.

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

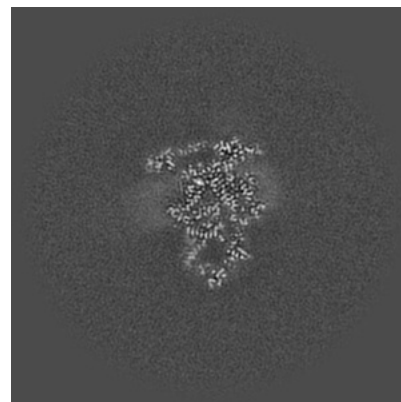
### 6.3.1 Primary map



X Index: 280

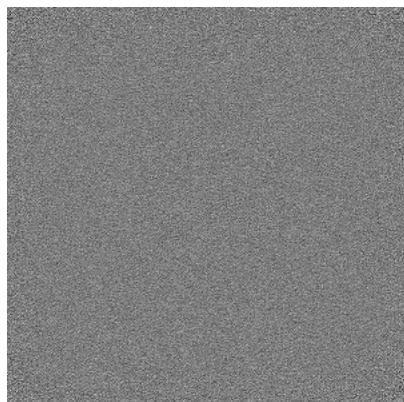


Y Index: 242

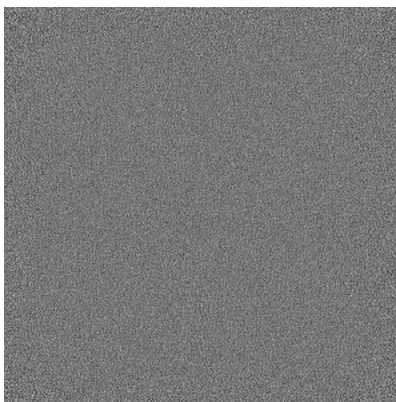


Z Index: 275

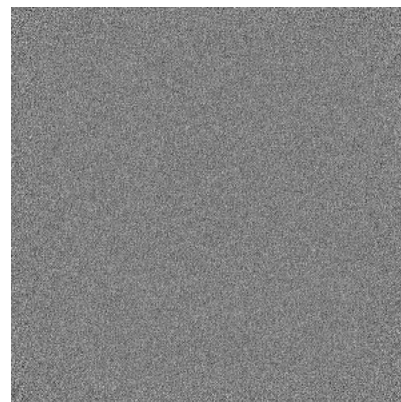
### 6.3.2 Raw map



X Index: 0



Y Index: 0

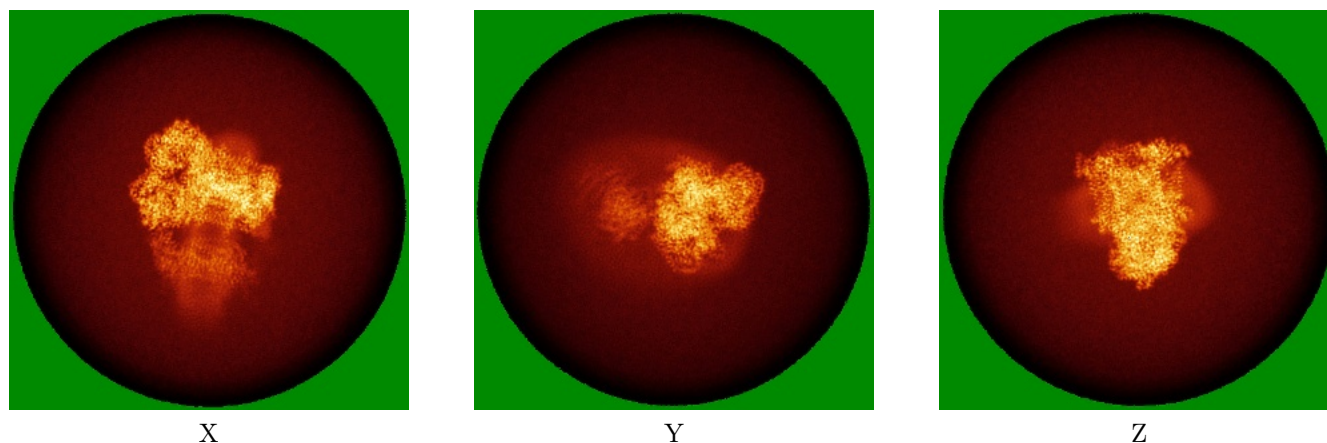


Z Index: 511

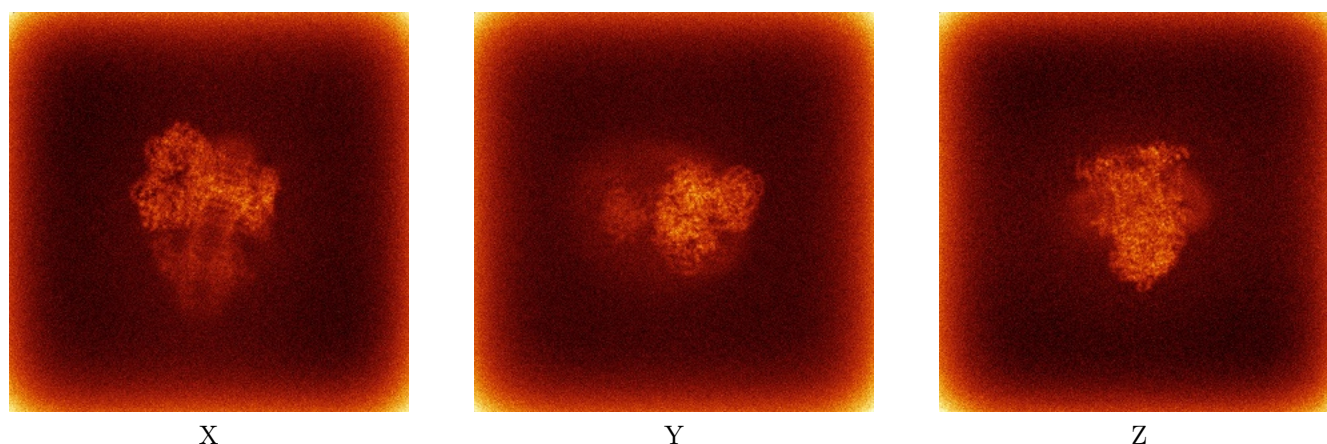
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

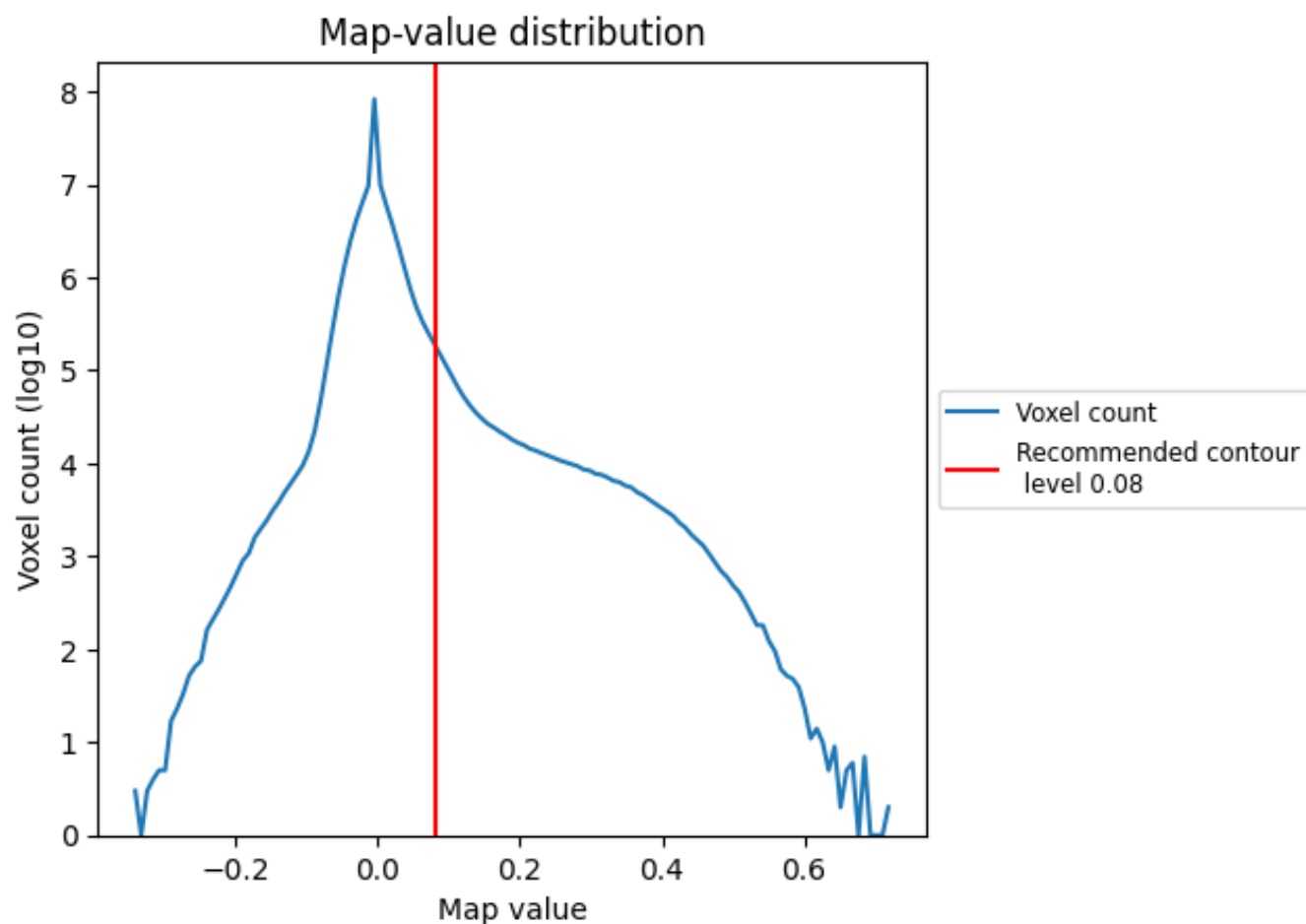
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

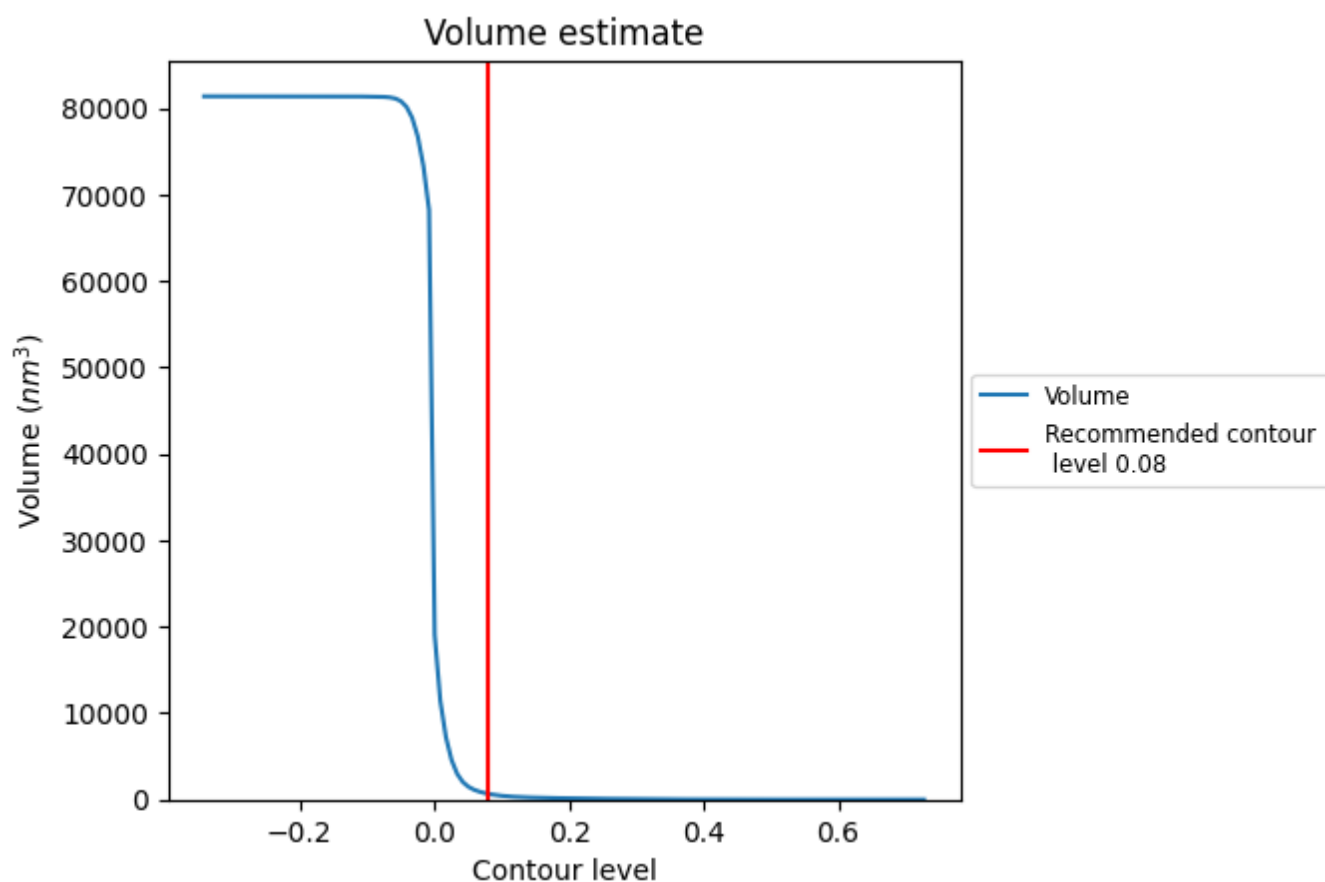
This section contains the results of statistical analysis of the map.

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



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

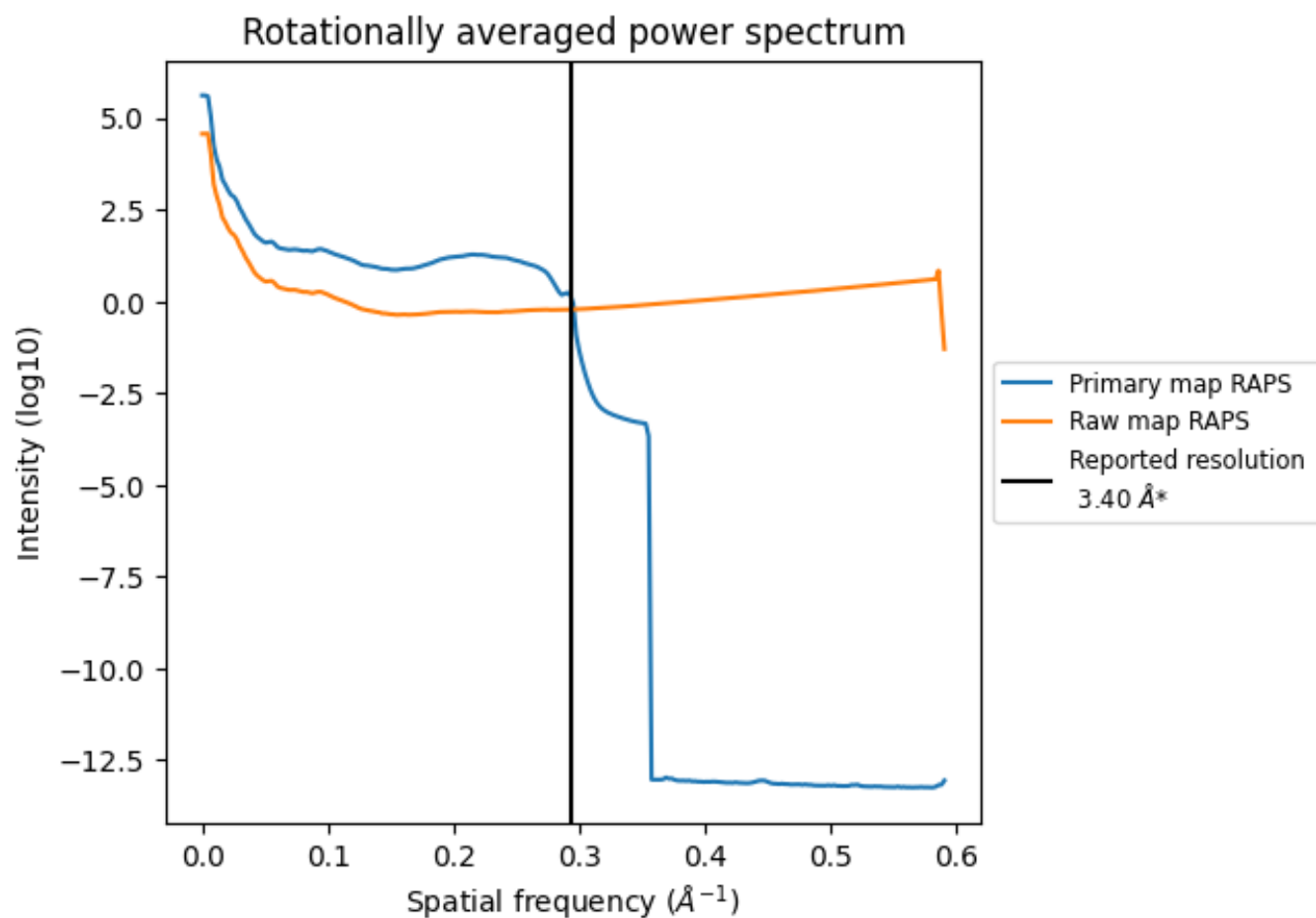
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 667  $\text{nm}^3$ ; this corresponds to an approximate mass of 602 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 ⓘ

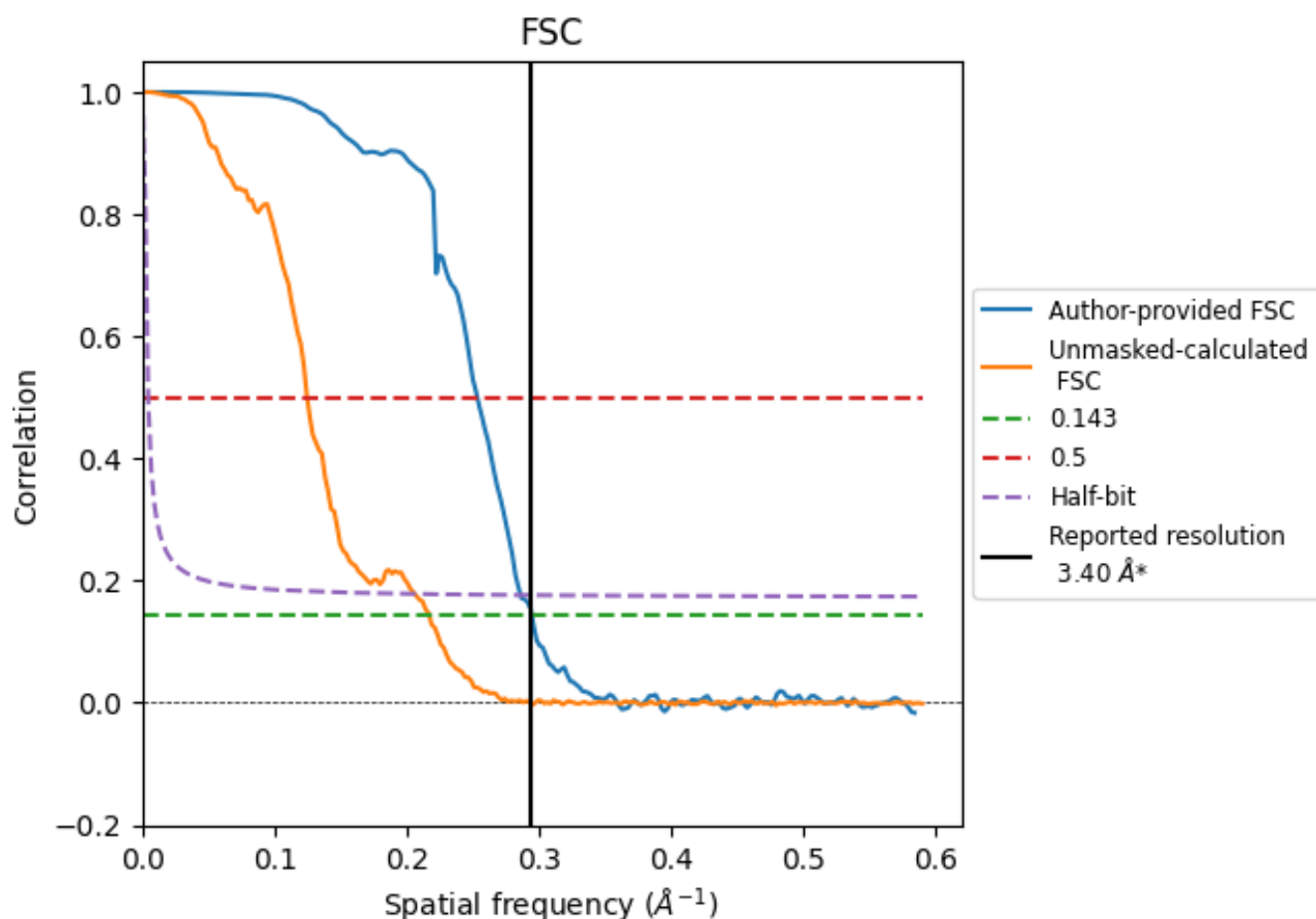


\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

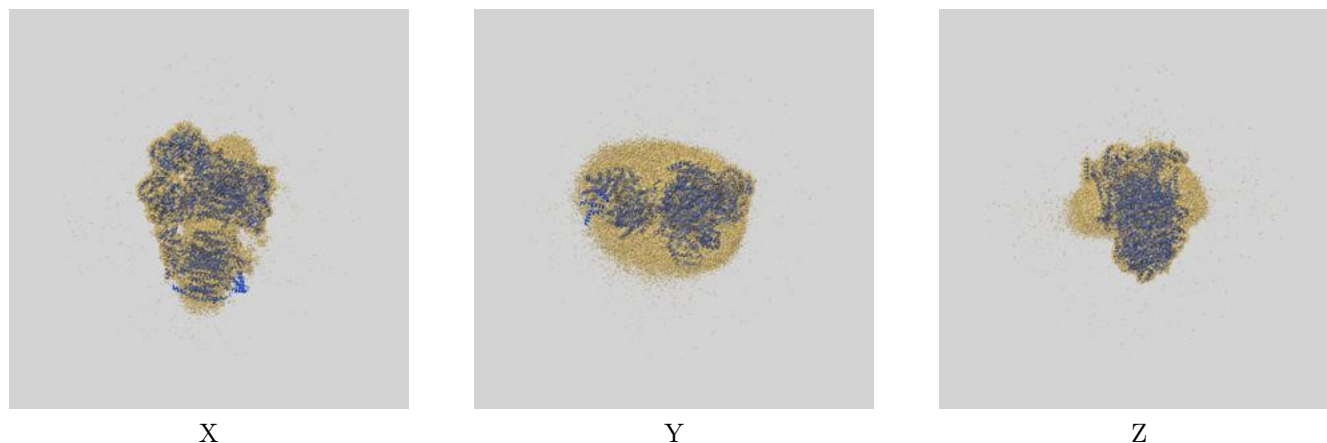
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.40                               | -    | -        |
| Author-provided FSC curve | 3.39                               | 3.94 | 3.49     |
| Unmasked-calculated*      | 4.60                               | 8.01 | 4.84     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.60 differs from the reported value 3.4 by more than 10 %

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

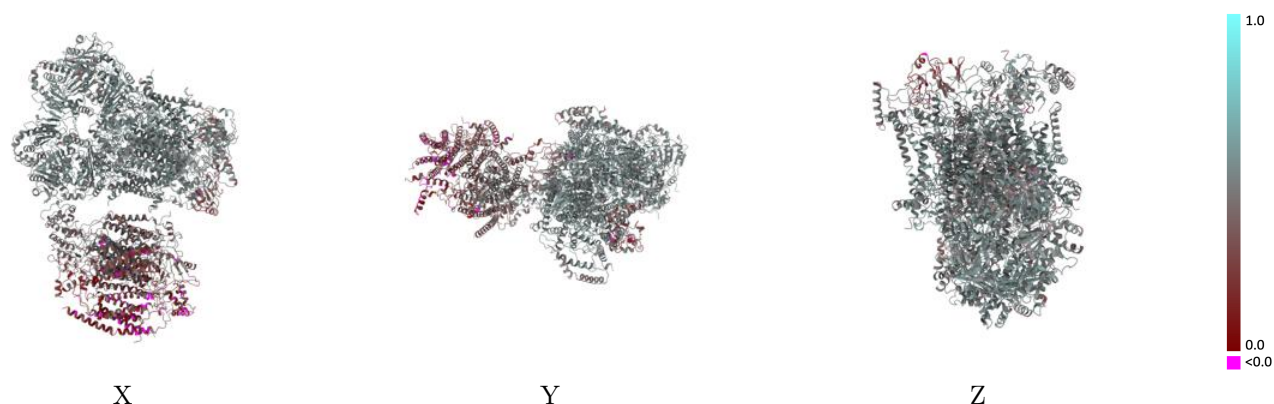
This section contains information regarding the fit between EMDB map EMD-18062 and PDB model 8Q1B. Per-residue inclusion information can be found in section [3](#) on page [17](#).

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



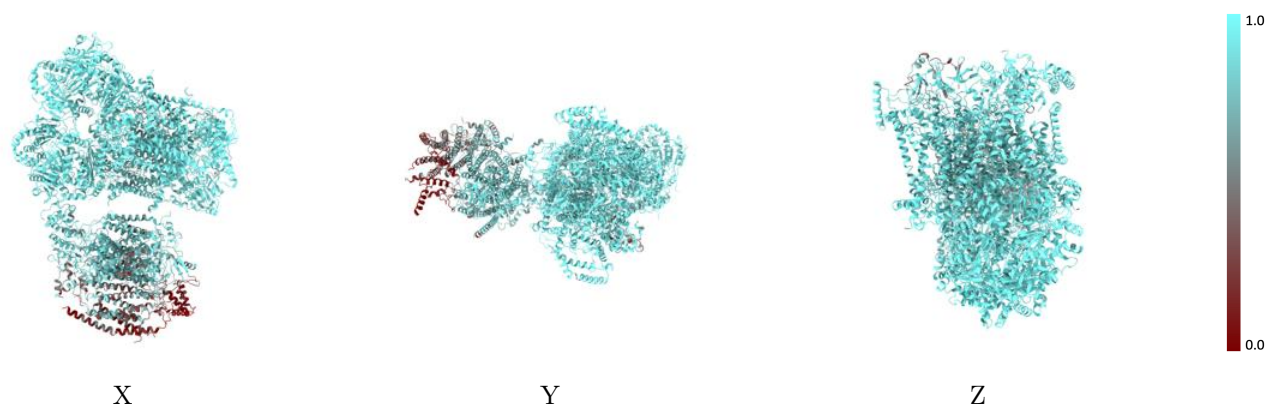
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



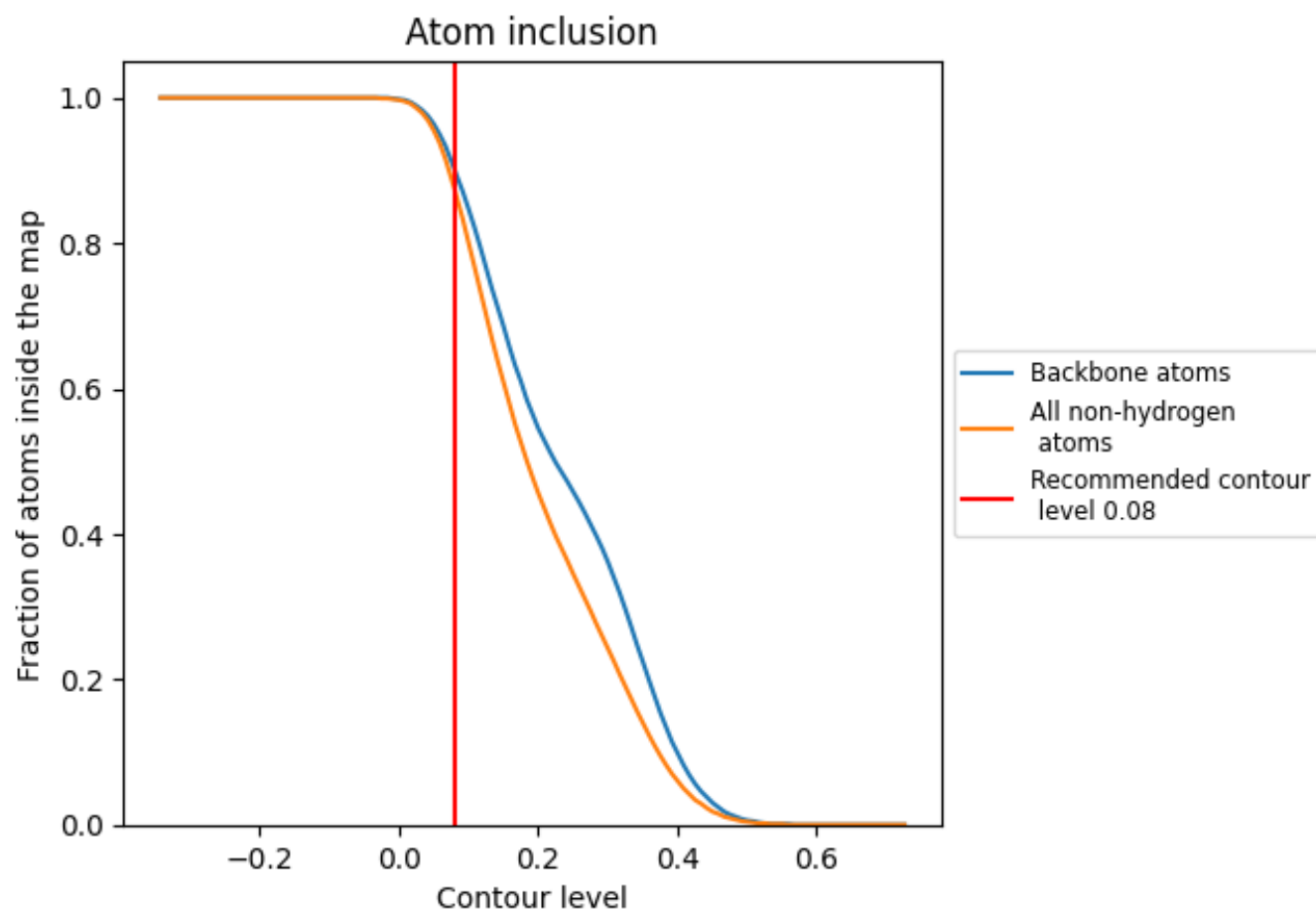
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.08) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8760   |  0.4600   |
| A     |  0.9660   |  0.5260   |
| B     |  0.9830   |  0.5310   |
| C     |  0.9570   |  0.5290   |
| D     |  0.9730   |  0.5290   |
| E     |  0.9000   |  0.3990   |
| F     |  0.9340   |  0.4650   |
| G     |  0.9680   |  0.5160   |
| H     |  0.9700   |  0.5360   |
| I     |  0.9440   |  0.5070   |
| J     |  0.9340   |  0.5040   |
| L     |  0.9670   |  0.5230   |
| M     |  0.9810   |  0.5330   |
| N     |  0.9460   |  0.5300   |
| O     |  0.9720  |  0.5360  |
| P     |  0.7930 |  0.3470 |
| Q     |  0.9420 |  0.4530 |
| R     |  0.9680 |  0.5280 |
| S     |  0.9800 |  0.5400 |
| T     |  0.9360 |  0.5040 |
| U     |  0.9490 |  0.4940 |
| a     |  0.8450 |  0.4010 |
| b     |  0.7870 |  0.3750 |
| c     |  0.5790 |  0.2470 |
| d     |  0.7080 |  0.3410 |
| e     |  0.9020 |  0.4490 |
| f     |  0.8810 |  0.3920 |
| g     |  0.6650 |  0.2740 |
| h     |  0.7820 |  0.3390 |
| i     |  0.7920 |  0.3760 |
| j     |  0.1370 |  0.2290 |
| k     |  0.2460 |  0.2410 |
| l     |  0.2720 |  0.1770 |
| m     |  0.0230 |  0.1830 |

