



## Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:16 AM EDT

PDB ID : 8UGF / pdb\_00008ugf  
EMDB ID : EMD-42223  
Title : In-situ complex III, state III  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-05  
Resolution : 3.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

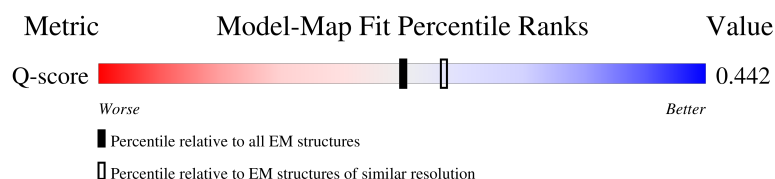
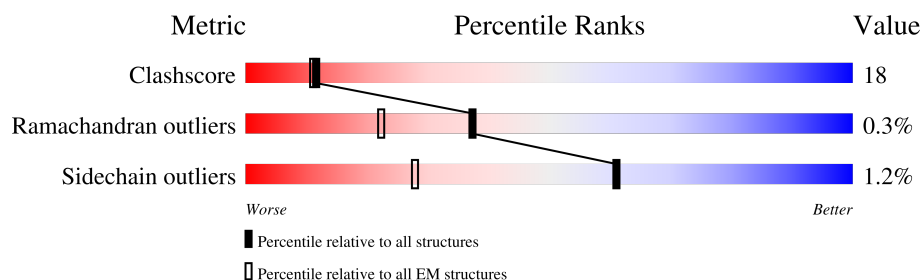
EMDB validation analysis : 0.0.1.dev133  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



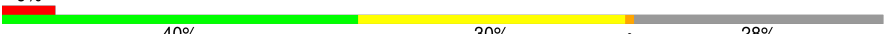
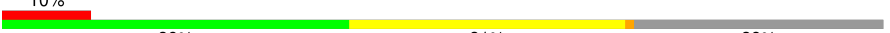
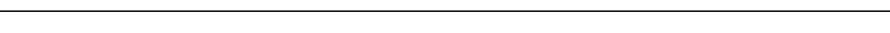
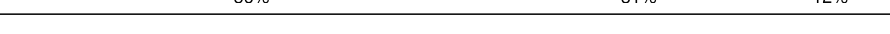
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 12797 ( 3.10 - 4.10 )                                    |

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   | 3A    | 480    |                  |
| 1   | 3N    | 480    |                  |
| 2   | 3B    | 453    |                  |
| 2   | 3O    | 453    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | 3C    | 379    |    |
| 3   | 3P    | 379    |    |
| 4   | 3D    | 325    |    |
| 4   | 3Q    | 325    |    |
| 5   | 3E    | 274    |    |
| 5   | 3I    | 274    |    |
| 5   | 3R    | 274    |    |
| 5   | 3V    | 274    |    |
| 6   | 3F    | 111    |    |
| 6   | 3S    | 111    |    |
| 7   | 3G    | 82     |    |
| 7   | 3T    | 82     |    |
| 8   | 3H    | 91     |  |
| 8   | 3U    | 91     |  |
| 9   | 3J    | 64     |  |
| 9   | 3W    | 64     |  |
| 10  | 3X    | 56     |  |
| 10  | 3Y    | 56     |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15  | HEC  | 3D    | 501 | X         | -        | -       | -                |
| 15  | HEC  | 3Q    | 501 | X         | -        | -       | -                |
| 16  | FES  | 3E    | 301 | -         | -        | X       | -                |

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 33551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 3A    | 440      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3411  | 2131 | 599 | 662 | 19 |         |       |
| 1   | 3N    | 445      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3424  | 2162 | 606 | 637 | 19 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 3B    | 418      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3138  | 1965 | 555 | 610 | 8 |         |       |
| 2   | 3O    | 417      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3124  | 1960 | 554 | 602 | 8 |         |       |

- Molecule 3 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 3C    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3025  | 2031 | 471 | 502 | 21 |         |       |
| 3   | 3P    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3024  | 2031 | 471 | 501 | 21 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 3D    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1888  | 1205 | 325 | 342 | 16 |         |       |
| 4   | 3Q    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1904  | 1215 | 327 | 346 | 16 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 3E    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 955 | 265 | 291 | 7 |         |       |
| 5   | 3I    | 47       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 337   | 210 | 62  | 64  | 1 |         |       |
| 5   | 3R    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 955 | 265 | 291 | 7 |         |       |
| 5   | 3V    | 31       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 223   | 137 | 45  | 40  | 1 |         |       |

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | 3F    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 557 | 152 | 157 | 2 |         |       |
| 6   | 3S    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 557 | 152 | 157 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 7   | 3G    | 74       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 628   | 411 | 116 | 99 | 2 |         |       |
| 7   | 3T    | 74       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 628   | 411 | 116 | 99 | 2 |         |       |

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 8   | 3H    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 533   | 325 | 97 | 106 | 5 |         |       |
| 8   | 3U    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 533   | 325 | 97 | 106 | 5 |         |       |

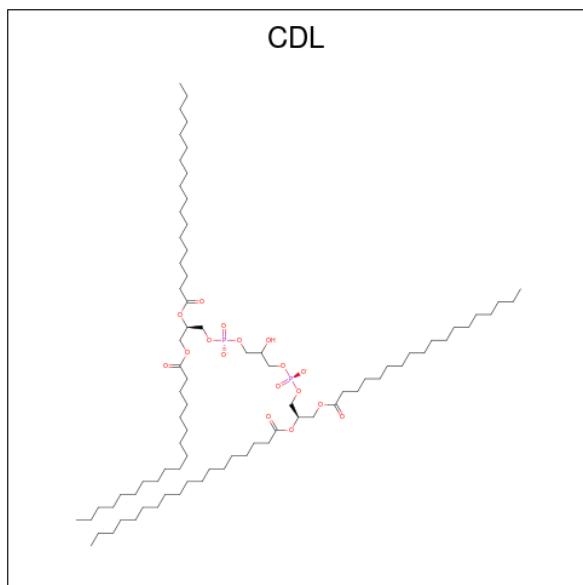
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | 3J    | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 464   | 305 | 82 | 77 |         |       |
| 9   | 3W    | 56       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 464   | 305 | 82 | 77 |         |       |

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

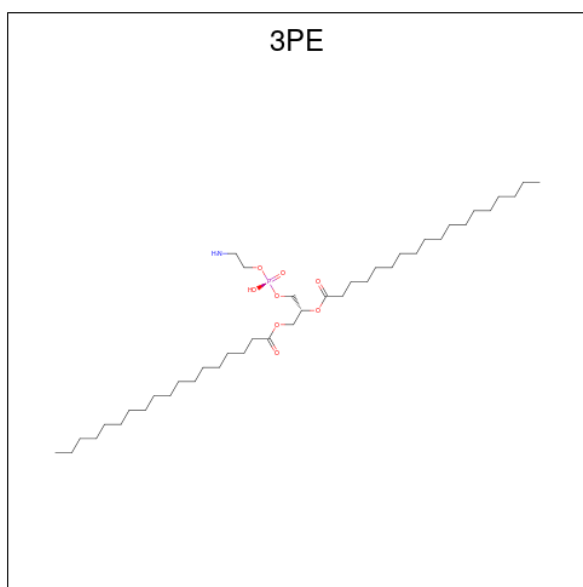
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | 3X    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 286 | 75 | 66 | 2 |         |       |
| 10  | 3Y    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 421   | 281 | 74 | 65 | 1 |         |       |

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



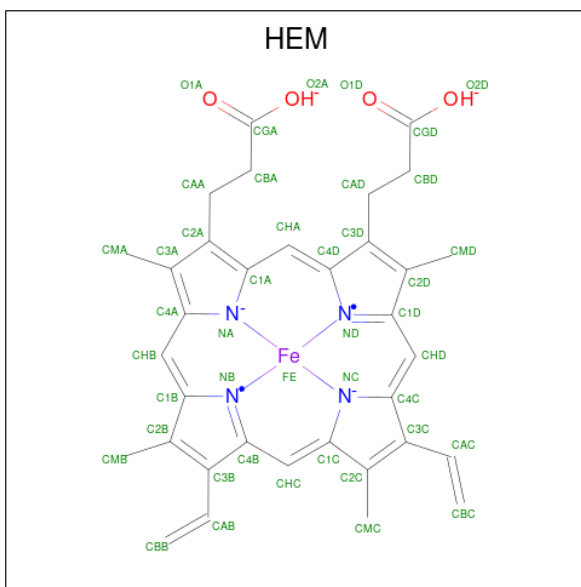
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 11  | 3A    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 58    | 39 | 17 | 2 |         |
| 11  | 3C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 52    | 33 | 17 | 2 |         |
| 11  | 3G    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 56    | 37 | 17 | 2 |         |
| 11  | 3N    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 24 | 17 | 2 |         |
| 11  | 3T    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 11  | 3T    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 56    | 37 | 17 | 2 |         |

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



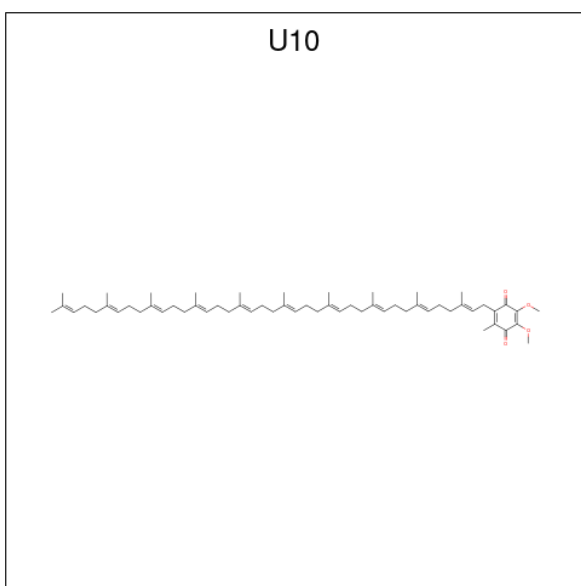
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 12  | 3A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 27    | 17 | 1 | 8 | 1 |         |
| 12  | 3A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 12  | 3C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 12  | 3C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 34    | 24 | 1 | 8 | 1 |         |
| 12  | 3E    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 12  | 3G    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 12  | 3N    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 12  | 3N    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 25    | 15 | 1 | 8 | 1 |         |
| 12  | 3P    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 12  | 3R    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 12  | 3Y    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



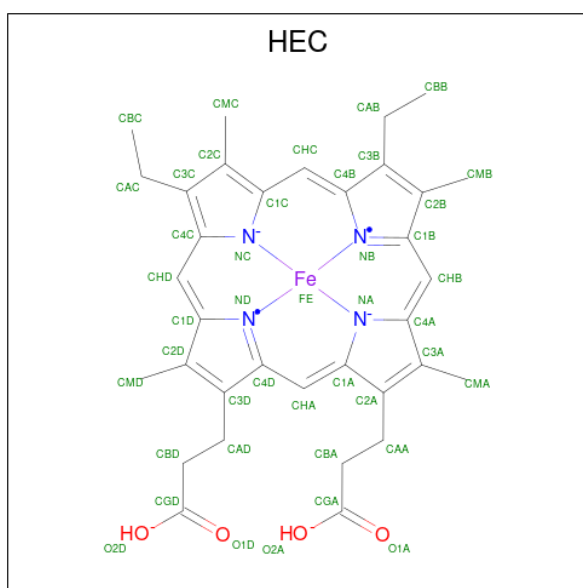
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 13  | 3C    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 13  | 3C    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 13  | 3P    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 13  | 3P    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 14 is UBIQUINONE-10 (CCD ID: U10) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



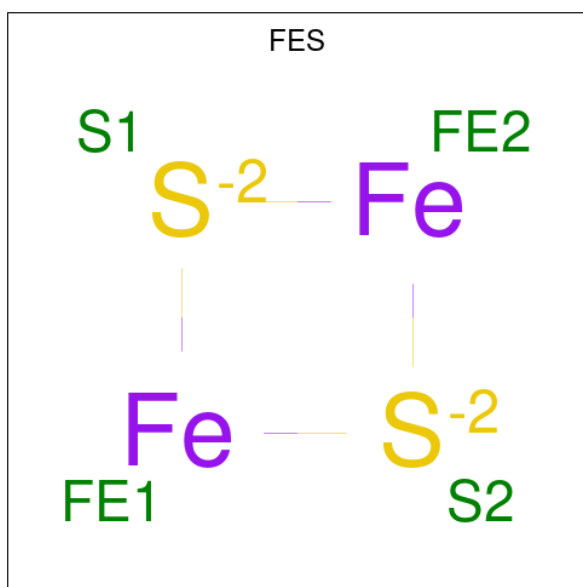
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 14  | 3C    | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 24 | 4 |         |
| 14  | 3C    | 1        | Total | C  | O | 0       |
|     |       |          | 23    | 19 | 4 |         |
| 14  | 3P    | 1        | Total | C  | O | 0       |
|     |       |          | 32    | 28 | 4 |         |
| 14  | 3P    | 1        | Total | C  | O | 0       |
|     |       |          | 32    | 28 | 4 |         |

- Molecule 15 is HEME C (CCD ID: HEC) (formula:  $C_{34}H_{36}FeN_4O_4$ ).



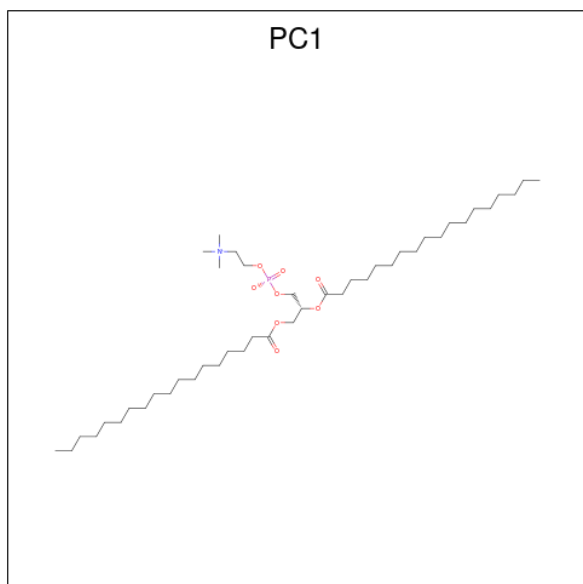
| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 15  | 3D    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 15  | 3Q    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $Fe_2S_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | 3E    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 16  | 3R    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 17  | 3E    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |

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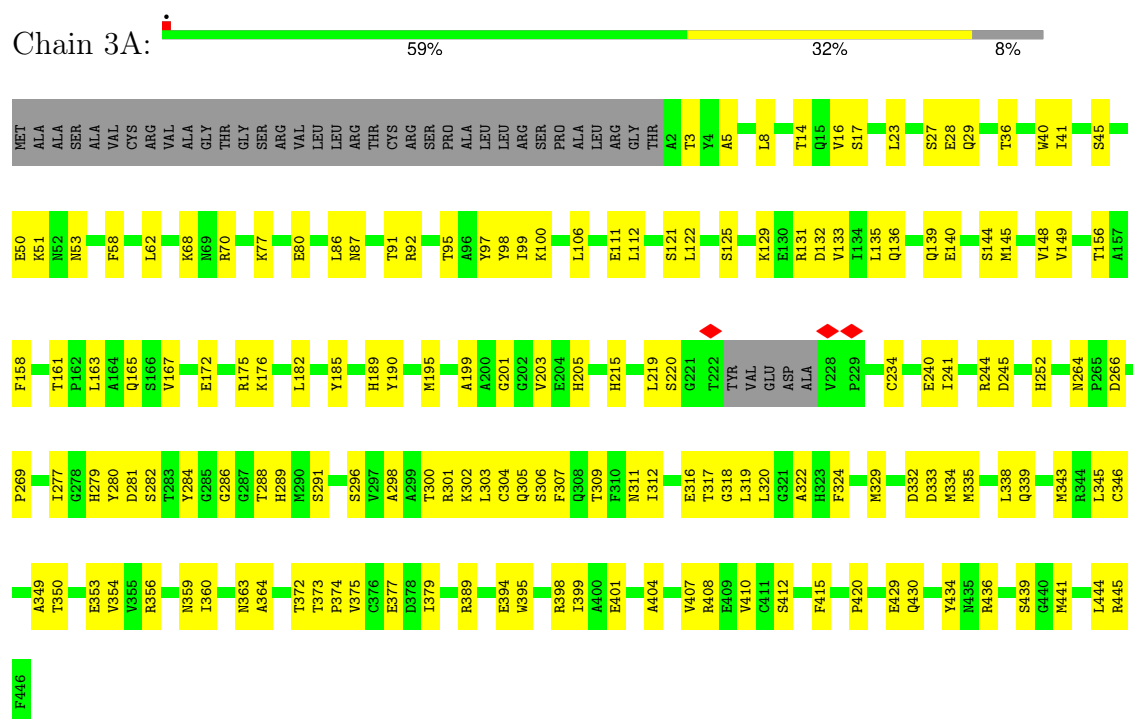
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 17  | 3R    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 17  | 3X    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |

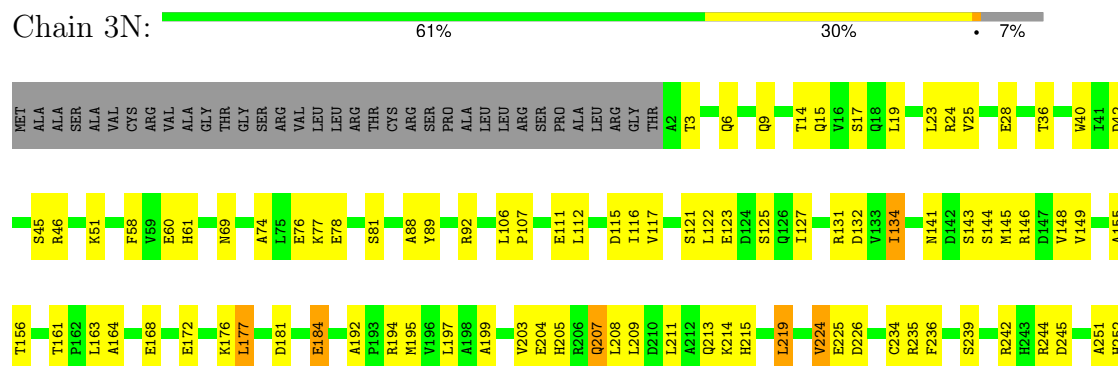
### 3 Residue-property plots

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

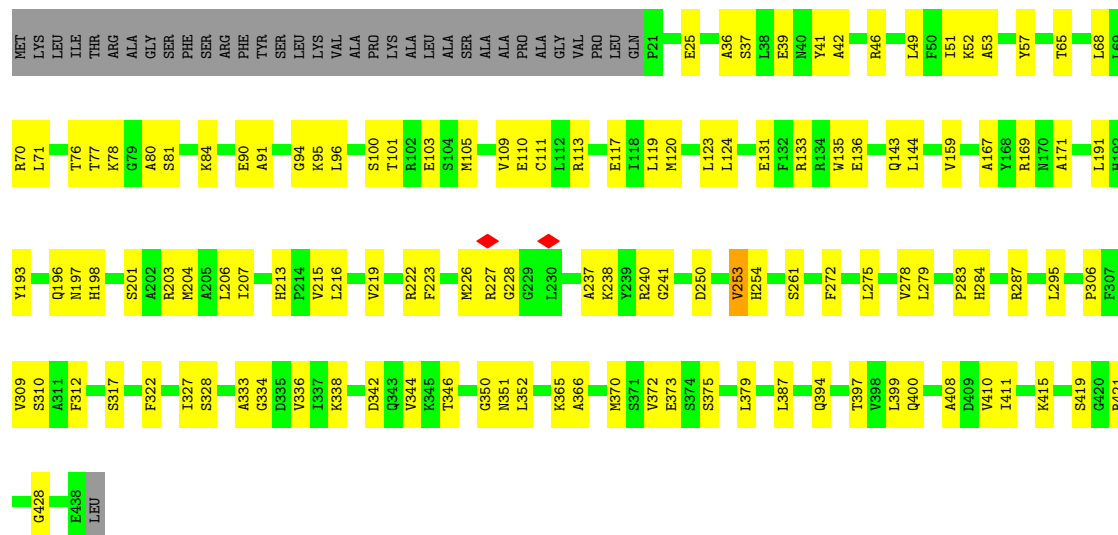
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



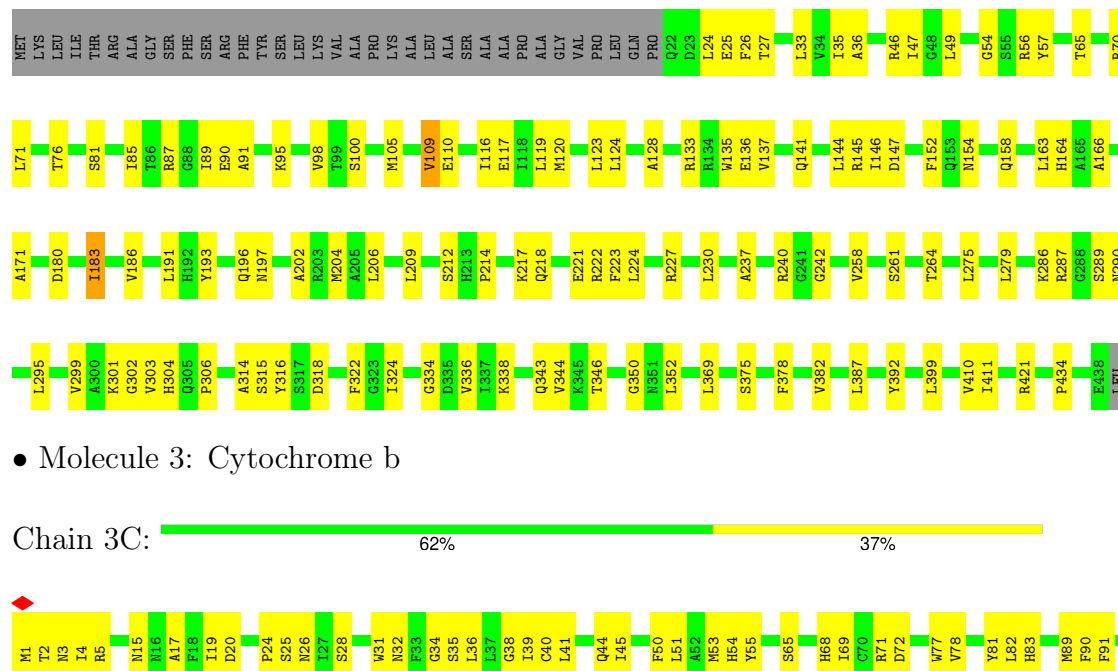
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

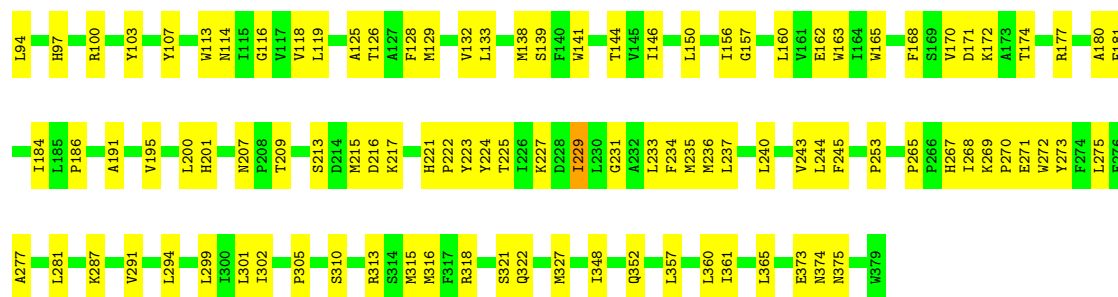


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



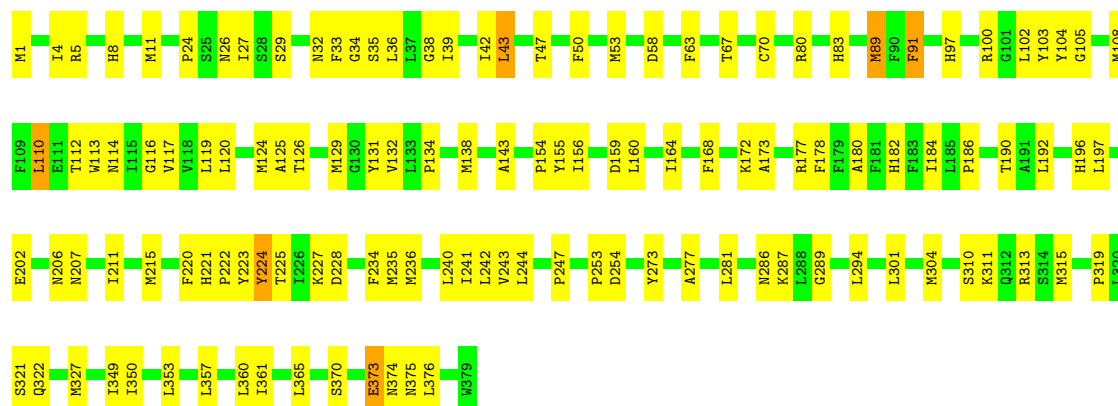
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





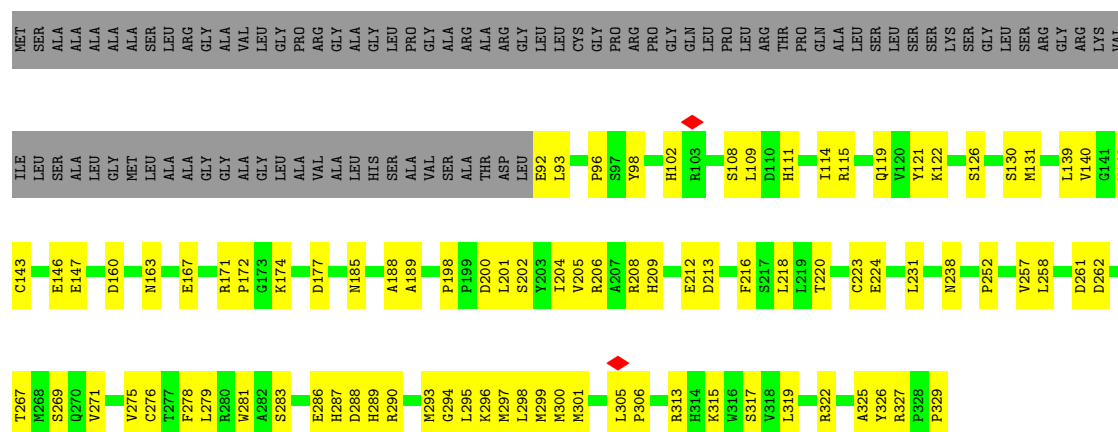
• Molecule 3: Cytochrome b

Chain 3P: 67% 31%



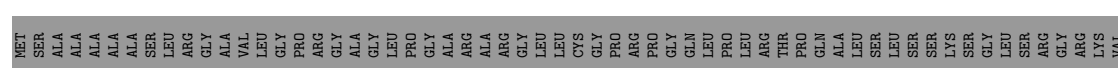
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

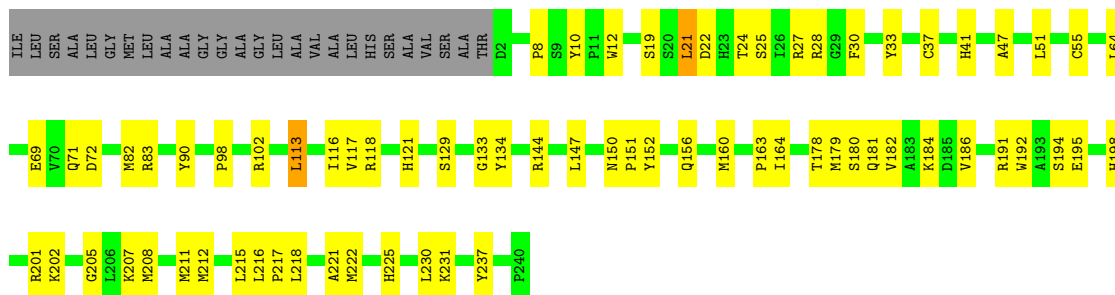
Chain 3D: 46% 27% 27%



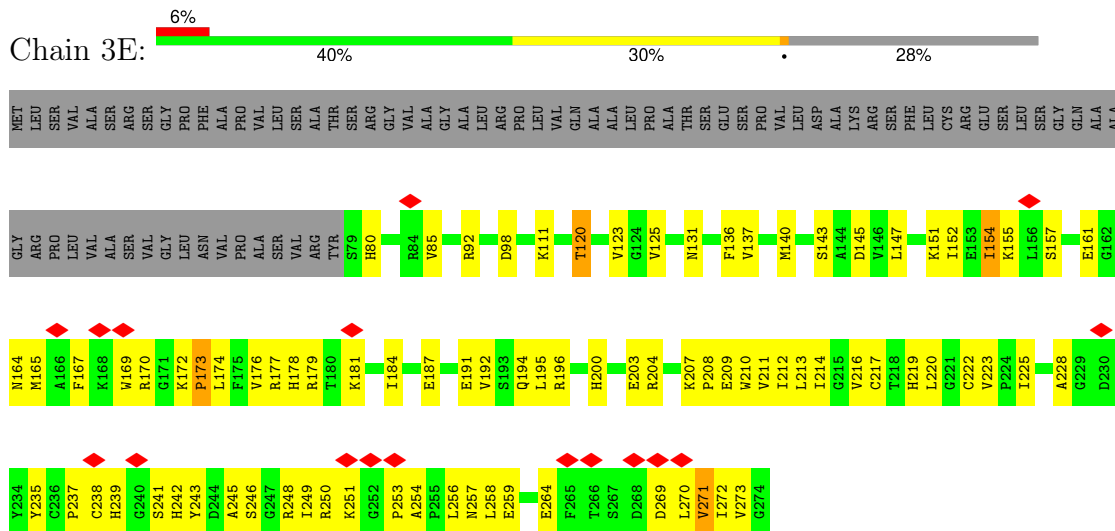
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain 3Q: 51% 22% 26%

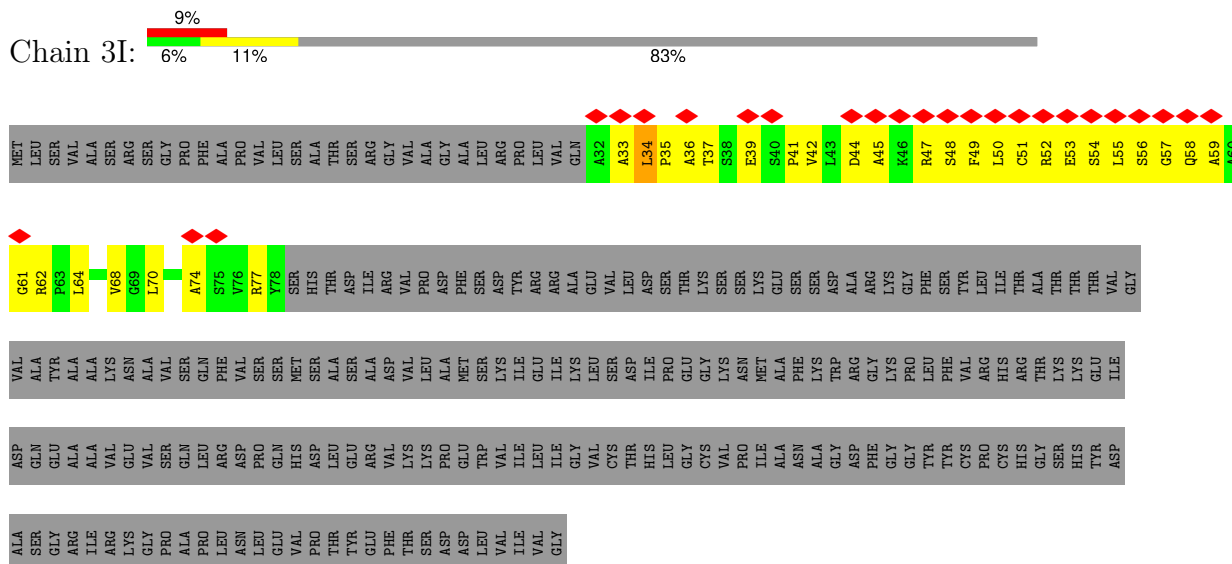




- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

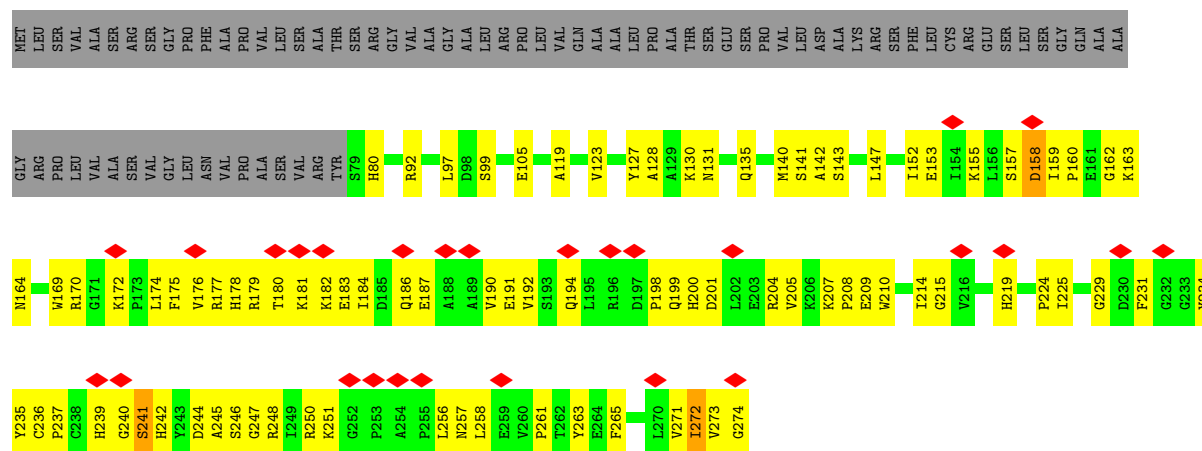


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

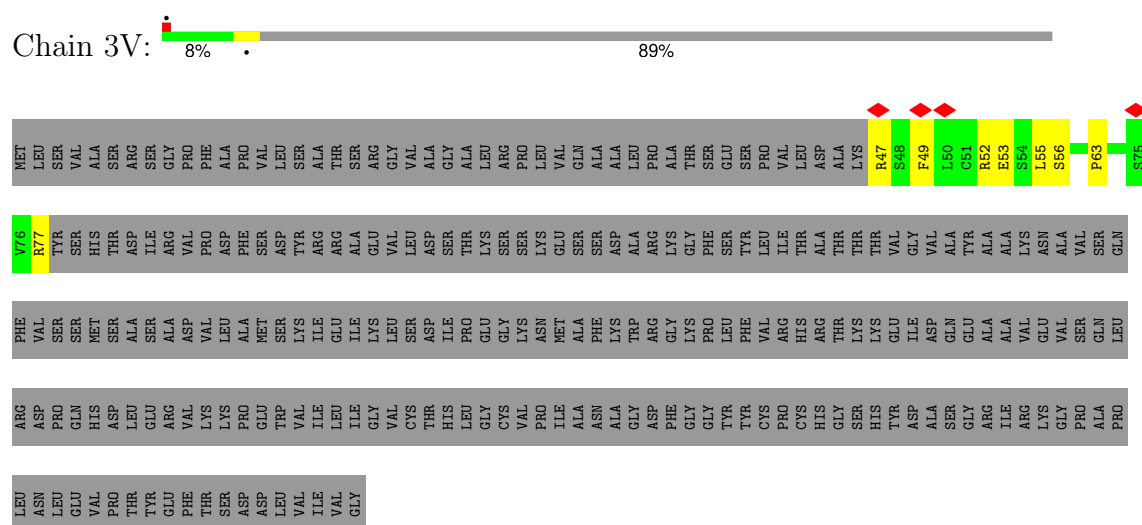


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

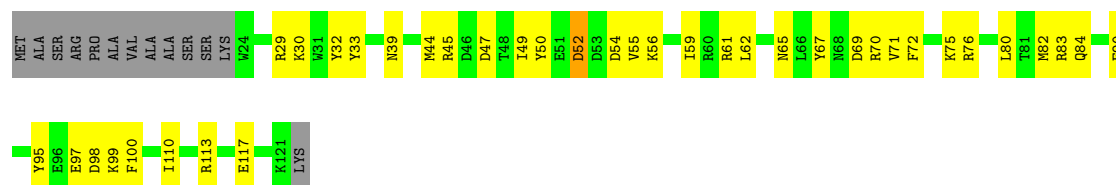




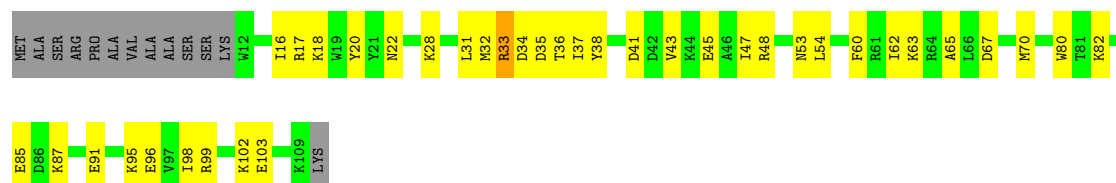
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 6: Cytochrome b-c1 complex subunit 7



- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain 3G: 

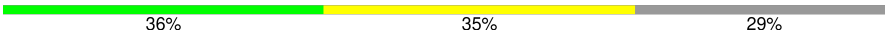


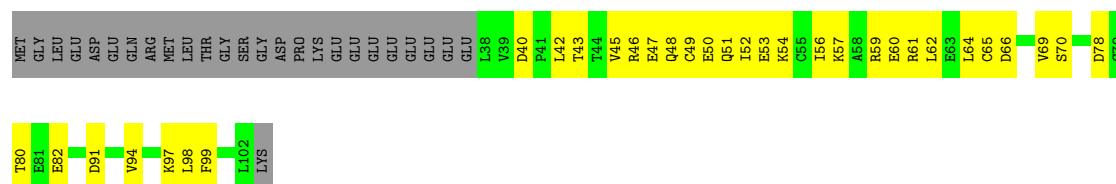
- Molecule 7: Cytochrome b-c1 complex subunit 8

Chain 3T: 

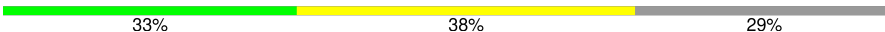


- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H: 



- Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U: 



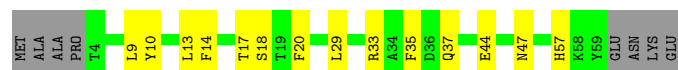
- Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J: 

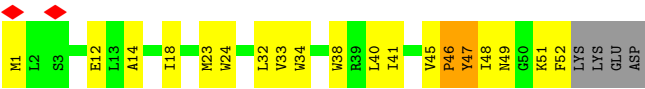


- Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W: 



- Molecule 10: Cytochrome b-c1 complex subunit 10



● Molecule 10: Cytochrome b-c1 complex subunit 10



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 60000                                   | 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 ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1300                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.763                                   | Depositor |
| Minimum map value                    | -0.290                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.027                                   | Depositor |
| Recommended contour level            | 0.12                                    | Depositor |
| Map size (Å)                         | 425.6, 425.6, 425.6                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.33, 1.33, 1.33                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, U10, FES, CDL, HEC, HEM, PC1

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   | 3A    | 0.20         | 0/3481         | 0.37        | 0/4722          |
| 1   | 3N    | 0.20         | 0/3496         | 0.37        | 0/4723          |
| 2   | 3B    | 0.20         | 0/3190         | 0.35        | 0/4317          |
| 2   | 3O    | 0.18         | 0/3175         | 0.32        | 0/4292          |
| 3   | 3C    | 0.24         | 0/3123         | 0.39        | 0/4269          |
| 3   | 3P    | 0.22         | 0/3122         | 0.38        | 0/4269          |
| 4   | 3D    | 0.21         | 0/1946         | 0.42        | 0/2641          |
| 4   | 3Q    | 0.20         | 0/1962         | 0.36        | 0/2663          |
| 5   | 3E    | 0.40         | 2/1551 (0.1%)  | 0.61        | 3/2098 (0.1%)   |
| 5   | 3I    | 0.87         | 2/342 (0.6%)   | 1.74        | 4/465 (0.9%)    |
| 5   | 3R    | 0.43         | 2/1551 (0.1%)  | 0.92        | 6/2098 (0.3%)   |
| 5   | 3V    | 0.20         | 0/225          | 0.47        | 0/303           |
| 6   | 3F    | 0.21         | 0/888          | 0.45        | 0/1193          |
| 6   | 3S    | 0.20         | 0/888          | 0.36        | 0/1193          |
| 7   | 3G    | 0.21         | 0/648          | 0.42        | 0/874           |
| 7   | 3T    | 0.21         | 0/649          | 0.52        | 0/878           |
| 8   | 3H    | 0.23         | 0/539          | 0.56        | 0/724           |
| 8   | 3U    | 0.21         | 0/539          | 0.54        | 0/724           |
| 9   | 3J    | 0.22         | 0/476          | 0.45        | 0/641           |
| 9   | 3W    | 0.22         | 0/476          | 0.46        | 1/641 (0.2%)    |
| 10  | 3X    | 0.21         | 0/445          | 0.56        | 1/608 (0.2%)    |
| 10  | 3Y    | 0.21         | 0/437          | 0.54        | 0/598           |
| All | All   | 0.25         | 6/33149 (0.0%) | 0.48        | 15/44934 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 5   | 3R    | 198 | PRO  | CG-CD | -11.64 | 1.11        | 1.50     |
| 5   | 3I    | 41  | PRO  | CG-CD | -10.41 | 1.15        | 1.50     |
| 5   | 3E    | 173 | PRO  | CG-CD | -10.23 | 1.16        | 1.50     |
| 5   | 3I    | 41  | PRO  | CB-CG | -8.94  | 1.04        | 1.49     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | 3R    | 198 | PRO  | CB-CG | -7.38 | 1.12        | 1.49     |
| 5   | 3E    | 173 | PRO  | N-CD  | 6.08  | 1.56        | 1.47     |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 5   | 3I    | 41  | PRO  | CB-CG-CD | 23.05  | 179.87      | 106.10   |
| 5   | 3R    | 198 | PRO  | CB-CG-CD | 21.68  | 175.49      | 106.10   |
| 5   | 3R    | 198 | PRO  | N-CD-CG  | -20.16 | 72.96       | 103.20   |
| 5   | 3I    | 41  | PRO  | N-CD-CG  | -18.36 | 75.66       | 103.20   |
| 5   | 3I    | 41  | PRO  | CA-CB-CG | -15.94 | 74.21       | 104.50   |
| 5   | 3R    | 198 | PRO  | CA-CB-CG | -15.87 | 74.36       | 104.50   |
| 5   | 3E    | 173 | PRO  | CA-N-CD  | -12.17 | 94.96       | 112.00   |
| 5   | 3E    | 173 | PRO  | N-CD-CG  | -11.17 | 86.44       | 103.20   |
| 5   | 3I    | 41  | PRO  | CA-N-CD  | -6.63  | 102.72      | 112.00   |
| 5   | 3E    | 173 | PRO  | CA-CB-CG | -6.57  | 92.02       | 104.50   |
| 5   | 3R    | 198 | PRO  | CA-N-CD  | -5.77  | 103.92      | 112.00   |
| 9   | 3W    | 44  | GLU  | CA-CB-CG | 5.45   | 125.00      | 114.10   |
| 5   | 3R    | 272 | ILE  | CA-C-N   | -5.41  | 117.67      | 122.97   |
| 5   | 3R    | 272 | ILE  | C-N-CA   | -5.41  | 117.67      | 122.97   |
| 10  | 3X    | 1   | MET  | CB-CG-SD | 5.12   | 128.04      | 112.70   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 3A    | 3411  | 0        | 3309     | 120     | 0            |
| 1   | 3N    | 3424  | 0        | 3350     | 121     | 0            |
| 2   | 3B    | 3138  | 0        | 3116     | 93      | 0            |
| 2   | 3O    | 3124  | 0        | 3108     | 84      | 0            |
| 3   | 3C    | 3025  | 0        | 3090     | 137     | 0            |
| 3   | 3P    | 3024  | 0        | 3090     | 108     | 0            |
| 4   | 3D    | 1888  | 0        | 1834     | 81      | 0            |
| 4   | 3Q    | 1904  | 0        | 1848     | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 3E    | 1518  | 0        | 1498     | 91      | 0            |
| 5   | 3I    | 337   | 0        | 347      | 33      | 0            |
| 5   | 3R    | 1518  | 0        | 1500     | 89      | 0            |
| 5   | 3V    | 223   | 0        | 233      | 12      | 0            |
| 6   | 3F    | 868   | 0        | 857      | 37      | 0            |
| 6   | 3S    | 868   | 0        | 857      | 31      | 0            |
| 7   | 3G    | 628   | 0        | 634      | 30      | 0            |
| 7   | 3T    | 628   | 0        | 632      | 32      | 0            |
| 8   | 3H    | 533   | 0        | 513      | 26      | 0            |
| 8   | 3U    | 533   | 0        | 513      | 32      | 0            |
| 9   | 3J    | 464   | 0        | 467      | 24      | 0            |
| 9   | 3W    | 464   | 0        | 467      | 15      | 0            |
| 10  | 3X    | 429   | 0        | 430      | 16      | 0            |
| 10  | 3Y    | 421   | 0        | 418      | 12      | 0            |
| 11  | 3A    | 58    | 0        | 60       | 4       | 0            |
| 11  | 3C    | 52    | 0        | 48       | 5       | 0            |
| 11  | 3G    | 56    | 0        | 56       | 7       | 0            |
| 11  | 3N    | 43    | 0        | 30       | 5       | 0            |
| 11  | 3T    | 113   | 0        | 114      | 17      | 0            |
| 12  | 3A    | 59    | 0        | 66       | 9       | 0            |
| 12  | 3C    | 69    | 0        | 86       | 7       | 0            |
| 12  | 3E    | 33    | 0        | 40       | 6       | 0            |
| 12  | 3G    | 29    | 0        | 32       | 2       | 0            |
| 12  | 3N    | 58    | 0        | 62       | 15      | 0            |
| 12  | 3P    | 33    | 0        | 40       | 0       | 0            |
| 12  | 3R    | 47    | 0        | 71       | 8       | 0            |
| 12  | 3Y    | 30    | 0        | 34       | 4       | 0            |
| 13  | 3C    | 86    | 0        | 60       | 10      | 0            |
| 13  | 3P    | 86    | 0        | 60       | 7       | 0            |
| 14  | 3C    | 51    | 0        | 54       | 10      | 0            |
| 14  | 3P    | 64    | 0        | 78       | 12      | 0            |
| 15  | 3D    | 42    | 0        | 32       | 1       | 0            |
| 15  | 3Q    | 43    | 0        | 32       | 3       | 0            |
| 16  | 3E    | 4     | 0        | 0        | 4       | 0            |
| 16  | 3R    | 4     | 0        | 0        | 1       | 0            |
| 17  | 3E    | 47    | 0        | 68       | 7       | 0            |
| 17  | 3R    | 45    | 0        | 64       | 5       | 0            |
| 17  | 3X    | 29    | 0        | 32       | 4       | 0            |
| All | All   | 33551 | 0        | 33330    | 1182    | 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 18.

All (1182) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:3J:53:TRP:O      | 9:3J:57:LYS:HE3    | 1.42                     | 1.19              |
| 9:3J:53:TRP:CE2    | 9:3J:57:LYS:HG2    | 1.91                     | 1.05              |
| 5:3E:217:CYS:HB3   | 16:3E:301:FES:S1   | 1.99                     | 1.02              |
| 14:3P:503:U10:H4M3 | 14:3P:503:U10:H3M3 | 1.46                     | 0.96              |
| 14:3C:503:U10:H4M2 | 14:3C:503:U10:H3M2 | 1.49                     | 0.92              |
| 5:3E:217:CYS:CB    | 16:3E:301:FES:S1   | 2.57                     | 0.89              |
| 5:3E:167:PHE:HB2   | 5:3E:174:LEU:HB3   | 1.57                     | 0.85              |
| 9:3J:53:TRP:O      | 9:3J:57:LYS:CE     | 2.24                     | 0.85              |
| 2:3B:226:MET:HG3   | 2:3B:227:ARG:H     | 1.44                     | 0.82              |
| 3:3C:146:ILE:HG13  | 14:3C:504:U10:H4M2 | 1.60                     | 0.82              |
| 5:3E:219:HIS:CE1   | 5:3E:239:HIS:ND1   | 2.48                     | 0.82              |
| 2:3B:397:THR:HA    | 2:3B:400:GLN:HE22  | 1.45                     | 0.80              |
| 3:3P:310:SER:HA    | 3:3P:374:ASN:HD21  | 1.47                     | 0.80              |
| 9:3J:53:TRP:NE1    | 9:3J:57:LYS:HG2    | 1.93                     | 0.79              |
| 8:3H:50:GLU:OE1    | 8:3H:51:GLN:NE2    | 2.16                     | 0.79              |
| 3:3C:53:MET:SD     | 5:3E:140:MET:HE1   | 2.23                     | 0.78              |
| 5:3E:219:HIS:ND1   | 5:3E:239:HIS:ND1   | 2.31                     | 0.78              |
| 5:3E:239:HIS:HD2   | 5:3E:253:PRO:HD2   | 1.47                     | 0.78              |
| 5:3I:47:ARG:O      | 5:3I:49:PHE:CE2    | 2.36                     | 0.78              |
| 5:3R:181:LYS:HD2   | 5:3R:184:ILE:HD12  | 1.65                     | 0.77              |
| 11:3G:102:CDL:H532 | 11:3G:102:CDL:H722 | 1.66                     | 0.77              |
| 3:3C:17:ALA:HA     | 3:3C:201:HIS:HE1   | 1.50                     | 0.77              |
| 1:3A:131:ARG:HD3   | 1:3A:175:ARG:HA    | 1.68                     | 0.76              |
| 11:3G:102:CDL:HA31 | 11:3G:102:CDL:HB22 | 1.68                     | 0.76              |
| 2:3O:124:LEU:HD22  | 2:3O:224:LEU:HD21  | 1.68                     | 0.75              |
| 3:3P:221:HIS:O     | 3:3P:225:THR:OG1   | 2.04                     | 0.75              |
| 5:3E:196:ARG:HB2   | 5:3E:251:LYS:HA    | 1.67                     | 0.75              |
| 3:3P:126:THR:HG21  | 13:3P:501:HEM:HBB2 | 1.67                     | 0.74              |
| 5:3E:151:LYS:HD2   | 5:3E:152:ILE:HG13  | 1.68                     | 0.74              |
| 3:3P:8:HIS:HB3     | 3:3P:11:MET:HB2    | 1.69                     | 0.74              |
| 2:3B:46:ARG:HE     | 2:3B:110:GLU:HB2   | 1.51                     | 0.74              |
| 1:3A:372:THR:N     | 2:3B:373:GLU:OE2   | 2.20                     | 0.74              |
| 5:3R:164:ASN:HB2   | 5:3R:177:ARG:HD2   | 1.68                     | 0.74              |
| 1:3A:304:CYS:HB2   | 1:3A:334:MET:HE1   | 1.69                     | 0.74              |
| 3:3C:281:LEU:HB2   | 3:3C:294:LEU:HD21  | 1.69                     | 0.73              |
| 1:3A:279:HIS:CG    | 5:3I:35:PRO:HB3    | 2.24                     | 0.73              |
| 10:3Y:39:ARG:HH21  | 10:3Y:52:PHE:HB2   | 1.52                     | 0.73              |
| 5:3E:155:LYS:HB2   | 5:3E:271:VAL:HG13  | 1.70                     | 0.73              |
| 3:3P:119:LEU:HD11  | 3:3P:192:LEU:HB3   | 1.69                     | 0.73              |
| 2:3B:124:LEU:HB3   | 2:3B:223:PHE:HD2   | 1.52                     | 0.73              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:3N:184:GLU:OE2  | 1:3N:184:GLU:N     | 2.22                     | 0.72              |
| 1:3A:286:GLY:H    | 5:3I:70:LEU:HD23   | 1.53                     | 0.72              |
| 9:3J:11:TYR:HA    | 9:3J:15:PHE:HB2    | 1.71                     | 0.72              |
| 3:3P:120:LEU:O    | 3:3P:124:MET:HG3   | 1.89                     | 0.72              |
| 3:3C:35:SER:HB3   | 14:3C:503:U10:H1M1 | 1.70                     | 0.72              |
| 2:3B:124:LEU:HB3  | 2:3B:223:PHE:CD2   | 2.24                     | 0.72              |
| 1:3N:60:GLU:OE1   | 2:3O:287:ARG:NH2   | 2.22                     | 0.71              |
| 6:3S:32:MET:O     | 6:3S:34:ASP:N      | 2.23                     | 0.71              |
| 5:3E:200:HIS:HB3  | 5:3E:203:GLU:HG2   | 1.72                     | 0.71              |
| 12:3A:503:3PE:N   | 3:3C:3:ASN:OD1     | 2.24                     | 0.71              |
| 3:3C:221:HIS:O    | 3:3C:225:THR:OG1   | 2.06                     | 0.71              |
| 2:3B:36:ALA:HB3   | 2:3B:207:ILE:HG13  | 1.73                     | 0.71              |
| 3:3C:229:ILE:HG23 | 17:3E:303:PC1:H3A1 | 1.73                     | 0.71              |
| 4:3D:223:CYS:SG   | 4:3D:224:GLU:N     | 2.64                     | 0.71              |
| 6:3F:90:GLU:OE1   | 6:3F:90:GLU:N      | 2.22                     | 0.71              |
| 1:3A:339:GLN:O    | 1:3A:343:MET:HG2   | 1.91                     | 0.70              |
| 5:3E:164:ASN:ND2  | 5:3E:164:ASN:O     | 2.23                     | 0.70              |
| 2:3B:350:GLY:HA2  | 2:3B:411:ILE:HD11  | 1.73                     | 0.70              |
| 1:3N:335:MET:HE3  | 1:3N:335:MET:HA    | 1.72                     | 0.70              |
| 3:3C:38:GLY:HA3   | 14:3C:503:U10:H13  | 1.73                     | 0.70              |
| 10:3X:38:TRP:HA   | 17:3X:101:PC1:H32  | 1.73                     | 0.70              |
| 1:3N:14:THR:HG21  | 1:3N:389:ARG:HB3   | 1.71                     | 0.70              |
| 9:3W:10:TYR:HA    | 9:3W:14:PHE:HB2    | 1.74                     | 0.70              |
| 2:3O:334:GLY:HA2  | 2:3O:434:PRO:HD3   | 1.74                     | 0.70              |
| 3:3P:224:TYR:O    | 3:3P:228:ASP:N     | 2.20                     | 0.70              |
| 4:3Q:41:HIS:HE1   | 15:3Q:501:HEC:NA   | 1.87                     | 0.69              |
| 2:3B:101:THR:HG23 | 2:3B:103:GLU:H     | 1.58                     | 0.69              |
| 2:3B:95:LYS:O     | 2:3B:109:VAL:HA    | 1.93                     | 0.69              |
| 1:3A:445:ARG:HD3  | 12:3A:503:3PE:H231 | 1.75                     | 0.69              |
| 5:3R:177:ARG:HG2  | 5:3R:179:ARG:HG3   | 1.75                     | 0.69              |
| 3:3C:25:SER:OG    | 3:3C:216:ASP:OD2   | 2.10                     | 0.68              |
| 5:3I:47:ARG:O     | 5:3I:49:PHE:CD2    | 2.45                     | 0.68              |
| 3:3P:155:TYR:OH   | 12:3Y:101:3PE:N    | 2.24                     | 0.68              |
| 10:3X:33:VAL:HG23 | 10:3X:38:TRP:HB3   | 1.75                     | 0.68              |
| 4:3Q:69:GLU:HB3   | 4:3Q:82:MET:HE2    | 1.75                     | 0.68              |
| 10:3X:14:ALA:O    | 10:3X:18:ILE:HG12  | 1.93                     | 0.68              |
| 9:3J:17:ARG:HB2   | 9:3J:20:THR:HG23   | 1.75                     | 0.68              |
| 4:3Q:8:PRO:HG3    | 8:3U:66:ASP:HB3    | 1.76                     | 0.68              |
| 2:3O:76:THR:HG23  | 2:3O:81:SER:HA     | 1.75                     | 0.67              |
| 5:3E:178:HIS:ND1  | 5:3E:209:GLU:O     | 2.25                     | 0.67              |
| 4:3D:296:LYS:NZ   | 12:3E:302:3PE:O12  | 2.28                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3N:141:ASN:ND2   | 1:3N:168:GLU:OE2   | 2.27                     | 0.67              |
| 9:3W:18:SER:HB2    | 10:3X:23:MET:SD    | 2.35                     | 0.67              |
| 2:3O:128:ALA:HA    | 2:3O:227:ARG:HH22  | 1.58                     | 0.67              |
| 1:3A:364:ALA:HB2   | 5:3I:33:ALA:HB3    | 1.77                     | 0.67              |
| 5:3R:199:GLN:O     | 5:3R:248:ARG:NH1   | 2.28                     | 0.66              |
| 4:3D:317:SER:O     | 7:3G:25:GLN:NE2    | 2.28                     | 0.66              |
| 4:3Q:118:ARG:NH1   | 4:3Q:195:GLU:OE1   | 2.27                     | 0.66              |
| 5:3R:169:TRP:HD1   | 5:3R:174:LEU:HD23  | 1.60                     | 0.66              |
| 3:3P:70:CYS:SG     | 3:3P:80:ARG:NH1    | 2.68                     | 0.66              |
| 1:3A:106:LEU:HD22  | 1:3A:203:VAL:HG12  | 1.76                     | 0.66              |
| 4:3D:163:ASN:HD21  | 4:3D:167:GLU:HB2   | 1.61                     | 0.66              |
| 1:3N:235:ARG:HE    | 5:3R:92:ARG:HH22   | 1.43                     | 0.66              |
| 12:3N:501:3PE:H352 | 3:3P:5:ARG:HG3     | 1.78                     | 0.66              |
| 3:3C:82:LEU:HD12   | 3:3C:243:VAL:HG21  | 1.77                     | 0.66              |
| 6:3S:43:VAL:O      | 6:3S:47:ILE:HD12   | 1.95                     | 0.66              |
| 7:3G:5:GLU:OE1     | 7:3G:8:HIS:NE2     | 2.28                     | 0.66              |
| 3:3C:34:GLY:HA3    | 13:3C:502:HEM:HBA2 | 1.78                     | 0.66              |
| 2:3O:46:ARG:HG3    | 2:3O:110:GLU:HB3   | 1.76                     | 0.66              |
| 4:3D:171:ARG:NH2   | 4:3D:177:ASP:OD2   | 2.30                     | 0.65              |
| 17:3R:303:PC1:H152 | 9:3W:17:THR:HG22   | 1.78                     | 0.65              |
| 5:3E:225:ILE:HD13  | 5:3E:228:ALA:H     | 1.59                     | 0.65              |
| 5:3R:162:GLY:N     | 5:3R:178:HIS:O     | 2.30                     | 0.65              |
| 2:3B:39:GLU:OE2    | 2:3B:113:ARG:NH2   | 2.29                     | 0.65              |
| 3:3C:233:LEU:HD21  | 4:3D:305:LEU:HD12  | 1.77                     | 0.65              |
| 1:3N:291:SER:N     | 2:3O:90:GLU:OE1    | 2.29                     | 0.65              |
| 6:3S:34:ASP:HA     | 6:3S:37:ILE:HD13   | 1.77                     | 0.65              |
| 10:3Y:14:ALA:O     | 10:3Y:18:ILE:HG12  | 1.96                     | 0.65              |
| 2:3B:287:ARG:HG2   | 5:3I:53:GLU:HB3    | 1.78                     | 0.65              |
| 3:3P:50:PHE:HA     | 3:3P:53:MET:HG3    | 1.78                     | 0.65              |
| 1:3N:19:LEU:HD23   | 1:3N:19:LEU:H      | 1.62                     | 0.65              |
| 2:3B:37:SER:HB3    | 2:3B:216:LEU:HD12  | 1.78                     | 0.64              |
| 3:3C:114:ASN:HD22  | 3:3C:302:ILE:HD11  | 1.62                     | 0.64              |
| 3:3C:116:GLY:HA2   | 3:3C:119:LEU:HD12  | 1.79                     | 0.64              |
| 1:3N:433:ASP:OD2   | 3:3P:223:TYR:OH    | 2.14                     | 0.64              |
| 1:3N:444:LEU:HD13  | 12:3N:503:3PE:H122 | 1.78                     | 0.64              |
| 5:3R:153:GLU:HG2   | 5:3R:169:TRP:HB3   | 1.80                     | 0.64              |
| 5:3R:219:HIS:O     | 5:3R:219:HIS:ND1   | 2.30                     | 0.64              |
| 8:3U:42:GLN:OE1    | 8:3U:42:GLN:N      | 2.29                     | 0.64              |
| 1:3A:301:ARG:HD2   | 1:3A:303:LEU:HD23  | 1.80                     | 0.64              |
| 8:3U:31:ILE:O      | 8:3U:35:GLU:HG2    | 1.98                     | 0.64              |
| 1:3N:106:LEU:HD22  | 1:3N:203:VAL:HG12  | 1.80                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:3P:234:PHE:HZ    | 11:3T:101:CDL:H562 | 1.63                     | 0.64              |
| 5:3R:175:PHE:CE2   | 5:3R:215:GLY:HA2   | 2.34                     | 0.63              |
| 5:3R:170:ARG:O     | 5:3R:172:LYS:NZ    | 2.29                     | 0.63              |
| 8:3U:19:THR:O      | 8:3U:23:GLN:NE2    | 2.32                     | 0.63              |
| 3:3P:223:TYR:O     | 3:3P:225:THR:N     | 2.31                     | 0.63              |
| 3:3P:102:LEU:HD21  | 3:3P:304:MET:HG3   | 1.81                     | 0.63              |
| 3:3C:373:GLU:OE2   | 6:3F:32:TYR:OH     | 2.16                     | 0.63              |
| 5:3R:159:ILE:HD12  | 5:3R:160:PRO:HD2   | 1.80                     | 0.63              |
| 1:3A:311:ASN:OD1   | 1:3A:320:LEU:HD12  | 1.98                     | 0.63              |
| 5:3E:167:PHE:HB3   | 5:3E:169:TRP:CD1   | 2.33                     | 0.63              |
| 8:3H:49:CYS:O      | 8:3H:52:ILE:HG22   | 1.99                     | 0.62              |
| 11:3N:502:CDL:OB4  | 12:3N:503:3PE:N    | 2.31                     | 0.62              |
| 2:3B:400:GLN:OE1   | 2:3B:400:GLN:N     | 2.31                     | 0.62              |
| 3:3C:119:LEU:HD22  | 13:3C:502:HEM:HBB2 | 1.80                     | 0.62              |
| 7:3T:37:VAL:HG21   | 11:3T:101:CDL:H311 | 1.81                     | 0.62              |
| 6:3F:59:ILE:HA     | 6:3F:62:LEU:HD12   | 1.81                     | 0.62              |
| 5:3R:153:GLU:OE1   | 5:3R:273:VAL:HG13  | 2.00                     | 0.62              |
| 7:3T:40:ARG:NH1    | 11:3T:101:CDL:OA3  | 2.33                     | 0.62              |
| 2:3B:117:GLU:HA    | 2:3B:120:MET:HE2   | 1.80                     | 0.62              |
| 3:3P:370:SER:O     | 3:3P:374:ASN:ND2   | 2.32                     | 0.62              |
| 1:3A:444:LEU:HD11  | 12:3A:502:3PE:H12  | 1.81                     | 0.62              |
| 3:3C:237:LEU:HD13  | 4:3D:301:MET:HG2   | 1.81                     | 0.62              |
| 1:3A:176:LYS:HE3   | 1:3A:176:LYS:HA    | 1.82                     | 0.61              |
| 3:3P:33:PHE:HA     | 3:3P:36:LEU:HB2    | 1.80                     | 0.61              |
| 5:3E:237:PRO:HB2   | 4:3Q:144:ARG:HD3   | 1.82                     | 0.61              |
| 1:3N:107:PRO:HA    | 1:3N:211:LEU:HD11  | 1.82                     | 0.61              |
| 3:3P:1:MET:HE3     | 3:3P:1:MET:HA      | 1.82                     | 0.61              |
| 4:3D:111:HIS:HD2   | 9:3J:52:LEU:HA     | 1.65                     | 0.61              |
| 3:3P:34:GLY:HA3    | 13:3P:502:HEM:HBA2 | 1.81                     | 0.61              |
| 6:3F:76:ARG:O      | 6:3F:80:LEU:HD22   | 1.99                     | 0.61              |
| 1:3N:280:TYR:HB3   | 1:3N:307:PHE:CE1   | 2.36                     | 0.61              |
| 5:3R:153:GLU:OE1   | 5:3R:274:GLY:N     | 2.31                     | 0.61              |
| 4:3D:313:ARG:HG3   | 7:3G:28:PHE:HE1    | 1.66                     | 0.61              |
| 9:3J:20:THR:HG22   | 10:3Y:23:MET:HE1   | 1.82                     | 0.61              |
| 1:3N:143:SER:O     | 5:3V:47:ARG:NH1    | 2.34                     | 0.61              |
| 1:3N:270:LEU:HD13  | 1:3N:320:LEU:HD22  | 1.81                     | 0.61              |
| 3:3P:47:THR:OG1    | 3:3P:83:HIS:ND1    | 2.32                     | 0.61              |
| 12:3A:503:3PE:H122 | 3:3C:4:ILE:HG12    | 1.82                     | 0.60              |
| 2:3O:209:LEU:HD11  | 2:3O:378:PHE:HD2   | 1.65                     | 0.60              |
| 3:3P:53:MET:HE1    | 5:3R:140:MET:HG3   | 1.83                     | 0.60              |
| 1:3A:28:GLU:OE1    | 1:3A:389:ARG:NH1   | 2.33                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:298:ALA:HB1   | 1:3A:304:CYS:HB3   | 1.81                     | 0.60              |
| 1:3N:235:ARG:HH21  | 5:3R:92:ARG:HH12   | 1.49                     | 0.60              |
| 2:3O:240:ARG:O     | 2:3O:421:ARG:NH1   | 2.34                     | 0.60              |
| 12:3N:503:3PE:H11  | 17:3R:303:PC1:H11  | 1.82                     | 0.60              |
| 2:3O:133:ARG:HB2   | 2:3O:136:GLU:HG3   | 1.83                     | 0.60              |
| 8:3U:60:ASP:OD1    | 8:3U:61:PHE:N      | 2.34                     | 0.60              |
| 5:3E:219:HIS:CG    | 5:3E:219:HIS:O     | 2.55                     | 0.60              |
| 3:3P:24:PRO:O      | 3:3P:224:TYR:OH    | 2.15                     | 0.60              |
| 3:3P:104:TYR:O     | 3:3P:206:ASN:ND2   | 2.34                     | 0.60              |
| 3:3P:322:GLN:OE1   | 7:3T:47:ARG:NH2    | 2.34                     | 0.60              |
| 8:3U:38:GLU:HA     | 8:3U:41:ASP:OD2    | 2.02                     | 0.60              |
| 2:3O:35:ILE:HD13   | 2:3O:206:LEU:HB3   | 1.84                     | 0.60              |
| 1:3N:42:ASP:HB3    | 1:3N:194:ARG:HB3   | 1.84                     | 0.60              |
| 5:3E:173:PRO:HD2   | 5:3E:173:PRO:O     | 2.01                     | 0.60              |
| 2:3B:222:ARG:HG2   | 2:3B:223:PHE:CD1   | 2.36                     | 0.59              |
| 3:3C:116:GLY:C     | 13:3C:502:HEM:HBC2 | 2.27                     | 0.59              |
| 2:3O:304:HIS:HA    | 5:3V:52:ARG:HH22   | 1.66                     | 0.59              |
| 11:3A:501:CDL:H141 | 11:3A:501:CDL:H542 | 1.84                     | 0.59              |
| 3:3C:125:ALA:HB2   | 14:3C:504:U10:H13  | 1.83                     | 0.59              |
| 1:3N:350:THR:HA    | 10:3X:12:GLU:OE1   | 2.03                     | 0.59              |
| 4:3Q:21:LEU:H      | 4:3Q:21:LEU:HD12   | 1.67                     | 0.59              |
| 1:3N:244:ARG:NH2   | 1:3N:429:GLU:OE1   | 2.36                     | 0.59              |
| 10:3Y:8:PRO:O      | 10:3Y:11:ARG:HG2   | 2.01                     | 0.59              |
| 1:3A:301:ARG:HH21  | 3:3C:2:THR:HG22    | 1.68                     | 0.59              |
| 3:3C:51:LEU:HD13   | 13:3C:501:HEM:HBD1 | 1.85                     | 0.59              |
| 8:3H:45:VAL:HG12   | 8:3H:94:VAL:HG22   | 1.85                     | 0.59              |
| 1:3N:276:ILE:HG21  | 1:3N:345:LEU:HD21  | 1.84                     | 0.59              |
| 2:3O:145:ARG:HD2   | 2:3O:146:ILE:HD12  | 1.84                     | 0.59              |
| 3:3P:361:ILE:HA    | 3:3P:365:LEU:HB2   | 1.85                     | 0.59              |
| 4:3Q:82:MET:HE3    | 4:3Q:83:ARG:N      | 2.17                     | 0.59              |
| 4:3D:171:ARG:NH1   | 4:3D:172:PRO:O     | 2.35                     | 0.59              |
| 3:3P:236:MET:HB3   | 4:3Q:212:MET:HE1   | 1.84                     | 0.59              |
| 1:3N:24:ARG:NH2    | 1:3N:383:LEU:O     | 2.36                     | 0.58              |
| 3:3C:5:ARG:NH1     | 3:3C:20:ASP:OD2    | 2.35                     | 0.58              |
| 5:3E:131:ASN:ND2   | 12:3E:302:3PE:O11  | 2.31                     | 0.58              |
| 5:3E:173:PRO:HD3   | 5:3E:216:VAL:HG13  | 1.85                     | 0.58              |
| 3:3P:126:THR:HG23  | 3:3P:182:HIS:CD2   | 2.37                     | 0.58              |
| 3:3C:207:ASN:ND2   | 3:3C:209:THR:OG1   | 2.36                     | 0.58              |
| 5:3V:53:GLU:O      | 5:3V:56:SER:OG     | 2.18                     | 0.58              |
| 12:3A:502:3PE:H351 | 17:3E:303:PC1:H341 | 1.85                     | 0.58              |
| 6:3F:30:LYS:HD2    | 6:3F:95:TYR:HD2    | 1.67                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:3F:33:TYR:OH    | 6:3F:98:ASP:OD2    | 2.20                     | 0.58              |
| 6:3F:80:LEU:O     | 6:3F:84:GLN:N      | 2.37                     | 0.58              |
| 1:3N:209:LEU:HG   | 1:3N:213:GLN:HE21  | 1.68                     | 0.58              |
| 4:3Q:211:MET:HE1  | 5:3R:127:TYR:CE2   | 2.38                     | 0.58              |
| 3:3C:227:LYS:HE3  | 11:3G:102:CDL:HB61 | 1.84                     | 0.58              |
| 4:3D:185:ASN:OD1  | 4:3D:188:ALA:N     | 2.34                     | 0.58              |
| 5:3E:194:GLN:NE2  | 5:3E:250:ARG:HH11  | 2.01                     | 0.58              |
| 3:3C:103:TYR:OH   | 3:3C:322:GLN:NE2   | 2.35                     | 0.58              |
| 4:3D:300:MET:HG2  | 12:3E:302:3PE:H331 | 1.86                     | 0.58              |
| 5:3E:264:GLU:N    | 5:3E:272:ILE:O     | 2.36                     | 0.58              |
| 6:3F:45:ARG:HE    | 6:3F:100:PHE:HE2   | 1.50                     | 0.58              |
| 1:3N:235:ARG:HE   | 5:3R:92:ARG:NH2    | 2.01                     | 0.58              |
| 10:3X:45:VAL:O    | 10:3X:49:ASN:ND2   | 2.36                     | 0.58              |
| 2:3O:299:VAL:HG11 | 2:3O:336:VAL:HG13  | 1.85                     | 0.58              |
| 3:3P:38:GLY:HA3   | 14:3P:503:U10:H122 | 1.84                     | 0.58              |
| 5:3E:172:LYS:HD2  | 5:3E:214:ILE:HD13  | 1.86                     | 0.58              |
| 1:3N:304:CYS:HB3  | 1:3N:334:MET:HE1   | 1.84                     | 0.58              |
| 4:3Q:47:ALA:HA    | 4:3Q:90:TYR:HA     | 1.85                     | 0.58              |
| 5:3R:160:PRO:HG2  | 5:3R:163:LYS:HD3   | 1.84                     | 0.58              |
| 2:3B:41:TYR:HA    | 2:3B:113:ARG:HH22  | 1.69                     | 0.58              |
| 3:3C:172:LYS:H    | 3:3C:172:LYS:HD3   | 1.69                     | 0.58              |
| 3:3C:269:LYS:HB2  | 3:3C:275:LEU:HD21  | 1.85                     | 0.58              |
| 6:3F:33:TYR:HE1   | 6:3F:39:ASN:HB3    | 1.68                     | 0.58              |
| 3:3P:132:VAL:HG11 | 3:3P:178:PHE:HD2   | 1.69                     | 0.58              |
| 2:3B:394:GLN:O    | 2:3B:397:THR:OG1   | 2.20                     | 0.57              |
| 12:3N:501:3PE:O12 | 12:3N:501:3PE:N    | 2.31                     | 0.57              |
| 8:3H:78:ASP:HB3   | 8:3H:80:THR:HG23   | 1.85                     | 0.57              |
| 6:3S:82:LYS:HB2   | 6:3S:85:GLU:HG2    | 1.87                     | 0.57              |
| 1:3A:439:SER:O    | 12:3A:502:3PE:N    | 2.37                     | 0.57              |
| 11:3C:505:CDL:OB7 | 7:3G:42:ARG:NH2    | 2.37                     | 0.57              |
| 2:3O:54:GLY:H     | 2:3O:57:TYR:HD2    | 1.52                     | 0.57              |
| 8:3U:48:SER:OG    | 8:3U:49:GLN:OE1    | 2.22                     | 0.57              |
| 2:3B:94:GLY:HA3   | 2:3B:119:LEU:HD21  | 1.87                     | 0.57              |
| 4:3Q:152:TYR:OH   | 8:3U:66:ASP:OD2    | 2.22                     | 0.57              |
| 3:3C:245:PHE:O    | 4:3D:290:ARG:NH2   | 2.38                     | 0.57              |
| 1:3N:225:GLU:HG3  | 1:3N:226:ASP:H     | 1.68                     | 0.57              |
| 1:3A:70:ARG:HH21  | 1:3A:112:LEU:HD12  | 1.69                     | 0.57              |
| 3:3C:71:ARG:NH2   | 4:3D:202:SER:OG    | 2.38                     | 0.57              |
| 4:3D:325:ALA:HB3  | 7:3G:16:ILE:HB     | 1.85                     | 0.57              |
| 5:3E:239:HIS:CD2  | 5:3E:253:PRO:HD2   | 2.36                     | 0.57              |
| 1:3N:281:ASP:OD1  | 1:3N:282:SER:N     | 2.37                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:3P:281:LEU:HB2  | 3:3P:294:LEU:HD12  | 1.86                     | 0.57              |
| 8:3U:29:LYS:HA    | 8:3U:29:LYS:HE3    | 1.85                     | 0.57              |
| 1:3A:86:LEU:HD13  | 1:3A:99:ILE:HB     | 1.87                     | 0.57              |
| 6:3F:69:ASP:OD1   | 6:3F:70:ARG:N      | 2.37                     | 0.57              |
| 6:3F:30:LYS:HD2   | 6:3F:95:TYR:CD2    | 2.40                     | 0.57              |
| 8:3H:60:GLU:O     | 8:3H:64:LEU:HG     | 2.05                     | 0.57              |
| 4:3Q:82:MET:HE3   | 4:3Q:83:ARG:H      | 1.70                     | 0.56              |
| 1:3A:156:THR:HB   | 1:3A:241:ILE:HG13  | 1.86                     | 0.56              |
| 1:3N:359:ASN:O    | 1:3N:363:ASN:ND2   | 2.39                     | 0.56              |
| 5:3R:182:LYS:O    | 5:3R:182:LYS:NZ    | 2.35                     | 0.56              |
| 5:3R:205:VAL:HG22 | 5:3R:207:LYS:H     | 1.70                     | 0.56              |
| 11:3T:102:CDL:HA4 | 11:3T:102:CDL:H522 | 1.88                     | 0.56              |
| 1:3A:420:PRO:O    | 1:3A:434:TYR:OH    | 2.20                     | 0.56              |
| 3:3C:17:ALA:HA    | 3:3C:201:HIS:CE1   | 2.37                     | 0.56              |
| 2:3O:46:ARG:NH1   | 2:3O:375:SER:OG    | 2.27                     | 0.56              |
| 4:3D:262:ASP:OD1  | 4:3D:262:ASP:N     | 2.39                     | 0.56              |
| 3:3P:129:MET:HE2  | 14:3P:504:U10:H151 | 1.88                     | 0.56              |
| 5:3R:235:TYR:HA   | 5:3R:242:HIS:HB3   | 1.88                     | 0.56              |
| 2:3B:241:GLY:O    | 2:3B:421:ARG:NH2   | 2.38                     | 0.56              |
| 4:3D:98:TYR:HB3   | 8:3H:99:PHE:CE2    | 2.40                     | 0.56              |
| 4:3D:174:LYS:N    | 4:3D:177:ASP:OD1   | 2.38                     | 0.56              |
| 5:3I:62:ARG:HB2   | 5:3I:77:ARG:HH22   | 1.69                     | 0.56              |
| 3:3C:237:LEU:HD22 | 4:3D:305:LEU:HD21  | 1.87                     | 0.56              |
| 1:3N:131:ARG:HH12 | 1:3N:177:LEU:H     | 1.53                     | 0.56              |
| 3:3C:97:HIS:NE2   | 13:3C:502:HEM:O1A  | 2.32                     | 0.56              |
| 3:3C:201:HIS:CD2  | 14:3C:503:U10:H4M1 | 2.41                     | 0.56              |
| 5:3E:249:ILE:HG23 | 5:3E:257:ASN:HA    | 1.88                     | 0.56              |
| 8:3U:29:LYS:NZ    | 8:3U:32:LYS:HD2    | 2.21                     | 0.56              |
| 2:3B:226:MET:HG3  | 2:3B:227:ARG:N     | 2.19                     | 0.56              |
| 4:3D:114:ILE:HD12 | 4:3D:278:PHE:HA    | 1.88                     | 0.56              |
| 1:3N:307:PHE:HA   | 1:3N:324:PHE:HA    | 1.88                     | 0.56              |
| 2:3O:116:ILE:HG22 | 2:3O:120:MET:HE2   | 1.87                     | 0.56              |
| 2:3O:117:GLU:HA   | 2:3O:120:MET:HE3   | 1.88                     | 0.56              |
| 7:3T:46:LEU:HD12  | 7:3T:47:ARG:HG3    | 1.88                     | 0.56              |
| 4:3D:271:VAL:O    | 4:3D:275:VAL:HG12  | 2.06                     | 0.55              |
| 3:3P:186:PRO:HG2  | 13:3P:501:HEM:HMC3 | 1.89                     | 0.55              |
| 2:3B:222:ARG:HG2  | 2:3B:223:PHE:CE1   | 2.42                     | 0.55              |
| 2:3B:346:THR:O    | 2:3B:351:ASN:ND2   | 2.26                     | 0.55              |
| 4:3D:300:MET:HE2  | 4:3D:300:MET:HA    | 1.88                     | 0.55              |
| 5:3E:167:PHE:HD2  | 5:3E:174:LEU:HD12  | 1.71                     | 0.55              |
| 12:3N:503:3PE:H32 | 3:3P:221:HIS:HE1   | 1.71                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3O:369:LEU:HD11  | 2:3O:399:LEU:HD11  | 1.87                     | 0.55              |
| 5:3R:192:VAL:HG11  | 5:3R:200:HIS:CD2   | 2.41                     | 0.55              |
| 9:3J:23:LEU:O      | 9:3J:27:VAL:HG12   | 2.06                     | 0.55              |
| 2:3B:70:ARG:HD3    | 2:3B:100:SER:HB3   | 1.87                     | 0.55              |
| 5:3E:163:LYS:NZ    | 5:3E:165:MET:SD    | 2.80                     | 0.55              |
| 17:3E:303:PC1:H11  | 17:3E:303:PC1:H111 | 1.88                     | 0.55              |
| 7:3G:28:PHE:HE2    | 12:3G:101:3PE:H351 | 1.71                     | 0.55              |
| 8:3H:57:LYS:HA     | 8:3H:60:GLU:HG2    | 1.88                     | 0.55              |
| 1:3N:327:ASP:OD1   | 1:3N:330:SER:OG    | 2.25                     | 0.55              |
| 10:3X:32:LEU:HD21  | 17:3X:101:PC1:H342 | 1.88                     | 0.55              |
| 1:3N:40:TRP:NE1    | 1:3N:89:TYR:OH     | 2.37                     | 0.55              |
| 3:3P:182:HIS:HE1   | 13:3P:501:HEM:NA   | 2.05                     | 0.55              |
| 1:3A:282:SER:O     | 2:3B:143:GLN:NE2   | 2.40                     | 0.55              |
| 1:3N:242:ARG:HB3   | 1:3N:428:ILE:HD11  | 1.87                     | 0.55              |
| 12:3N:503:3PE:H332 | 17:3R:303:PC1:H351 | 1.89                     | 0.55              |
| 4:3Q:118:ARG:HB2   | 4:3Q:194:SER:OG    | 2.07                     | 0.55              |
| 11:3C:505:CDL:H722 | 7:3G:43:THR:OG1    | 2.05                     | 0.55              |
| 1:3A:281:ASP:H     | 1:3A:284:TYR:HD2   | 1.54                     | 0.55              |
| 1:3A:322:ALA:HB3   | 1:3A:338:LEU:HD21  | 1.88                     | 0.55              |
| 1:3N:436:ARG:HD3   | 3:3P:222:PRO:HD3   | 1.89                     | 0.55              |
| 2:3O:350:GLY:HA2   | 2:3O:411:ILE:HD12  | 1.87                     | 0.55              |
| 3:3C:31:TRP:NE1    | 13:3C:502:HEM:O2D  | 2.34                     | 0.55              |
| 1:3N:46:ARG:NH2    | 1:3N:316:GLU:OE2   | 2.39                     | 0.55              |
| 7:3T:40:ARG:HH21   | 11:3T:102:CDL:HB21 | 1.72                     | 0.55              |
| 7:3T:56:TYR:O      | 7:3T:60:THR:HG22   | 2.07                     | 0.55              |
| 1:3A:324:PHE:CD1   | 1:3A:334:MET:HG2   | 2.41                     | 0.54              |
| 5:3E:192:VAL:HA    | 5:3E:195:LEU:HD12  | 1.87                     | 0.54              |
| 1:3N:77:LYS:O      | 1:3N:81:SER:OG     | 2.20                     | 0.54              |
| 10:3X:46:PRO:O     | 10:3X:48:ILE:N     | 2.40                     | 0.54              |
| 2:3B:65:THR:HG23   | 2:3B:191:LEU:HD23  | 1.89                     | 0.54              |
| 3:3C:361:ILE:HA    | 3:3C:365:LEU:HB2   | 1.89                     | 0.54              |
| 3:3P:24:PRO:HB2    | 3:3P:27:ILE:HG12   | 1.89                     | 0.54              |
| 4:3Q:195:GLU:OE2   | 4:3Q:201:ARG:NE    | 2.40                     | 0.54              |
| 5:3R:199:GLN:OE1   | 5:3R:204:ARG:NE    | 2.23                     | 0.54              |
| 1:3A:132:ASP:OD1   | 1:3A:133:VAL:N     | 2.41                     | 0.54              |
| 8:3H:53:GLU:HA     | 8:3H:56:ILE:HB     | 1.89                     | 0.54              |
| 4:3Q:24:THR:OG1    | 4:3Q:28:ARG:NH1    | 2.35                     | 0.54              |
| 7:3T:27:PRO:O      | 7:3T:28:HIS:ND1    | 2.41                     | 0.54              |
| 10:3Y:33:VAL:HG23  | 10:3Y:38:TRP:HB3   | 1.89                     | 0.54              |
| 1:3A:288:THR:O     | 1:3A:289:HIS:ND1   | 2.41                     | 0.54              |
| 2:3B:196:GLN:HA    | 2:3B:226:MET:HE2   | 1.88                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:3C:40:CYS:O      | 3:3C:44:GLN:N      | 2.33                     | 0.54              |
| 4:3D:317:SER:HB2   | 7:3G:25:GLN:HE21   | 1.73                     | 0.54              |
| 1:3N:446:PHE:O     | 9:3W:18:SER:OG     | 2.20                     | 0.54              |
| 4:3D:109:LEU:HD11  | 4:3D:287:HIS:HB3   | 1.89                     | 0.54              |
| 7:3G:61:TYR:O      | 7:3G:65:THR:HG23   | 2.08                     | 0.54              |
| 1:3N:25:VAL:HG12   | 1:3N:197:LEU:HB3   | 1.90                     | 0.54              |
| 1:3A:14:THR:OG1    | 1:3A:389:ARG:NH1   | 2.38                     | 0.54              |
| 3:3P:373:GLU:HB3   | 6:3S:20:TYR:CZ     | 2.43                     | 0.54              |
| 3:3C:186:PRO:HG2   | 13:3C:501:HEM:HMC1 | 1.90                     | 0.54              |
| 5:3E:179:ARG:HG2   | 5:3E:184:ILE:HG13  | 1.89                     | 0.54              |
| 2:3O:302:GLY:O     | 2:3O:304:HIS:ND1   | 2.41                     | 0.54              |
| 1:3A:172:GLU:HA    | 1:3A:175:ARG:HH21  | 1.72                     | 0.53              |
| 3:3C:316:MET:HG3   | 12:3C:506:3PE:H112 | 1.90                     | 0.53              |
| 5:3E:239:HIS:HE2   | 5:3E:254:ALA:HB2   | 1.73                     | 0.53              |
| 3:3C:348:ILE:O     | 3:3C:352:GLN:HG2   | 2.07                     | 0.53              |
| 5:3E:219:HIS:ND1   | 5:3E:239:HIS:CE1   | 2.75                     | 0.53              |
| 8:3U:41:ASP:OD1    | 8:3U:42:GLN:N      | 2.41                     | 0.53              |
| 2:3B:253:VAL:HG21  | 2:3B:333:ALA:HB2   | 1.90                     | 0.53              |
| 3:3C:26:ASN:HD21   | 3:3C:207:ASN:HB2   | 1.73                     | 0.53              |
| 4:3D:293:MET:HE2   | 12:3E:302:3PE:H12  | 1.90                     | 0.53              |
| 8:3H:42:LEU:O      | 8:3H:46:ARG:HG3    | 2.08                     | 0.53              |
| 11:3T:101:CDL:H132 | 11:3T:102:CDL:H111 | 1.91                     | 0.53              |
| 1:3A:58:PHE:HB3    | 1:3A:182:LEU:HD11  | 1.91                     | 0.53              |
| 3:3C:129:MET:HE1   | 3:3C:181:PHE:HB3   | 1.89                     | 0.53              |
| 12:3C:507:3PE:O22  | 12:3C:507:3PE:N    | 2.41                     | 0.53              |
| 1:3N:445:ARG:NH1   | 11:3N:502:CDL:OB2  | 2.41                     | 0.53              |
| 12:3R:302:3PE:H3B1 | 17:3R:303:PC1:H3D2 | 1.90                     | 0.53              |
| 1:3A:445:ARG:NH2   | 12:3A:503:3PE:O14  | 2.42                     | 0.53              |
| 5:3E:194:GLN:HE22  | 5:3E:250:ARG:HD2   | 1.72                     | 0.53              |
| 2:3O:352:LEU:HB3   | 2:3O:411:ILE:HD11  | 1.89                     | 0.53              |
| 1:3A:100:LYS:HE2   | 1:3A:373:THR:OG1   | 2.09                     | 0.53              |
| 1:3A:354:VAL:HG21  | 1:3A:404:ALA:HA    | 1.91                     | 0.53              |
| 3:3P:103:TYR:O     | 3:3P:315:MET:HG3   | 2.08                     | 0.53              |
| 4:3Q:98:PRO:O      | 4:3Q:102:ARG:HG3   | 2.09                     | 0.53              |
| 7:3T:3:GLU:N       | 7:3T:3:GLU:OE1     | 2.39                     | 0.53              |
| 3:3C:97:HIS:CE1    | 3:3C:100:ARG:HH22  | 2.26                     | 0.53              |
| 12:3C:507:3PE:N    | 12:3C:507:3PE:O14  | 2.39                     | 0.53              |
| 4:3D:267:THR:O     | 4:3D:271:VAL:HG12  | 2.08                     | 0.53              |
| 6:3F:45:ARG:HG2    | 6:3F:45:ARG:HH11   | 1.73                     | 0.53              |
| 7:3T:68:LYS:HE3    | 7:3T:68:LYS:HA     | 1.90                     | 0.53              |
| 2:3O:141:GLN:HE22  | 2:3O:186:VAL:HB    | 1.74                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:3P:116:GLY:C     | 13:3P:502:HEM:HBC2 | 2.33                     | 0.53              |
| 5:3R:191:GLU:HB2   | 5:3R:194:GLN:HE22  | 1.73                     | 0.53              |
| 5:3R:239:HIS:HB3   | 16:3R:301:FES:S1   | 2.49                     | 0.53              |
| 5:3I:68:VAL:HG23   | 5:3I:74:ALA:HB2    | 1.91                     | 0.53              |
| 1:3A:23:LEU:HD21   | 1:3A:219:LEU:HD23  | 1.90                     | 0.52              |
| 1:3A:324:PHE:HE2   | 1:3A:335:MET:HE2   | 1.74                     | 0.52              |
| 1:3N:156:THR:OG1   | 1:3N:239:SER:OG    | 2.23                     | 0.52              |
| 1:3N:269:PRO:HB2   | 1:3N:410:VAL:HG11  | 1.90                     | 0.52              |
| 2:3O:27:THR:HG21   | 2:3O:217:LYS:HZ2   | 1.74                     | 0.52              |
| 1:3A:317:THR:OG1   | 1:3A:318:GLY:N     | 2.42                     | 0.52              |
| 3:3C:234:PHE:HB3   | 11:3G:102:CDL:H772 | 1.90                     | 0.52              |
| 1:3N:148:VAL:HG12  | 5:3R:80:HIS:CD2    | 2.44                     | 0.52              |
| 2:3O:217:LYS:O     | 2:3O:221:GLU:HG3   | 2.08                     | 0.52              |
| 9:3W:18:SER:HB3    | 10:3X:24:TRP:CE2   | 2.44                     | 0.52              |
| 4:3D:306:PRO:HB3   | 12:3G:101:3PE:H361 | 1.92                     | 0.52              |
| 1:3N:3:THR:N       | 1:3N:6:GLN:OE1     | 2.40                     | 0.52              |
| 2:3O:303:VAL:O     | 5:3V:52:ARG:NH2    | 2.42                     | 0.52              |
| 7:3T:44:CYS:SG     | 11:3T:102:CDL:HB32 | 2.50                     | 0.52              |
| 2:3B:120:MET:SD    | 2:3B:219:VAL:HG11  | 2.49                     | 0.52              |
| 3:3C:15:ASN:HA     | 3:3C:19:ILE:HB     | 1.92                     | 0.52              |
| 6:3F:113:ARG:O     | 6:3F:117:GLU:HG2   | 2.08                     | 0.52              |
| 1:3N:235:ARG:HH21  | 5:3R:92:ARG:NH1    | 2.07                     | 0.52              |
| 4:3Q:134:TYR:OH    | 4:3Q:160:MET:HB3   | 2.09                     | 0.52              |
| 6:3S:22:ASN:O      | 6:3S:28:LYS:NZ     | 2.43                     | 0.52              |
| 3:3P:110:LEU:O     | 3:3P:114:ASN:ND2   | 2.42                     | 0.52              |
| 5:3R:204:ARG:NH1   | 5:3R:246:SER:O     | 2.43                     | 0.52              |
| 2:3B:71:LEU:HD12   | 5:3I:68:VAL:HG11   | 1.90                     | 0.52              |
| 2:3B:171:ALA:HB3   | 2:3B:237:ALA:HB2   | 1.92                     | 0.52              |
| 3:3P:375:ASN:O     | 6:3S:17:ARG:NH1    | 2.37                     | 0.52              |
| 5:3R:105:GLU:OE1   | 5:3R:105:GLU:N     | 2.43                     | 0.52              |
| 12:3Y:101:3PE:H371 | 12:3Y:101:3PE:O32  | 2.10                     | 0.52              |
| 1:3A:356:ARG:HG3   | 2:3B:91:ALA:HA     | 1.92                     | 0.52              |
| 3:3C:310:SER:HA    | 3:3C:374:ASN:HD21  | 1.75                     | 0.52              |
| 4:3D:140:VAL:HG22  | 4:3D:146:GLU:HA    | 1.91                     | 0.52              |
| 3:3P:190:THR:HG21  | 14:3P:503:U10:H252 | 1.92                     | 0.52              |
| 10:3Y:39:ARG:NH2   | 10:3Y:52:PHE:HB2   | 2.22                     | 0.52              |
| 2:3B:109:VAL:HG21  | 2:3B:123:LEU:HB2   | 1.92                     | 0.52              |
| 1:3N:146:ARG:C     | 1:3N:146:ARG:HD2   | 2.35                     | 0.52              |
| 2:3O:303:VAL:HG21  | 2:3O:336:VAL:HG22  | 1.91                     | 0.52              |
| 1:3N:58:PHE:HE2    | 1:3N:127:ILE:HG23  | 1.74                     | 0.52              |
| 4:3Q:211:MET:HE1   | 5:3R:127:TYR:CD2   | 2.45                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3B:71:LEU:HD22   | 2:3B:144:LEU:HD23  | 1.92                     | 0.51              |
| 1:3N:226:ASP:OD1   | 1:3N:226:ASP:N     | 2.42                     | 0.51              |
| 2:3O:212:SER:OG    | 2:3O:214:PRO:HD2   | 2.09                     | 0.51              |
| 3:3P:244:LEU:HD13  | 4:3Q:205:GLY:HA2   | 1.91                     | 0.51              |
| 6:3S:67:ASP:HA     | 6:3S:70:MET:HE2    | 1.92                     | 0.51              |
| 1:3A:245:ASP:OD1   | 7:3G:13:ARG:NH1    | 2.43                     | 0.51              |
| 3:3C:40:CYS:HB2    | 3:3C:90:PHE:HD2    | 1.75                     | 0.51              |
| 3:3C:316:MET:HG3   | 12:3C:506:3PE:C11  | 2.40                     | 0.51              |
| 4:3D:115:ARG:HB2   | 4:3D:143:CYS:HB2   | 1.91                     | 0.51              |
| 1:3N:224:VAL:HG22  | 1:3N:225:GLU:H     | 1.75                     | 0.51              |
| 3:3P:35:SER:OG     | 14:3P:503:U10:O5   | 2.26                     | 0.51              |
| 5:3R:155:LYS:NZ    | 5:3R:158:ASP:OD2   | 2.44                     | 0.51              |
| 11:3A:501:CDL:H712 | 11:3A:501:CDL:H541 | 1.90                     | 0.51              |
| 12:3A:502:3PE:H2   | 17:3E:303:PC1:H31  | 1.92                     | 0.51              |
| 2:3B:52:LYS:HE3    | 2:3B:203:ARG:HG2   | 1.92                     | 0.51              |
| 3:3C:44:GLN:HB3    | 13:3C:501:HEM:HAB  | 1.92                     | 0.51              |
| 3:3C:156:ILE:HG21  | 17:3X:101:PC1:H322 | 1.91                     | 0.51              |
| 5:3E:152:ILE:HB    | 5:3E:272:ILE:HG23  | 1.91                     | 0.51              |
| 1:3N:25:VAL:HG21   | 1:3N:209:LEU:HD13  | 1.91                     | 0.51              |
| 1:3N:235:ARG:HH11  | 5:3R:99:SER:HA     | 1.76                     | 0.51              |
| 10:3Y:9:ARG:HA     | 10:3Y:12:GLU:OE1   | 2.09                     | 0.51              |
| 1:3A:349:ALA:H     | 1:3A:408:ARG:HH11  | 1.56                     | 0.51              |
| 5:3I:55:LEU:O      | 5:3I:56:SER:C      | 2.53                     | 0.51              |
| 3:3P:63:PHE:O      | 3:3P:67:THR:HG23   | 2.09                     | 0.51              |
| 7:3T:29:TYR:CE1    | 11:3T:101:CDL:HA61 | 2.45                     | 0.51              |
| 4:3D:289:HIS:O     | 4:3D:293:MET:HG3   | 2.11                     | 0.51              |
| 1:3N:209:LEU:HG    | 1:3N:213:GLN:NE2   | 2.26                     | 0.51              |
| 12:3N:501:3PE:H332 | 11:3N:502:CDL:HA21 | 1.92                     | 0.51              |
| 2:3O:163:LEU:HD21  | 2:3O:258:VAL:HG21  | 1.92                     | 0.51              |
| 5:3R:141:SER:OG    | 5:3R:142:ALA:N     | 2.42                     | 0.51              |
| 2:3B:133:ARG:HD2   | 2:3B:135:TRP:CZ2   | 2.46                     | 0.51              |
| 3:3C:50:PHE:CE2    | 5:3E:136:PHE:HB3   | 2.45                     | 0.51              |
| 1:3N:36:THR:HG21   | 1:3N:373:THR:HA    | 1.92                     | 0.51              |
| 1:3N:204:GLU:HG3   | 1:3N:207[A]:GLN:H  | 1.76                     | 0.51              |
| 4:3D:218:LEU:O     | 4:3D:238:ASN:ND2   | 2.42                     | 0.51              |
| 5:3E:204:ARG:NH2   | 5:3E:246:SER:O     | 2.29                     | 0.51              |
| 3:3P:132:VAL:HG22  | 3:3P:143:ALA:HB2   | 1.92                     | 0.51              |
| 3:3P:159:ASP:OD1   | 3:3P:160:LEU:N     | 2.44                     | 0.51              |
| 5:3R:214:ILE:HD11  | 5:3R:261:PRO:HB3   | 1.92                     | 0.51              |
| 5:3R:263:TYR:HB3   | 5:3R:273:VAL:HA    | 1.93                     | 0.51              |
| 1:3A:145:MET:HB3   | 1:3A:252:HIS:CE1   | 2.46                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:3P:211:ILE:HG21  | 6:3S:62:ILE:HD13   | 1.93                     | 0.51              |
| 5:3R:152:ILE:O     | 5:3R:152:ILE:HG13  | 2.10                     | 0.51              |
| 6:3S:98:ILE:O      | 6:3S:102:LYS:HG2   | 2.11                     | 0.51              |
| 1:3N:316:GLU:OE1   | 1:3N:316:GLU:N     | 2.40                     | 0.51              |
| 2:3O:109:VAL:HG12  | 2:3O:123:LEU:HD13  | 1.92                     | 0.51              |
| 1:3A:97:TYR:OH     | 1:3A:190:TYR:OH    | 2.15                     | 0.51              |
| 1:3A:360:ILE:HG23  | 5:3I:33:ALA:HB2    | 1.93                     | 0.51              |
| 1:3N:111:GLU:HA    | 1:3N:215:HIS:HD2   | 1.76                     | 0.51              |
| 4:3Q:8:PRO:HG2     | 4:3Q:10:TYR:HE1    | 1.75                     | 0.51              |
| 4:3Q:178:THR:HG22  | 8:3U:13:LEU:HD21   | 1.92                     | 0.51              |
| 5:3R:179:ARG:HH22  | 5:3R:208:PRO:HB3   | 1.76                     | 0.51              |
| 2:3B:328:SER:HB2   | 2:3B:336:VAL:HG21  | 1.93                     | 0.50              |
| 4:3D:257:VAL:HG13  | 4:3D:258:LEU:HG    | 1.91                     | 0.50              |
| 2:3O:324:ILE:HD11  | 2:3O:344:VAL:HG21  | 1.94                     | 0.50              |
| 2:3B:167:ALA:O     | 2:3B:240:ARG:N     | 2.42                     | 0.50              |
| 3:3C:171:ASP:OD1   | 3:3C:172:LYS:HD3   | 2.12                     | 0.50              |
| 4:3D:297:MET:HA    | 12:3E:302:3PE:H321 | 1.93                     | 0.50              |
| 9:3J:5:THR:N       | 9:3J:9:ARG:HH21    | 2.09                     | 0.50              |
| 5:3R:179:ARG:HD2   | 5:3R:245:ALA:HB1   | 1.94                     | 0.50              |
| 12:3C:507:3PE:H2B2 | 5:3R:130:LYS:HA    | 1.92                     | 0.50              |
| 4:3D:92:GLU:OE2    | 4:3D:92:GLU:N      | 2.45                     | 0.50              |
| 2:3B:51:ILE:HG12   | 2:3B:204:MET:HG2   | 1.94                     | 0.50              |
| 3:3C:44:GLN:OE1    | 3:3C:44:GLN:HA     | 2.11                     | 0.50              |
| 3:3C:165:TRP:O     | 3:3C:174:THR:OG1   | 2.20                     | 0.50              |
| 2:3O:137:VAL:O     | 2:3O:141:GLN:HG2   | 2.11                     | 0.50              |
| 3:3P:215:MET:HE1   | 6:3S:63:LYS:N      | 2.25                     | 0.50              |
| 7:3T:71:ARG:NE     | 8:3U:56:GLU:OE2    | 2.33                     | 0.50              |
| 1:3A:140:GLU:HA    | 5:3I:48:SER:HB2    | 1.92                     | 0.50              |
| 4:3D:108:SER:HB2   | 4:3D:288:ASP:OD1   | 2.11                     | 0.50              |
| 1:3N:375:VAL:O     | 1:3N:379:ILE:HG13  | 2.10                     | 0.50              |
| 2:3O:301:LYS:HG3   | 2:3O:301:LYS:O     | 2.11                     | 0.50              |
| 4:3Q:186:VAL:HG21  | 15:3Q:501:HEC:HBB3 | 1.92                     | 0.50              |
| 1:3A:429:GLU:OE2   | 7:3G:7:GLY:N       | 2.44                     | 0.50              |
| 4:3D:98:TYR:HB3    | 8:3H:99:PHE:HE2    | 1.76                     | 0.50              |
| 5:3I:53:GLU:O      | 5:3I:56:SER:HB3    | 2.12                     | 0.50              |
| 2:3O:275:LEU:HD13  | 2:3O:410:VAL:HG13  | 1.93                     | 0.50              |
| 3:3C:200:LEU:HD23  | 14:3C:503:U10:H4M3 | 1.92                     | 0.50              |
| 9:3J:33:GLU:OE2    | 10:3Y:34:TRP:NE1   | 2.44                     | 0.50              |
| 9:3J:50:GLY:H      | 9:3J:55:HIS:CE1    | 2.29                     | 0.50              |
| 1:3N:192:ALA:HB2   | 1:3N:219:LEU:HB3   | 1.94                     | 0.50              |
| 6:3S:31:LEU:HD11   | 6:3S:65:ALA:HB2    | 1.94                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:3U:27:ILE:HG22  | 8:3U:30:CYS:HB2    | 1.92                     | 0.50              |
| 2:3O:287:ARG:HA   | 5:3V:53:GLU:CD     | 2.37                     | 0.50              |
| 4:3Q:24:THR:HG1   | 4:3Q:28:ARG:HH12   | 1.56                     | 0.50              |
| 4:3Q:217:PRO:O    | 4:3Q:221:ALA:N     | 2.33                     | 0.50              |
| 2:3B:76:THR:HG21  | 2:3B:133:ARG:NH2   | 2.27                     | 0.50              |
| 5:3E:214:ILE:HB   | 5:3E:259:GLU:HB3   | 1.93                     | 0.50              |
| 3:3P:277:ALA:HB3  | 14:3P:504:U10:H3M1 | 1.93                     | 0.50              |
| 1:3A:401:GLU:OE1  | 1:3A:401:GLU:N     | 2.40                     | 0.49              |
| 2:3B:49:LEU:HD13  | 2:3B:206:LEU:HD13  | 1.94                     | 0.49              |
| 5:3E:167:PHE:HB3  | 5:3E:169:TRP:NE1   | 2.27                     | 0.49              |
| 8:3H:66:ASP:O     | 8:3H:70:SER:OG     | 2.22                     | 0.49              |
| 1:3N:58:PHE:CE2   | 1:3N:127:ILE:HG23  | 2.47                     | 0.49              |
| 2:3O:306:PRO:HA   | 5:3V:52:ARG:HG3    | 1.93                     | 0.49              |
| 1:3A:145:MET:HG2  | 1:3A:252:HIS:CD2   | 2.47                     | 0.49              |
| 1:3A:296:SER:O    | 1:3A:300:THR:OG1   | 2.27                     | 0.49              |
| 2:3B:308:ASP:OD1  | 2:3B:327:ILE:HB    | 2.12                     | 0.49              |
| 3:3C:267:HIS:NE2  | 3:3C:269:LYS:HD3   | 2.26                     | 0.49              |
| 4:3D:160:ASP:OD2  | 4:3D:171:ARG:NE    | 2.44                     | 0.49              |
| 9:3J:53:TRP:CE2   | 9:3J:57:LYS:CG     | 2.81                     | 0.49              |
| 3:3P:197:LEU:HD21 | 13:3P:502:HEM:HMA3 | 1.94                     | 0.49              |
| 5:3R:184:ILE:HD11 | 5:3R:209:GLU:HG3   | 1.95                     | 0.49              |
| 3:3C:81:TYR:OH    | 4:3D:206:ARG:NH1   | 2.46                     | 0.49              |
| 7:3G:19:SER:OG    | 7:3G:20:LEU:N      | 2.42                     | 0.49              |
| 4:3Q:181:GLN:HG2  | 8:3U:77:LEU:HD22   | 1.93                     | 0.49              |
| 3:3C:78:VAL:O     | 3:3C:82:LEU:HB2    | 2.12                     | 0.49              |
| 3:3C:231:GLY:HA2  | 11:3G:102:CDL:H721 | 1.93                     | 0.49              |
| 3:3C:272:TRP:HA   | 3:3C:275:LEU:HD12  | 1.93                     | 0.49              |
| 2:3O:193:TYR:O    | 2:3O:197:ASN:ND2   | 2.30                     | 0.49              |
| 2:3B:76:THR:HG23  | 2:3B:81:SER:HA     | 1.95                     | 0.49              |
| 2:3B:159:VAL:HG21 | 2:3B:254:HIS:HB2   | 1.93                     | 0.49              |
| 4:3Q:207:LYS:NZ   | 12:3R:302:3PE:O12  | 2.27                     | 0.49              |
| 5:3R:236:CYS:H    | 5:3R:242:HIS:HA    | 1.77                     | 0.49              |
| 6:3S:16:ILE:HD12  | 6:3S:16:ILE:H      | 1.77                     | 0.49              |
| 1:3N:304:CYS:SG   | 1:3N:305:GLN:N     | 2.86                     | 0.49              |
| 1:3A:3:THR:O      | 1:3A:5:ALA:N       | 2.42                     | 0.49              |
| 1:3A:269:PRO:HB2  | 1:3A:410:VAL:HG11  | 1.95                     | 0.49              |
| 2:3B:52:LYS:HG3   | 2:3B:387:LEU:HD22  | 1.94                     | 0.49              |
| 1:3N:149:VAL:HG21 | 1:3N:252:HIS:HB3   | 1.95                     | 0.49              |
| 1:3A:185:TYR:CE2  | 1:3A:189:HIS:HD2   | 2.30                     | 0.49              |
| 3:3C:240:LEU:O    | 3:3C:244:LEU:HB2   | 2.11                     | 0.49              |
| 3:3C:360:LEU:HG   | 3:3C:365:LEU:HD23  | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:3C:505:CDL:H712 | 11:3C:505:CDL:HB61 | 1.37                     | 0.49              |
| 5:3E:137:VAL:O     | 5:3E:140:MET:HB2   | 2.12                     | 0.49              |
| 1:3N:204:GLU:HG3   | 1:3N:207[B]:GLN:H  | 1.76                     | 0.49              |
| 2:3O:46:ARG:NE     | 2:3O:110:GLU:OE1   | 2.40                     | 0.49              |
| 5:3R:119:ALA:HB2   | 9:3W:20:PHE:HE1    | 1.78                     | 0.49              |
| 5:3R:153:GLU:OE2   | 5:3R:170:ARG:NE    | 2.46                     | 0.49              |
| 3:3C:55:TYR:OH     | 3:3C:133:LEU:O     | 2.25                     | 0.49              |
| 4:3D:205:VAL:HG13  | 4:3D:212:GLU:HG3   | 1.94                     | 0.49              |
| 2:3O:202:ALA:HB3   | 2:3O:230:LEU:HA    | 1.95                     | 0.49              |
| 3:3P:39:ILE:O      | 3:3P:43:LEU:HD22   | 2.13                     | 0.49              |
| 3:3P:50:PHE:O      | 3:3P:53:MET:HB2    | 2.13                     | 0.49              |
| 3:3P:119:LEU:CD1   | 3:3P:192:LEU:HB3   | 2.40                     | 0.49              |
| 7:3T:67:GLU:OE1    | 7:3T:68:LYS:HD2    | 2.13                     | 0.49              |
| 1:3A:394:GLU:O     | 1:3A:398:ARG:HG3   | 2.13                     | 0.49              |
| 2:3B:261:SER:HB3   | 2:3B:272:PHE:CD2   | 2.47                     | 0.49              |
| 3:3C:128:PHE:CD1   | 14:3C:504:U10:H4M1 | 2.48                     | 0.49              |
| 1:3A:332:ASP:OD1   | 1:3A:333:ASP:N     | 2.46                     | 0.48              |
| 2:3B:77:THR:OG1    | 2:3B:80:ALA:O      | 2.30                     | 0.48              |
| 3:3C:215:MET:HB2   | 7:3G:12:MET:HE2    | 1.95                     | 0.48              |
| 5:3E:219:HIS:NE2   | 5:3E:239:HIS:HB3   | 2.29                     | 0.48              |
| 8:3H:52:ILE:HD12   | 8:3H:53:GLU:H      | 1.78                     | 0.48              |
| 1:3A:359:ASN:O     | 1:3A:363:ASN:ND2   | 2.46                     | 0.48              |
| 5:3R:204:ARG:NH1   | 5:3R:257:ASN:OD1   | 2.45                     | 0.48              |
| 10:3X:51:LYS:HD2   | 10:3X:52:PHE:CE1   | 2.48                     | 0.48              |
| 10:3Y:38:TRP:CD2   | 12:3Y:101:3PE:H221 | 2.48                     | 0.48              |
| 5:3E:155:LYS:HE3   | 5:3E:273:VAL:HG22  | 1.94                     | 0.48              |
| 1:3N:343:MET:HG3   | 1:3N:443:TRP:CD1   | 2.48                     | 0.48              |
| 3:3P:224:TYR:HA    | 3:3P:227:LYS:HB3   | 1.96                     | 0.48              |
| 5:3R:187:GLU:HA    | 5:3R:190:VAL:HG23  | 1.95                     | 0.48              |
| 5:3R:258:LEU:HD12  | 5:3R:258:LEU:H     | 1.77                     | 0.48              |
| 8:3U:20:VAL:HG12   | 8:3U:69:VAL:HG22   | 1.95                     | 0.48              |
| 1:3N:444:LEU:HB3   | 11:3N:502:CDL:H712 | 1.95                     | 0.48              |
| 2:3O:33:LEU:HD11   | 2:3O:224:LEU:HB3   | 1.95                     | 0.48              |
| 3:3P:50:PHE:HA     | 3:3P:53:MET:CG     | 2.42                     | 0.48              |
| 3:3P:236:MET:HG2   | 12:3R:302:3PE:H3A2 | 1.95                     | 0.48              |
| 7:3T:40:ARG:NE     | 11:3T:102:CDL:OB4  | 2.47                     | 0.48              |
| 1:3A:277:ILE:HD11  | 1:3A:345:LEU:HD11  | 1.95                     | 0.48              |
| 3:3C:168:PHE:O     | 5:3R:172:LYS:NZ    | 2.42                     | 0.48              |
| 4:3D:119:GLN:NE2   | 4:3D:261:ASP:OD2   | 2.43                     | 0.48              |
| 3:3C:141:TRP:CD1   | 3:3C:265:PRO:HD3   | 2.49                     | 0.48              |
| 4:3Q:207:LYS:HB3   | 9:3W:35:PHE:HE2    | 1.78                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:306:SER:HB3   | 5:3I:39:GLU:HG2    | 1.95                     | 0.48              |
| 1:3A:264:ASN:O     | 1:3A:266:ASP:N     | 2.47                     | 0.48              |
| 6:3F:39:ASN:N      | 6:3F:39:ASN:OD1    | 2.47                     | 0.48              |
| 1:3N:172:GLU:HG3   | 1:3N:176:LYS:NZ    | 2.29                     | 0.48              |
| 2:3O:47:ILE:HG22   | 2:3O:123:LEU:HD22  | 1.95                     | 0.48              |
| 5:3R:157:SER:O     | 5:3R:159:ILE:N     | 2.47                     | 0.48              |
| 11:3T:102:CDL:H351 | 11:3T:102:CDL:H311 | 1.96                     | 0.48              |
| 5:3R:92:ARG:HB2    | 5:3R:97:LEU:HD13   | 1.95                     | 0.48              |
| 7:3G:38:ASN:O      | 7:3G:42:ARG:HG3    | 2.13                     | 0.47              |
| 1:3N:350:THR:O     | 1:3N:353:GLU:HG2   | 2.13                     | 0.47              |
| 4:3Q:179:MET:N     | 8:3U:15:ASP:OD2    | 2.47                     | 0.47              |
| 1:3A:70:ARG:HH21   | 1:3A:112:LEU:HA    | 1.79                     | 0.47              |
| 1:3A:70:ARG:HH22   | 1:3A:111:GLU:HG2   | 1.78                     | 0.47              |
| 5:3E:181:LYS:HA    | 5:3E:184:ILE:HD12  | 1.96                     | 0.47              |
| 7:3T:18:LEU:HB3    | 7:3T:23:GLN:NE2    | 2.29                     | 0.47              |
| 1:3A:339:GLN:NE2   | 1:3A:441:MET:SD    | 2.87                     | 0.47              |
| 4:3D:295:LEU:O     | 4:3D:299:MET:HE3   | 2.14                     | 0.47              |
| 4:3D:326:TYR:HB2   | 6:3F:72:PHE:CE1    | 2.48                     | 0.47              |
| 5:3E:155:LYS:HD3   | 5:3E:155:LYS:HA    | 1.64                     | 0.47              |
| 5:3E:207:LYS:CG    | 5:3E:210:TRP:HE3   | 2.27                     | 0.47              |
| 6:3F:45:ARG:HG2    | 6:3F:45:ARG:NH1    | 2.28                     | 0.47              |
| 1:3N:144:SER:HA    | 5:3V:47:ARG:CZ     | 2.44                     | 0.47              |
| 7:3T:33:GLY:HA3    | 11:3T:101:CDL:HA62 | 1.96                     | 0.47              |
| 8:3U:17:LEU:HD13   | 8:3U:21:ARG:HD3    | 1.96                     | 0.47              |
| 3:3C:126:THR:HG21  | 13:3C:501:HEM:HBB2 | 1.96                     | 0.47              |
| 1:3N:74:ALA:O      | 1:3N:78:GLU:HG2    | 2.14                     | 0.47              |
| 1:3N:294:LEU:HD12  | 1:3N:307:PHE:CE2   | 2.49                     | 0.47              |
| 3:3C:26:ASN:ND2    | 3:3C:207:ASN:HB2   | 2.29                     | 0.47              |
| 3:3C:32:ASN:O      | 3:3C:36:LEU:HG     | 2.14                     | 0.47              |
| 4:3Q:12:TRP:CZ3    | 4:3Q:184:LYS:HG2   | 2.50                     | 0.47              |
| 1:3A:50:GLU:OE2    | 1:3A:51:LYS:HG3    | 2.15                     | 0.47              |
| 1:3A:298:ALA:O     | 1:3A:302:LYS:N     | 2.44                     | 0.47              |
| 3:3C:65:SER:O      | 3:3C:69:ILE:HG13   | 2.15                     | 0.47              |
| 3:3C:313:ARG:HB3   | 6:3F:50:TYR:HB2    | 1.95                     | 0.47              |
| 5:3E:196:ARG:O     | 5:3E:196:ARG:NH1   | 2.38                     | 0.47              |
| 3:3P:244:LEU:HD23  | 4:3Q:201:ARG:HG3   | 1.96                     | 0.47              |
| 4:3Q:222:MET:O     | 4:3Q:225:HIS:HB3   | 2.14                     | 0.47              |
| 1:3A:62:LEU:HD23   | 1:3A:122:LEU:HA    | 1.97                     | 0.47              |
| 1:3A:172:GLU:O     | 1:3A:176:LYS:HG2   | 2.15                     | 0.47              |
| 2:3B:372:VAL:HG12  | 2:3B:372:VAL:O     | 2.14                     | 0.47              |
| 3:3C:191:ALA:O     | 3:3C:195:VAL:HG23  | 2.14                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:3D:269:SER:HB3   | 8:3H:42:LEU:HB2    | 1.97                     | 0.47              |
| 5:3E:181:LYS:HB2   | 5:3E:181:LYS:HE2   | 1.59                     | 0.47              |
| 9:3J:43:ILE:O      | 9:3J:47:ILE:HG23   | 2.15                     | 0.47              |
| 9:3J:47:ILE:HG13   | 9:3J:48:ASN:ND2    | 2.29                     | 0.47              |
| 1:3N:273:ALA:O     | 1:3N:276:ILE:HB    | 2.15                     | 0.47              |
| 2:3O:81:SER:O      | 2:3O:85:ILE:HG13   | 2.14                     | 0.47              |
| 2:3O:120:MET:O     | 2:3O:124:LEU:HG    | 2.15                     | 0.47              |
| 3:3P:39:ILE:HA     | 3:3P:42:ILE:HD12   | 1.97                     | 0.47              |
| 8:3U:72:LYS:HA     | 8:3U:75:ASN:HD21   | 1.79                     | 0.47              |
| 3:3C:253:PRO:HG2   | 4:3D:209:HIS:CD2   | 2.50                     | 0.47              |
| 13:3C:501:HEM:O1D  | 13:3C:501:HEM:HHA  | 2.15                     | 0.47              |
| 1:3N:19:LEU:HD21   | 1:3N:23:LEU:HD23   | 1.96                     | 0.47              |
| 1:3N:76:GLU:OE2    | 2:3O:290:ASN:N     | 2.47                     | 0.47              |
| 3:3P:373:GLU:HA    | 3:3P:376:LEU:HB2   | 1.97                     | 0.47              |
| 3:3C:40:CYS:HB2    | 3:3C:90:PHE:CD2    | 2.50                     | 0.47              |
| 12:3C:507:3PE:H261 | 12:3C:507:3PE:H222 | 1.97                     | 0.47              |
| 4:3D:298:LEU:HA    | 4:3D:298:LEU:HD23  | 1.74                     | 0.47              |
| 5:3I:64:LEU:HD12   | 5:3I:64:LEU:HA     | 1.77                     | 0.47              |
| 2:3O:217:LYS:HB2   | 2:3O:217:LYS:HE2   | 1.67                     | 0.47              |
| 3:3P:105:GLY:O     | 3:3P:313:ARG:NE    | 2.48                     | 0.47              |
| 7:3T:60:THR:OG1    | 7:3T:64:GLN:NE2    | 2.48                     | 0.47              |
| 1:3A:144:SER:HA    | 5:3I:47:ARG:HD2    | 1.95                     | 0.47              |
| 5:3E:125:VAL:HG11  | 17:3E:303:PC1:H371 | 1.96                     | 0.47              |
| 7:3G:20:LEU:HD21   | 7:3G:24:GLU:HB2    | 1.97                     | 0.47              |
| 2:3O:89:ILE:HG12   | 2:3O:119:LEU:HD23  | 1.97                     | 0.47              |
| 4:3Q:33:TYR:HA     | 4:3Q:37:CYS:HB2    | 1.97                     | 0.47              |
| 5:3R:164:ASN:HA    | 5:3R:177:ARG:HA    | 1.96                     | 0.47              |
| 1:3A:53:ASN:HB2    | 1:3A:165:GLN:HE21  | 1.80                     | 0.46              |
| 2:3B:42:ALA:O      | 2:3B:113:ARG:NH1   | 2.48                     | 0.46              |
| 2:3B:295:LEU:HD13  | 2:3B:309:VAL:HG22  | 1.97                     | 0.46              |
| 3:3C:172:LYS:HD3   | 3:3C:172:LYS:N     | 2.29                     | 0.46              |
| 5:3E:120:THR:HA    | 5:3E:123:VAL:HG12  | 1.97                     | 0.46              |
| 3:3C:35:SER:O      | 3:3C:39:ILE:HG12   | 2.15                     | 0.46              |
| 3:3C:68:HIS:NE2    | 5:3E:145:ASP:OD2   | 2.48                     | 0.46              |
| 3:3C:234:PHE:CE2   | 11:3G:102:CDL:H542 | 2.51                     | 0.46              |
| 3:3C:315:MET:HE1   | 3:3C:321:SER:O     | 2.15                     | 0.46              |
| 8:3H:56:ILE:HD13   | 8:3H:59:ARG:HH21   | 1.81                     | 0.46              |
| 1:3A:163:LEU:HD13  | 1:3A:234:CYS:SG    | 2.56                     | 0.46              |
| 4:3D:206:ARG:HB2   | 4:3D:283:SER:OG    | 2.15                     | 0.46              |
| 5:3I:44:ASP:OD1    | 5:3I:45:ALA:N      | 2.47                     | 0.46              |
| 2:3O:95:LYS:O      | 2:3O:109:VAL:HA    | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:3Q:22:ASP:HB3    | 4:3Q:25:SER:HB3    | 1.96                     | 0.46              |
| 4:3Q:218:LEU:O     | 4:3Q:222:MET:N     | 2.47                     | 0.46              |
| 5:3R:201:ASP:HB3   | 5:3R:246:SER:HB2   | 1.98                     | 0.46              |
| 2:3B:111:CYS:HB3   | 2:3B:119:LEU:HD22  | 1.97                     | 0.46              |
| 1:3N:199:ALA:HB1   | 1:3N:203:VAL:HG11  | 1.96                     | 0.46              |
| 4:3D:111:HIS:ND1   | 4:3D:142:VAL:O     | 2.48                     | 0.46              |
| 5:3E:125:VAL:HG21  | 17:3E:303:PC1:H362 | 1.97                     | 0.46              |
| 5:3E:177:ARG:HG2   | 5:3E:211:VAL:HG13  | 1.96                     | 0.46              |
| 1:3N:123:GLU:OE2   | 1:3N:125:SER:HB3   | 2.15                     | 0.46              |
| 3:3P:241:ILE:HG13  | 4:3Q:208:MET:HE1   | 1.98                     | 0.46              |
| 5:3R:224:PRO:HB2   | 5:3R:234:TYR:HD2   | 1.81                     | 0.46              |
| 8:3U:27:ILE:HG23   | 8:3U:30:CYS:H      | 1.81                     | 0.46              |
| 11:3A:501:CDL:H151 | 11:3A:501:CDL:H312 | 1.98                     | 0.46              |
| 3:3C:107:TYR:HB2   | 3:3C:305:PRO:HG3   | 1.97                     | 0.46              |
| 3:3C:375:ASN:O     | 6:3F:29:ARG:NH2    | 2.49                     | 0.46              |
| 4:3D:297:MET:HE3   | 4:3D:297:MET:HB3   | 1.85                     | 0.46              |
| 5:3E:217:CYS:HB2   | 16:3E:301:FES:S1   | 2.42                     | 0.46              |
| 2:3O:70:ARG:O      | 2:3O:98:VAL:HG21   | 2.15                     | 0.46              |
| 3:3P:202:GLU:OE2   | 3:3P:202:GLU:HA    | 2.15                     | 0.46              |
| 3:3C:277:ALA:HB1   | 3:3C:294:LEU:HD13  | 1.98                     | 0.46              |
| 5:3E:194:GLN:HE21  | 5:3E:250:ARG:HH11  | 1.64                     | 0.46              |
| 6:3F:33:TYR:CE1    | 6:3F:39:ASN:HB3    | 2.49                     | 0.46              |
| 2:3O:180:ASP:HA    | 2:3O:183:ILE:HG13  | 1.98                     | 0.46              |
| 5:3V:77:ARG:HD2    | 5:3V:77:ARG:C      | 2.41                     | 0.46              |
| 7:3T:61:TRP:HA     | 7:3T:64:GLN:OE1    | 2.15                     | 0.46              |
| 11:3A:501:CDL:H331 | 11:3A:501:CDL:H372 | 1.98                     | 0.46              |
| 4:3D:261:ASP:OD1   | 4:3D:261:ASP:N     | 2.48                     | 0.46              |
| 7:3G:6:PHE:HA      | 7:3G:9:LEU:HD21    | 1.97                     | 0.46              |
| 8:3H:91:ASP:OD1    | 8:3H:91:ASP:C      | 2.58                     | 0.46              |
| 5:3I:62:ARG:HB2    | 5:3I:77:ARG:NH2    | 2.31                     | 0.46              |
| 3:3P:29:SER:HB3    | 11:3T:101:CDL:HB62 | 1.98                     | 0.46              |
| 3:3P:138:MET:HE2   | 3:3P:254:ASP:HB2   | 1.98                     | 0.46              |
| 4:3Q:72:ASP:HB2    | 4:3Q:83:ARG:HG2    | 1.98                     | 0.46              |
| 5:3R:256:LEU:HD23  | 5:3R:256:LEU:HA    | 1.80                     | 0.46              |
| 1:3A:41:ILE:N      | 1:3A:95:THR:O      | 2.49                     | 0.46              |
| 1:3A:301:ARG:NH2   | 3:3C:1:MET:O       | 2.44                     | 0.46              |
| 5:3E:187:GLU:OE1   | 5:3E:248:ARG:NH1   | 2.46                     | 0.46              |
| 5:3E:248:ARG:HA    | 5:3E:257:ASN:HB3   | 1.99                     | 0.46              |
| 8:3H:57:LYS:HA     | 8:3H:57:LYS:HE2    | 1.96                     | 0.46              |
| 5:3R:131:ASN:HD21  | 12:3R:302:3PE:H112 | 1.81                     | 0.46              |
| 5:3R:152:ILE:HB    | 5:3R:272:ILE:HD12  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:3A:135:LEU:O    | 1:3A:139:GLN:HG3   | 2.16                     | 0.45              |
| 2:3B:334:GLY:O    | 2:3B:338:LYS:HG2   | 2.15                     | 0.45              |
| 2:3B:408:ALA:O    | 2:3B:411:ILE:HG22  | 2.16                     | 0.45              |
| 3:3C:170:VAL:HG13 | 3:3C:174:THR:HG21  | 1.98                     | 0.45              |
| 5:3E:98:ASP:OD1   | 5:3E:98:ASP:N      | 2.50                     | 0.45              |
| 7:3G:39:VAL:HG22  | 7:3G:42:ARG:NH2    | 2.31                     | 0.45              |
| 2:3O:100:SER:HB2  | 2:3O:105:MET:HG3   | 1.98                     | 0.45              |
| 1:3A:316:GLU:HG2  | 1:3A:317:THR:HG22  | 1.97                     | 0.45              |
| 5:3E:241:SER:HB3  | 5:3E:249:ILE:HB    | 1.98                     | 0.45              |
| 7:3G:75:ASN:HB2   | 7:3G:82:PRO:HD2    | 1.96                     | 0.45              |
| 8:3H:54:LYS:H     | 8:3H:54:LYS:HD2    | 1.81                     | 0.45              |
| 8:3U:53:ASP:OD1   | 8:3U:53:ASP:N      | 2.48                     | 0.45              |
| 4:3D:216:PHE:HB2  | 4:3D:276:CYS:SG    | 2.56                     | 0.45              |
| 5:3E:243:TYR:CZ   | 5:3E:258:LEU:HG    | 2.52                     | 0.45              |
| 5:3E:256:LEU:HD12 | 5:3E:256:LEU:HA    | 1.86                     | 0.45              |
| 3:3P:207:ASN:ND2  | 3:3P:211:ILE:O     | 2.39                     | 0.45              |
| 4:3Q:30:PHE:CZ    | 4:3Q:64:LEU:HD21   | 2.51                     | 0.45              |
| 8:3U:29:LYS:HZ1   | 8:3U:32:LYS:HD2    | 1.82                     | 0.45              |
| 1:3A:125:SER:O    | 1:3A:129:LYS:HE3   | 2.16                     | 0.45              |
| 2:3B:253:VAL:HG12 | 2:3B:428:GLY:HA3   | 1.96                     | 0.45              |
| 4:3D:327:ARG:HD2  | 4:3D:327:ARG:HA    | 1.71                     | 0.45              |
| 5:3E:170:ARG:NH1  | 3:3P:168:PHE:HB3   | 2.31                     | 0.45              |
| 1:3N:204:GLU:OE2  | 1:3N:205:HIS:N     | 2.49                     | 0.45              |
| 12:3R:302:3PE:O12 | 12:3R:302:3PE:H32  | 2.17                     | 0.45              |
| 1:3A:329:MET:HE1  | 7:3G:8:HIS:CD2     | 2.52                     | 0.45              |
| 3:3C:113:TRP:NE1  | 3:3C:301:LEU:O     | 2.37                     | 0.45              |
| 1:3N:334:MET:HB2  | 1:3N:334:MET:HE2   | 1.83                     | 0.45              |
| 1:3N:444:LEU:HA   | 9:3W:17:THR:HG21   | 1.99                     | 0.45              |
| 3:3P:32:ASN:HD22  | 11:3T:101:CDL:H721 | 1.82                     | 0.45              |
| 3:3P:242:LEU:HD23 | 3:3P:242:LEU:HA    | 1.77                     | 0.45              |
| 5:3R:159:ILE:HG23 | 5:3R:210:TRP:HZ3   | 1.80                     | 0.45              |
| 2:3B:342:ASP:O    | 2:3B:346:THR:HG23  | 2.16                     | 0.45              |
| 3:3C:128:PHE:O    | 3:3C:132:VAL:HG23  | 2.16                     | 0.45              |
| 4:3D:130:SER:O    | 4:3D:200:ASP:HA    | 2.17                     | 0.45              |
| 5:3E:92:ARG:HA    | 7:3G:25:GLN:HA     | 1.99                     | 0.45              |
| 1:3N:429:GLU:OE2  | 7:3T:7:LEU:HB2     | 2.17                     | 0.45              |
| 2:3O:214:PRO:O    | 2:3O:218:GLN:HG2   | 2.17                     | 0.45              |
| 3:3P:349:ILE:O    | 3:3P:353:LEU:HD12  | 2.16                     | 0.45              |
| 5:3R:247:GLY:O    | 5:3R:257:ASN:HB2   | 2.15                     | 0.45              |
| 2:3B:375:SER:O    | 2:3B:379:LEU:HB2   | 2.16                     | 0.45              |
| 3:3C:114:ASN:HD22 | 3:3C:302:ILE:CD1   | 2.27                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:3C:327:MET:HA   | 7:3G:53:PRO:HB3    | 1.99                     | 0.45              |
| 8:3H:98:LEU:HD23  | 8:3H:98:LEU:HA     | 1.82                     | 0.45              |
| 5:3R:153:GLU:OE1  | 5:3R:153:GLU:N     | 2.49                     | 0.45              |
| 6:3S:31:LEU:HD23  | 6:3S:36:THR:HG22   | 1.99                     | 0.45              |
| 8:3U:31:ILE:HD13  | 8:3U:34:ARG:HH22   | 1.82                     | 0.45              |
| 1:3A:111:GLU:HB2  | 1:3A:215:HIS:CE1   | 2.52                     | 0.45              |
| 1:3A:436:ARG:HH11 | 3:3C:222:PRO:HD3   | 1.81                     | 0.45              |
| 3:3C:215:MET:SD   | 3:3C:215:MET:N     | 2.78                     | 0.45              |
| 2:3O:218:GLN:O    | 2:3O:222:ARG:HB2   | 2.16                     | 0.45              |
| 2:3O:287:ARG:HA   | 5:3V:53:GLU:OE1    | 2.17                     | 0.45              |
| 3:3P:26:ASN:HA    | 6:3S:70:MET:HB2    | 1.98                     | 0.45              |
| 3:3P:58:ASP:OD2   | 3:3P:172:LYS:HE3   | 2.16                     | 0.45              |
| 5:3R:131:ASN:O    | 5:3R:135:GLN:HG2   | 2.16                     | 0.45              |
| 3:3C:163:TRP:O    | 3:3C:177:ARG:NH1   | 2.49                     | 0.45              |
| 4:3D:201:LEU:HA   | 4:3D:204:ILE:HG12  | 1.98                     | 0.45              |
| 1:3A:291:SER:N    | 2:3B:90:GLU:OE2    | 2.37                     | 0.45              |
| 2:3B:25:GLU:HB3   | 2:3B:213:HIS:ND1   | 2.32                     | 0.45              |
| 4:3D:96:PRO:O     | 4:3D:213:ASP:HB3   | 2.16                     | 0.45              |
| 4:3D:122:LYS:O    | 4:3D:126:SER:OG    | 2.31                     | 0.45              |
| 5:3E:157:SER:H    | 5:3E:269:ASP:HA    | 1.81                     | 0.45              |
| 9:3J:47:ILE:HG13  | 9:3J:48:ASN:N      | 2.32                     | 0.45              |
| 14:3P:504:U10:O5  | 14:3P:504:U10:H4M2 | 2.17                     | 0.45              |
| 4:3Q:21:LEU:HD22  | 4:3Q:192:TRP:HB2   | 1.99                     | 0.45              |
| 5:3R:155:LYS:HG3  | 5:3R:271:VAL:HG13  | 1.98                     | 0.45              |
| 9:3W:18:SER:HB3   | 10:3X:24:TRP:NE1   | 2.31                     | 0.45              |
| 9:3W:29:LEU:HD22  | 10:3X:34:TRP:CD1   | 2.52                     | 0.45              |
| 1:3A:80:GLU:HG2   | 2:3B:284:HIS:HB2   | 1.99                     | 0.44              |
| 1:3A:373:THR:HB   | 1:3A:374:PRO:HD3   | 1.98                     | 0.44              |
| 2:3B:254:HIS:CD2  | 2:3B:327:ILE:HG12  | 2.51                     | 0.44              |
| 4:3D:139:LEU:HD23 | 4:3D:139:LEU:HA    | 1.80                     | 0.44              |
| 6:3F:52:ASP:O     | 6:3F:56:LYS:NZ     | 2.50                     | 0.44              |
| 7:3G:74:LYS:NZ    | 8:3H:82:GLU:OE2    | 2.49                     | 0.44              |
| 2:3O:196:GLN:HA   | 2:3O:227:ARG:HD2   | 1.98                     | 0.44              |
| 3:3P:287:LYS:HB2  | 3:3P:287:LYS:HE2   | 1.77                     | 0.44              |
| 1:3A:29:GLN:HA    | 1:3A:201:GLY:O     | 2.17                     | 0.44              |
| 1:3A:158:PHE:O    | 1:3A:161:THR:OG1   | 2.34                     | 0.44              |
| 1:3A:280:TYR:HB3  | 1:3A:307:PHE:CE1   | 2.52                     | 0.44              |
| 3:3C:223:TYR:CZ   | 4:3D:319:LEU:HD11  | 2.52                     | 0.44              |
| 2:3O:343:GLN:O    | 2:3O:346:THR:OG1   | 2.23                     | 0.44              |
| 3:3P:319:PRO:HD2  | 6:3S:20:TYR:CE1    | 2.52                     | 0.44              |
| 4:3Q:129:SER:O    | 4:3Q:133:GLY:N     | 2.50                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:364:ALA:HB2   | 5:3I:33:ALA:CB     | 2.47                     | 0.44              |
| 1:3A:407:VAL:HA    | 1:3A:410:VAL:HG12  | 2.00                     | 0.44              |
| 2:3B:78:LYS:HE3    | 2:3B:78:LYS:HB2    | 1.71                     | 0.44              |
| 3:3C:41:LEU:O      | 3:3C:45:ILE:N      | 2.41                     | 0.44              |
| 8:3H:57:LYS:O      | 8:3H:61:ARG:HG3    | 2.17                     | 0.44              |
| 2:3O:87:ARG:HD3    | 2:3O:87:ARG:HA     | 1.76                     | 0.44              |
| 2:3O:314:ALA:HA    | 5:3V:63:PRO:HD3    | 1.98                     | 0.44              |
| 4:3Q:8:PRO:HG2     | 4:3Q:10:TYR:CE1    | 2.52                     | 0.44              |
| 2:3B:84:LYS:HG3    | 6:3S:103:GLU:OE2   | 2.17                     | 0.44              |
| 2:3B:133:ARG:HB2   | 2:3B:136:GLU:HG3   | 1.98                     | 0.44              |
| 3:3C:236:MET:HG2   | 12:3E:302:3PE:H382 | 1.97                     | 0.44              |
| 5:3E:242:HIS:O     | 5:3E:250:ARG:N     | 2.51                     | 0.44              |
| 1:3N:17:SER:OG     | 1:3N:205:HIS:NE2   | 2.37                     | 0.44              |
| 1:3N:161:THR:HG21  | 1:3N:234:CYS:HA    | 1.99                     | 0.44              |
| 4:3Q:41:HIS:HB3    | 4:3Q:113:LEU:HD21  | 1.98                     | 0.44              |
| 5:3R:263:TYR:HA    | 5:3R:273:VAL:O     | 2.17                     | 0.44              |
| 1:3A:332:ASP:OD2   | 1:3A:430:GLN:NE2   | 2.50                     | 0.44              |
| 12:3A:502:3PE:H2   | 12:3A:502:3PE:H221 | 1.64                     | 0.44              |
| 2:3B:366:ALA:O     | 2:3B:370:MET:HB2   | 2.17                     | 0.44              |
| 3:3C:5:ARG:NH1     | 3:3C:15:ASN:OD1    | 2.48                     | 0.44              |
| 3:3C:244:LEU:HD23  | 4:3D:294:GLY:HA2   | 1.99                     | 0.44              |
| 9:3J:52:LEU:HD12   | 9:3J:55:HIS:HE1    | 1.82                     | 0.44              |
| 1:3N:76:GLU:CD     | 2:3O:289:SER:H     | 2.24                     | 0.44              |
| 2:3O:338:LYS:HE3   | 2:3O:338:LYS:HB2   | 1.75                     | 0.44              |
| 14:3P:504:U10:H72  | 14:3P:504:U10:H1M1 | 1.74                     | 0.44              |
| 7:3T:50:PRO:HA     | 7:3T:53:VAL:HG12   | 1.99                     | 0.44              |
| 3:3C:50:PHE:CE2    | 5:3E:140:MET:HE3   | 2.53                     | 0.44              |
| 3:3C:233:LEU:HG    | 4:3D:301:MET:HE3   | 1.99                     | 0.44              |
| 6:3F:67:TYR:O      | 6:3F:71:VAL:HG22   | 2.17                     | 0.44              |
| 1:3N:333:ASP:O     | 1:3N:336:PHE:HB3   | 2.16                     | 0.44              |
| 3:3P:360:LEU:HG    | 3:3P:365:LEU:HG    | 1.99                     | 0.44              |
| 7:3T:49:ALA:N      | 7:3T:50:PRO:HD2    | 2.33                     | 0.44              |
| 1:3A:324:PHE:CE2   | 1:3A:335:MET:HE2   | 2.52                     | 0.44              |
| 1:3A:379:ILE:HG12  | 1:3A:389:ARG:HD3   | 1.97                     | 0.44              |
| 2:3B:96:LEU:O      | 5:3I:70:LEU:N      | 2.50                     | 0.44              |
| 2:3B:415:LYS:O     | 2:3B:419:SER:OG    | 2.29                     | 0.44              |
| 11:3C:505:CDL:H121 | 11:3C:505:CDL:H511 | 1.99                     | 0.44              |
| 12:3C:507:3PE:H231 | 12:3C:507:3PE:H332 | 2.00                     | 0.44              |
| 1:3N:245:ASP:OD1   | 7:3T:11:ARG:HG2    | 2.17                     | 0.44              |
| 5:3R:174:LEU:HD13  | 5:3R:214:ILE:HD13  | 2.00                     | 0.44              |
| 5:3R:199:GLN:HB3   | 5:3R:204:ARG:HH21  | 1.81                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:3B:117:GLU:OE1   | 2:3B:117:GLU:N     | 2.49                     | 0.44              |
| 4:3D:231:LEU:HD23  | 4:3D:231:LEU:HA    | 1.79                     | 0.44              |
| 4:3D:329:PRO:HD3   | 7:3G:14:HIS:CD2    | 2.53                     | 0.44              |
| 7:3G:20:LEU:HD23   | 7:3G:21:SER:N      | 2.32                     | 0.44              |
| 11:3G:102:CDL:H111 | 11:3G:102:CDL:HA4  | 1.62                     | 0.44              |
| 1:3N:439:SER:OG    | 12:3N:503:3PE:H112 | 2.18                     | 0.44              |
| 4:3Q:208:MET:O     | 4:3Q:212:MET:HB2   | 2.18                     | 0.44              |
| 3:3C:138:MET:HE1   | 3:3C:267:HIS:O     | 2.18                     | 0.44              |
| 6:3F:44:MET:HE1    | 6:3F:99:LYS:HB2    | 2.00                     | 0.44              |
| 5:3I:34:LEU:HD22   | 5:3I:34:LEU:H      | 1.82                     | 0.44              |
| 1:3N:15:GLN:OE1    | 1:3N:15:GLN:N      | 2.51                     | 0.44              |
| 1:3N:24:ARG:HH21   | 1:3N:383:LEU:HB3   | 1.82                     | 0.44              |
| 2:3O:56:ARG:HH12   | 2:3O:318:ASP:CG    | 2.26                     | 0.44              |
| 4:3Q:41:HIS:HE1    | 15:3Q:501:HEC:C1A  | 2.29                     | 0.44              |
| 5:3R:240:GLY:O     | 5:3R:242:HIS:N     | 2.51                     | 0.44              |
| 3:3C:213:SER:OG    | 3:3C:217:LYS:NZ    | 2.51                     | 0.43              |
| 1:3N:145:MET:HE2   | 1:3N:252:HIS:CD2   | 2.52                     | 0.43              |
| 5:3R:183:GLU:O     | 5:3R:186:GLN:HG2   | 2.18                     | 0.43              |
| 5:3R:224:PRO:HA    | 5:3R:237:PRO:HD3   | 2.00                     | 0.43              |
| 5:3R:231:PHE:O     | 5:3R:250:ARG:NH1   | 2.50                     | 0.43              |
| 6:3S:95:LYS:HE2    | 6:3S:95:LYS:HB2    | 1.71                     | 0.43              |
| 8:3U:21:ARG:HG3    | 8:3U:65:ARG:HD2    | 2.00                     | 0.43              |
| 1:3A:77:LYS:HE3    | 1:3A:77:LYS:HB2    | 1.67                     | 0.43              |
| 5:3E:209:GLU:OE1   | 5:3E:209:GLU:N     | 2.43                     | 0.43              |
| 8:3H:40:ASP:OD2    | 8:3H:43:THR:N      | 2.50                     | 0.43              |
| 5:3R:240:GLY:HA2   | 5:3R:242:HIS:CE1   | 2.53                     | 0.43              |
| 10:3X:40:LEU:HD23  | 10:3X:41:ILE:CD1   | 2.48                     | 0.43              |
| 3:3C:54:HIS:O      | 3:3C:65:SER:OG     | 2.36                     | 0.43              |
| 4:3D:319:LEU:HA    | 4:3D:322:ARG:HD3   | 2.00                     | 0.43              |
| 6:3F:50:TYR:CD1    | 6:3F:50:TYR:C      | 2.96                     | 0.43              |
| 6:3F:69:ASP:OD1    | 6:3F:69:ASP:C      | 2.61                     | 0.43              |
| 1:3N:303:LEU:HD22  | 1:3N:330:SER:HB3   | 2.00                     | 0.43              |
| 2:3O:166:ALA:O     | 2:3O:242:GLY:N     | 2.48                     | 0.43              |
| 3:3P:132:VAL:HG11  | 3:3P:178:PHE:CD2   | 2.51                     | 0.43              |
| 3:3P:160:LEU:HD12  | 3:3P:160:LEU:HA    | 1.82                     | 0.43              |
| 1:3A:241:ILE:HD11  | 5:3E:85:VAL:HG22   | 2.00                     | 0.43              |
| 2:3B:68:LEU:HD13   | 2:3B:144:LEU:HD11  | 1.99                     | 0.43              |
| 2:3B:100:SER:HB2   | 2:3B:105:MET:HG2   | 2.00                     | 0.43              |
| 2:3B:306:PRO:HA    | 5:3I:52:ARG:HB2    | 2.01                     | 0.43              |
| 3:3P:220:PHE:HE2   | 14:3P:503:U10:H3M2 | 1.83                     | 0.43              |
| 9:3W:33:ARG:HD2    | 9:3W:33:ARG:HA     | 1.81                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:145:MET:H     | 5:3I:47:ARG:NH1    | 2.16                     | 0.43              |
| 2:3B:279:LEU:HD11  | 2:3B:344:VAL:HG22  | 2.00                     | 0.43              |
| 3:3C:24:PRO:O      | 3:3C:224:TYR:OH    | 2.25                     | 0.43              |
| 1:3N:131:ARG:HH22  | 1:3N:177:LEU:C     | 2.26                     | 0.43              |
| 3:3P:125:ALA:O     | 3:3P:129:MET:HG3   | 2.19                     | 0.43              |
| 4:3Q:51:LEU:HD12   | 4:3Q:51:LEU:HA     | 1.81                     | 0.43              |
| 3:3C:89:MET:HE2    | 3:3C:89:MET:HB2    | 1.78                     | 0.43              |
| 5:3E:143:SER:O     | 5:3E:147:LEU:HG    | 2.18                     | 0.43              |
| 6:3F:54:ASP:OD1    | 6:3F:55:VAL:N      | 2.52                     | 0.43              |
| 7:3G:57:PHE:CD1    | 7:3G:57:PHE:C      | 2.97                     | 0.43              |
| 1:3N:255:ILE:HG21  | 1:3N:335:MET:HE1   | 1.99                     | 0.43              |
| 10:3X:40:LEU:HD23  | 10:3X:41:ILE:HD12  | 2.01                     | 0.43              |
| 2:3B:365:LYS:HG2   | 2:3B:399:LEU:HD22  | 2.00                     | 0.43              |
| 7:3G:70:LYS:HE3    | 7:3G:70:LYS:HB2    | 1.85                     | 0.43              |
| 12:3N:503:3PE:H2   | 12:3N:503:3PE:H221 | 1.39                     | 0.43              |
| 2:3O:223:PHE:C     | 2:3O:223:PHE:CD1   | 2.96                     | 0.43              |
| 2:3O:279:LEU:HB3   | 2:3O:295:LEU:HG    | 2.00                     | 0.43              |
| 6:3S:45:GLU:OE1    | 6:3S:48:ARG:NH2    | 2.51                     | 0.43              |
| 7:3T:68:LYS:HA     | 7:3T:71:ARG:HG2    | 1.99                     | 0.43              |
| 3:3C:141:TRP:O     | 3:3C:144:THR:OG1   | 2.34                     | 0.43              |
| 4:3D:300:MET:HE3   | 9:3J:36:PHE:CE2    | 2.54                     | 0.43              |
| 9:3J:52:LEU:HD12   | 9:3J:52:LEU:H      | 1.82                     | 0.43              |
| 1:3N:45:SER:HB3    | 1:3N:92:ARG:HG2    | 2.00                     | 0.43              |
| 2:3O:27:THR:HG21   | 2:3O:217:LYS:NZ    | 2.34                     | 0.43              |
| 3:3P:32:ASN:ND2    | 11:3T:101:CDL:H721 | 2.34                     | 0.43              |
| 3:3P:350:ILE:HD11  | 7:3T:61:TRP:HZ3    | 1.83                     | 0.43              |
| 7:3T:53:VAL:O      | 7:3T:57:LEU:HG     | 2.18                     | 0.43              |
| 11:3T:102:CDL:HB62 | 11:3T:102:CDL:H712 | 1.22                     | 0.43              |
| 8:3U:35:GLU:HA     | 8:3U:38:GLU:OE2    | 2.18                     | 0.43              |
| 1:3A:17:SER:OG     | 1:3A:205:HIS:NE2   | 2.45                     | 0.43              |
| 2:3B:193:TYR:O     | 2:3B:197:ASN:ND2   | 2.39                     | 0.43              |
| 3:3C:302:ILE:HD12  | 3:3C:302:ILE:HA    | 1.81                     | 0.43              |
| 3:3C:360:LEU:HG    | 3:3C:365:LEU:CD2   | 2.48                     | 0.43              |
| 4:3D:108:SER:N     | 9:3J:48:ASN:OD1    | 2.51                     | 0.43              |
| 5:3E:187:GLU:HG2   | 5:3E:245:ALA:HB3   | 2.00                     | 0.43              |
| 6:3F:65:ASN:OD1    | 6:3F:65:ASN:N      | 2.52                     | 0.43              |
| 1:3N:280:TYR:HA    | 1:3N:284:TYR:CE2   | 2.54                     | 0.43              |
| 4:3Q:27:ARG:HB2    | 4:3Q:55:CYS:HB2    | 2.01                     | 0.43              |
| 5:3E:235:TYR:HD1   | 5:3E:242:HIS:HB3   | 1.84                     | 0.43              |
| 8:3H:40:ASP:OD2    | 8:3H:42:LEU:HB3    | 2.18                     | 0.43              |
| 1:3N:306:SER:O     | 1:3N:306:SER:OG    | 2.32                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3N:428:ILE:HD13  | 1:3N:431:LEU:HD23  | 2.00                     | 0.43              |
| 2:3O:261:SER:HB3   | 2:3O:322:PHE:HB2   | 2.01                     | 0.43              |
| 6:3S:82:LYS:HD3    | 6:3S:82:LYS:N      | 2.34                     | 0.43              |
| 9:3W:37:GLN:OE1    | 10:3X:47:TYR:OH    | 2.29                     | 0.43              |
| 1:3A:244:ARG:CZ    | 1:3A:429:GLU:HB2   | 2.49                     | 0.42              |
| 1:3A:375:VAL:O     | 1:3A:379:ILE:HG13  | 2.18                     | 0.42              |
| 14:3C:503:U10:H172 | 14:3C:503:U10:H151 | 1.62                     | 0.42              |
| 5:3E:219:HIS:O     | 5:3E:220:LEU:HB2   | 2.19                     | 0.42              |
| 5:3E:222:CYS:HB3   | 5:3E:238:CYS:HB3   | 1.85                     | 0.42              |
| 6:3F:97:GLU:OE1    | 6:3F:97:GLU:HA     | 2.19                     | 0.42              |
| 7:3G:40:LEU:HD13   | 7:3G:40:LEU:HA     | 1.92                     | 0.42              |
| 1:3N:346:CYS:SG    | 1:3N:411:CYS:HB3   | 2.59                     | 0.42              |
| 2:3O:171:ALA:HB3   | 2:3O:237:ALA:HB2   | 2.00                     | 0.42              |
| 2:3O:387:LEU:HD23  | 2:3O:387:LEU:HA    | 1.77                     | 0.42              |
| 3:3P:286:ASN:OD1   | 3:3P:289:GLY:N     | 2.43                     | 0.42              |
| 3:3P:357:LEU:HD12  | 3:3P:361:ILE:HG13  | 2.01                     | 0.42              |
| 6:3S:53:ASN:OD1    | 6:3S:54:LEU:N      | 2.51                     | 0.42              |
| 7:3T:18:LEU:HA     | 7:3T:18:LEU:HD12   | 1.81                     | 0.42              |
| 8:3U:21:ARG:O      | 8:3U:25:GLU:HG3    | 2.18                     | 0.42              |
| 10:3Y:39:ARG:HG2   | 10:3Y:39:ARG:HH11  | 1.84                     | 0.42              |
| 5:3E:207:LYS:HD3   | 5:3E:207:LYS:HA    | 1.91                     | 0.42              |
| 6:3F:84:GLN:HG2    | 6:3F:84:GLN:O      | 2.19                     | 0.42              |
| 1:3N:235:ARG:NH1   | 5:3R:99:SER:HA     | 2.34                     | 0.42              |
| 1:3N:350:THR:O     | 1:3N:354:VAL:HG23  | 2.19                     | 0.42              |
| 2:3O:49:LEU:HD11   | 2:3O:204:MET:HE2   | 2.00                     | 0.42              |
| 5:3R:190:VAL:HG22  | 5:3R:250:ARG:NH1   | 2.34                     | 0.42              |
| 6:3S:41:ASP:OD1    | 6:3S:41:ASP:N      | 2.48                     | 0.42              |
| 3:3C:315:MET:HE1   | 3:3C:321:SER:C     | 2.44                     | 0.42              |
| 1:3N:15:GLN:CD     | 1:3N:15:GLN:H      | 2.27                     | 0.42              |
| 1:3N:329:MET:HE1   | 7:3T:6:HIS:CE1     | 2.55                     | 0.42              |
| 2:3O:71:LEU:HD22   | 2:3O:144:LEU:HD23  | 2.01                     | 0.42              |
| 2:3O:152:PHE:CD1   | 2:3O:158:GLN:HG2   | 2.54                     | 0.42              |
| 4:3Q:151:PRO:HA    | 4:3Q:156:GLN:HG3   | 2.01                     | 0.42              |
| 4:3Q:163:PRO:HG2   | 4:3Q:164:ILE:HG12  | 2.01                     | 0.42              |
| 5:3R:169:TRP:HB2   | 5:3R:170:ARG:HH21  | 1.85                     | 0.42              |
| 6:3S:18:LYS:O      | 6:3S:22:ASN:ND2    | 2.39                     | 0.42              |
| 7:3T:50:PRO:O      | 7:3T:54:VAL:HG13   | 2.19                     | 0.42              |
| 7:3T:61:TRP:CZ2    | 7:3T:65:GLU:HG3    | 2.54                     | 0.42              |
| 8:3U:19:THR:HG22   | 8:3U:23:GLN:HE21   | 1.83                     | 0.42              |
| 9:3W:57:HIS:CD2    | 9:3W:57:HIS:H      | 2.38                     | 0.42              |
| 10:3X:23:MET:HE2   | 10:3X:23:MET:HB2   | 1.94                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3A:149:VAL:HG21  | 1:3A:252:HIS:HB2   | 2.01                     | 0.42              |
| 2:3B:275:LEU:HD13  | 2:3B:410:VAL:HG12  | 2.01                     | 0.42              |
| 3:3C:28:SER:HB2    | 11:3C:505:CDL:HA21 | 2.00                     | 0.42              |
| 3:3C:94:LEU:HD23   | 3:3C:94:LEU:HA     | 1.81                     | 0.42              |
| 5:3E:208:PRO:HG2   | 5:3E:209:GLU:OE1   | 2.19                     | 0.42              |
| 5:3I:51:CYS:HB2    | 5:3I:54:SER:HB3    | 2.00                     | 0.42              |
| 1:3N:69:ASN:HB2    | 1:3N:115:ASP:OD2   | 2.20                     | 0.42              |
| 3:3P:160:LEU:O     | 3:3P:164:ILE:HG12  | 2.20                     | 0.42              |
| 3:3P:253:PRO:HD2   | 4:3Q:121:HIS:NE2   | 2.34                     | 0.42              |
| 5:3R:209:GLU:H     | 5:3R:209:GLU:CD    | 2.28                     | 0.42              |
| 12:3R:302:3PE:H2B1 | 12:3R:302:3PE:H271 | 2.01                     | 0.42              |
| 1:3A:281:ASP:HA    | 1:3A:306:SER:HA    | 2.01                     | 0.42              |
| 2:3B:327:ILE:HD13  | 5:3I:58:GLN:HB2    | 2.02                     | 0.42              |
| 3:3C:77:TRP:CE2    | 3:3C:78:VAL:HG23   | 2.54                     | 0.42              |
| 5:3E:207:LYS:HG2   | 5:3E:210:TRP:HE3   | 1.84                     | 0.42              |
| 6:3F:82:MET:HG3    | 6:3F:83:ARG:N      | 2.33                     | 0.42              |
| 1:3N:40:TRP:CZ2    | 1:3N:377:GLU:HA    | 2.55                     | 0.42              |
| 12:3N:501:3PE:O32  | 11:3N:502:CDL:H512 | 2.19                     | 0.42              |
| 4:3Q:237:TYR:HB2   | 6:3S:60:PHE:CE1    | 2.54                     | 0.42              |
| 7:3T:67:GLU:CD     | 7:3T:68:LYS:HD2    | 2.44                     | 0.42              |
| 8:3U:28:GLU:HA     | 8:3U:31:ILE:HB     | 2.01                     | 0.42              |
| 2:3B:283:PRO:HD3   | 5:3I:57:GLY:HA2    | 2.02                     | 0.42              |
| 2:3B:310:SER:HB3   | 5:3I:59:ALA:HB3    | 2.01                     | 0.42              |
| 4:3D:171:ARG:HH12  | 4:3D:174:LYS:H     | 1.67                     | 0.42              |
| 1:3N:163:LEU:HD23  | 1:3N:163:LEU:HA    | 1.80                     | 0.42              |
| 12:3N:501:3PE:H12  | 3:3P:4:ILE:HG13    | 2.01                     | 0.42              |
| 3:3P:97:HIS:CE1    | 3:3P:100:ARG:HH22  | 2.37                     | 0.42              |
| 3:3P:117:VAL:N     | 13:3P:502:HEM:HBC2 | 2.34                     | 0.42              |
| 3:3P:235:MET:SD    | 3:3P:236:MET:HE2   | 2.59                     | 0.42              |
| 4:3Q:178:THR:O     | 4:3Q:182:VAL:HG23  | 2.20                     | 0.42              |
| 5:3R:178:HIS:ND1   | 5:3R:209:GLU:O     | 2.34                     | 0.42              |
| 5:3R:242:HIS:ND1   | 5:3R:251:LYS:HB2   | 2.35                     | 0.42              |
| 6:3S:33:ARG:NH2    | 6:3S:91:GLU:OE2    | 2.53                     | 0.42              |
| 1:3A:5:ALA:HA      | 1:3A:8:LEU:HD12    | 2.01                     | 0.42              |
| 1:3A:324:PHE:CG    | 1:3A:334:MET:HG2   | 2.55                     | 0.42              |
| 1:3A:346:CYS:SG    | 1:3A:412:SER:HA    | 2.59                     | 0.42              |
| 1:3N:394:GLU:O     | 1:3N:398:ARG:HG3   | 2.19                     | 0.42              |
| 1:3N:442:PHE:CE2   | 12:3N:503:3PE:H111 | 2.54                     | 0.42              |
| 14:3P:503:U10:H1M1 | 14:3P:503:U10:H72  | 1.81                     | 0.42              |
| 5:3R:194:GLN:CD    | 5:3R:194:GLN:H     | 2.28                     | 0.42              |
| 1:3A:136:GLN:HB3   | 5:3I:50:LEU:HD12   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:3D:102:HIS:HB3  | 4:3D:109:LEU:HA   | 2.02                     | 0.42              |
| 5:3E:161:GLU:HA   | 5:3E:178:HIS:HB3  | 2.01                     | 0.42              |
| 2:3O:264:THR:HG22 | 2:3O:316:TYR:O    | 2.20                     | 0.42              |
| 4:3Q:212:MET:O    | 4:3Q:216:LEU:HB2  | 2.20                     | 0.42              |
| 5:3R:225:ILE:HD12 | 5:3R:229:GLY:HA2  | 2.02                     | 0.42              |
| 5:3V:49:PHE:HB3   | 5:3V:55:LEU:HD22  | 2.02                     | 0.42              |
| 1:3A:29:GLN:HB2   | 1:3A:203:VAL:O    | 2.19                     | 0.42              |
| 2:3B:261:SER:OG   | 2:3B:322:PHE:N    | 2.53                     | 0.42              |
| 2:3B:312:PHE:HA   | 5:3I:61:GLY:HA2   | 2.02                     | 0.42              |
| 3:3C:234:PHE:O    | 3:3C:237:LEU:HB3  | 2.20                     | 0.42              |
| 5:3E:223:VAL:HG11 | 4:3Q:147:LEU:HD21 | 2.02                     | 0.42              |
| 7:3G:52:PRO:HA    | 7:3G:55:VAL:HG22  | 2.01                     | 0.42              |
| 8:3H:53:GLU:OE2   | 8:3H:54:LYS:NZ    | 2.48                     | 0.42              |
| 1:3N:88:ALA:O     | 2:3O:286:LYS:NZ   | 2.43                     | 0.42              |
| 3:3P:243:VAL:O    | 3:3P:247:PRO:HG3  | 2.20                     | 0.42              |
| 3:3C:114:ASN:O    | 3:3C:118:VAL:HG23 | 2.20                     | 0.42              |
| 3:3C:162:GLU:OE1  | 3:3C:162:GLU:N    | 2.37                     | 0.42              |
| 3:3C:299:LEU:O    | 3:3C:302:ILE:HG22 | 2.19                     | 0.42              |
| 12:3N:503:3PE:H32 | 3:3P:221:HIS:CE1  | 2.53                     | 0.42              |
| 3:3C:318:ARG:HB3  | 3:3C:321:SER:HB2  | 2.02                     | 0.41              |
| 4:3D:93:LEU:H     | 4:3D:93:LEU:HD23  | 1.85                     | 0.41              |
| 4:3D:322:ARG:H    | 4:3D:322:ARG:HG3  | 1.71                     | 0.41              |
| 5:3E:167:PHE:HB3  | 5:3E:169:TRP:HE1  | 1.85                     | 0.41              |
| 1:3N:211:LEU:HA   | 1:3N:211:LEU:HD23 | 1.80                     | 0.41              |
| 1:3N:356:ARG:HG3  | 2:3O:91:ALA:HA    | 2.02                     | 0.41              |
| 2:3O:116:ILE:O    | 2:3O:117:GLU:C    | 2.63                     | 0.41              |
| 3:3P:131:TYR:O    | 3:3P:134:PRO:HD2  | 2.20                     | 0.41              |
| 4:3Q:198:HIS:NE2  | 4:3Q:202:LYS:HE2  | 2.35                     | 0.41              |
| 5:3R:159:ILE:HD11 | 5:3R:163:LYS:HB2  | 2.02                     | 0.41              |
| 5:3R:224:PRO:HB2  | 5:3R:234:TYR:HB3  | 2.02                     | 0.41              |
| 1:3A:395:TRP:O    | 1:3A:399:ILE:HD12 | 2.20                     | 0.41              |
| 2:3B:133:ARG:NH2  | 6:3S:96:GLU:OE2   | 2.53                     | 0.41              |
| 2:3B:397:THR:HA   | 2:3B:400:GLN:NE2  | 2.23                     | 0.41              |
| 4:3D:252:PRO:CB   | 15:3D:501:HEC:HHC | 2.50                     | 0.41              |
| 5:3E:155:LYS:N    | 5:3E:270:LEU:O    | 2.52                     | 0.41              |
| 8:3H:65:CYS:O     | 8:3H:69:VAL:HG22  | 2.20                     | 0.41              |
| 5:3R:205:VAL:HA   | 5:3R:263:TYR:OH   | 2.20                     | 0.41              |
| 1:3A:175:ARG:HE   | 1:3A:175:ARG:HB2  | 1.58                     | 0.41              |
| 2:3B:131:GLU:OE1  | 2:3B:133:ARG:NH1  | 2.53                     | 0.41              |
| 2:3B:278:VAL:HG11 | 2:3B:352:LEU:HD11 | 2.03                     | 0.41              |
| 4:3D:96:PRO:HG2   | 4:3D:98:TYR:CE2   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:3D:204:ILE:HG22 | 4:3D:208:ARG:HG2   | 2.03                     | 0.41              |
| 6:3F:110:ILE:HD13 | 6:3F:110:ILE:HA    | 1.92                     | 0.41              |
| 8:3H:48:GLN:HE22  | 8:3H:97:LYS:HE2    | 1.85                     | 0.41              |
| 1:3N:336:PHE:HZ   | 12:3N:501:3PE:H111 | 1.85                     | 0.41              |
| 2:3O:24:LEU:HD23  | 2:3O:392:TYR:CD2   | 2.54                     | 0.41              |
| 2:3O:378:PHE:O    | 2:3O:382:VAL:HG23  | 2.20                     | 0.41              |
| 3:3P:89:MET:HB3   | 3:3P:89:MET:HE3    | 1.62                     | 0.41              |
| 3:3P:91:PHE:CD2   | 3:3P:273:TYR:CG    | 3.08                     | 0.41              |
| 5:3R:205:VAL:HG21 | 5:3R:210:TRP:O     | 2.19                     | 0.41              |
| 1:3A:91:THR:OG1   | 1:3A:92:ARG:N      | 2.52                     | 0.41              |
| 1:3A:360:ILE:HG23 | 5:3I:33:ALA:CB     | 2.50                     | 0.41              |
| 2:3B:241:GLY:HA3  | 2:3B:421:ARG:NH1   | 2.35                     | 0.41              |
| 9:3J:9:ARG:H      | 9:3J:9:ARG:HG2     | 1.61                     | 0.41              |
| 1:3N:149:VAL:HG21 | 1:3N:252:HIS:CB    | 2.50                     | 0.41              |
| 3:3P:154:PRO:O    | 3:3P:156:ILE:N     | 2.51                     | 0.41              |
| 3:3P:313:ARG:HB2  | 6:3S:38:TYR:CD1    | 2.56                     | 0.41              |
| 4:3Q:211:MET:HG2  | 4:3Q:215:LEU:HD12  | 2.01                     | 0.41              |
| 17:3R:303:PC1:O14 | 17:3R:303:PC1:H121 | 2.20                     | 0.41              |
| 1:3A:301:ARG:NH2  | 3:3C:2:THR:HG22    | 2.33                     | 0.41              |
| 2:3B:53:ALA:O     | 2:3B:105:MET:HE2   | 2.21                     | 0.41              |
| 2:3B:57:TYR:HB3   | 2:3B:198:HIS:CE1   | 2.56                     | 0.41              |
| 2:3B:103:GLU:CD   | 2:3B:317:SER:H     | 2.28                     | 0.41              |
| 3:3C:68:HIS:HD2   | 3:3C:72:ASP:HB2    | 1.86                     | 0.41              |
| 4:3D:216:PHE:O    | 4:3D:220:THR:HG23  | 2.21                     | 0.41              |
| 1:3N:155:ALA:HA   | 1:3N:164:ALA:HB1   | 2.03                     | 0.41              |
| 1:3N:297:VAL:HG22 | 3:3P:1:MET:HE1     | 2.03                     | 0.41              |
| 3:3P:108:MET:HB2  | 3:3P:313:ARG:NH2   | 2.35                     | 0.41              |
| 3:3P:321:SER:OG   | 3:3P:373:GLU:OE2   | 2.38                     | 0.41              |
| 5:3R:119:ALA:O    | 5:3R:123:VAL:HG12  | 2.20                     | 0.41              |
| 8:3U:40:CYS:HA    | 8:3U:43:ARG:HH21   | 1.85                     | 0.41              |
| 1:3A:312:ILE:O    | 1:3A:319:LEU:N     | 2.47                     | 0.41              |
| 1:3A:436:ARG:NH2  | 3:3C:20:ASP:OD1    | 2.41                     | 0.41              |
| 2:3B:215:VAL:O    | 2:3B:219:VAL:HG12  | 2.20                     | 0.41              |
| 3:3C:313:ARG:HB3  | 6:3F:50:TYR:CG     | 2.55                     | 0.41              |
| 4:3D:111:HIS:CD2  | 9:3J:52:LEU:HA     | 2.50                     | 0.41              |
| 4:3D:189:ALA:HB1  | 4:3D:198:PRO:HD2   | 2.03                     | 0.41              |
| 4:3D:201:LEU:HB3  | 4:3D:279:LEU:HD11  | 2.03                     | 0.41              |
| 5:3E:155:LYS:HD2  | 5:3E:167:PHE:CD2   | 2.56                     | 0.41              |
| 5:3E:270:LEU:O    | 5:3E:271:VAL:C     | 2.63                     | 0.41              |
| 6:3F:49:ILE:HG21  | 6:3F:55:VAL:HG21   | 2.02                     | 0.41              |
| 1:3N:51:LYS:HB3   | 1:3N:51:LYS:HE2    | 1.89                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:3N:436:ARG:HD2   | 1:3N:436:ARG:HA    | 1.76                     | 0.41              |
| 2:3O:164:HIS:NE2   | 2:3O:316:TYR:OH    | 2.53                     | 0.41              |
| 3:3P:112:THR:HB    | 3:3P:196:HIS:HE1   | 1.86                     | 0.41              |
| 3:3P:287:LYS:H     | 3:3P:287:LYS:HD3   | 1.85                     | 0.41              |
| 4:3Q:19:SER:HA     | 9:3W:47:ASN:OD1    | 2.21                     | 0.41              |
| 4:3Q:231:LYS:NZ    | 11:3T:101:CDL:O1   | 2.53                     | 0.41              |
| 5:3R:242:HIS:O     | 5:3R:250:ARG:HB3   | 2.19                     | 0.41              |
| 1:3A:86:LEU:HD12   | 1:3A:87:ASN:H      | 1.86                     | 0.41              |
| 2:3B:169:ARG:HB3   | 2:3B:238:LYS:HB2   | 2.03                     | 0.41              |
| 3:3C:287:LYS:O     | 3:3C:291:VAL:HG23  | 2.21                     | 0.41              |
| 4:3D:121:TYR:OH    | 4:3D:131:MET:HB3   | 2.20                     | 0.41              |
| 9:3J:14:LEU:HD12   | 9:3J:15:PHE:CD1    | 2.56                     | 0.41              |
| 1:3N:61:HIS:CG     | 1:3N:134:ILE:HD11  | 2.56                     | 0.41              |
| 2:3O:24:LEU:HD12   | 2:3O:25:GLU:H      | 1.84                     | 0.41              |
| 5:3R:241:SER:N     | 5:3R:251:LYS:O     | 2.53                     | 0.41              |
| 7:3T:40:ARG:HB3    | 11:3T:102:CDL:HB31 | 2.02                     | 0.41              |
| 10:3Y:38:TRP:CG    | 12:3Y:101:3PE:H221 | 2.55                     | 0.41              |
| 1:3A:40:TRP:CZ2    | 1:3A:377:GLU:HA    | 2.55                     | 0.41              |
| 1:3A:277:ILE:HB    | 1:3A:309:THR:HG21  | 2.02                     | 0.41              |
| 3:3C:114:ASN:ND2   | 3:3C:302:ILE:HD11  | 2.34                     | 0.41              |
| 3:3C:270:PRO:HD2   | 3:3C:275:LEU:HD23  | 2.03                     | 0.41              |
| 5:3E:222:CYS:N     | 16:3E:301:FES:S2   | 2.94                     | 0.41              |
| 5:3E:241:SER:H     | 5:3E:251:LYS:C     | 2.23                     | 0.41              |
| 6:3F:44:MET:HB2    | 6:3F:47:ASP:OD2    | 2.20                     | 0.41              |
| 1:3N:214:LYS:HD3   | 1:3N:214:LYS:N     | 2.36                     | 0.41              |
| 3:3P:211:ILE:HG12  | 6:3S:35:ASP:O      | 2.21                     | 0.41              |
| 14:3P:503:U10:H3M3 | 14:3P:503:U10:C4M  | 2.33                     | 0.41              |
| 4:3Q:180:SER:HB2   | 8:3U:77:LEU:HD11   | 2.02                     | 0.41              |
| 6:3S:87:LYS:H      | 6:3S:87:LYS:HG2    | 1.73                     | 0.41              |
| 8:3U:17:LEU:HD11   | 8:3U:21:ARG:NH1    | 2.36                     | 0.41              |
| 1:3A:36:THR:O      | 1:3A:199:ALA:HA    | 2.20                     | 0.41              |
| 1:3A:87:ASN:HB3    | 1:3A:98:TYR:CE1    | 2.56                     | 0.41              |
| 1:3A:240:GLU:CD    | 7:3G:19:SER:HB3    | 2.46                     | 0.41              |
| 1:3A:353:GLU:H     | 1:3A:353:GLU:HG2   | 1.69                     | 0.41              |
| 2:3B:250:ASP:OD1   | 2:3B:428:GLY:HA2   | 2.21                     | 0.41              |
| 3:3C:51:LEU:HD12   | 3:3C:83:HIS:CD2    | 2.56                     | 0.41              |
| 3:3C:180:ALA:O     | 3:3C:184:ILE:HG22  | 2.20                     | 0.41              |
| 3:3C:235:MET:HE2   | 3:3C:235:MET:HB3   | 1.93                     | 0.41              |
| 3:3C:236:MET:HB2   | 3:3C:236:MET:HE2   | 1.82                     | 0.41              |
| 5:3E:154:ILE:HG23  | 5:3E:270:LEU:HG    | 2.03                     | 0.41              |
| 5:3E:173:PRO:HD3   | 5:3E:216:VAL:CG1   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:3E:174:LEU:HD22 | 5:3E:213:LEU:O     | 2.21                     | 0.41              |
| 5:3E:177:ARG:NH1  | 5:3E:233:GLY:HA3   | 2.36                     | 0.41              |
| 5:3E:191:GLU:HG3  | 5:3E:194:GLN:H     | 1.86                     | 0.41              |
| 5:3I:35:PRO:O     | 5:3I:36:ALA:C      | 2.63                     | 0.41              |
| 5:3I:62:ARG:HA    | 5:3I:62:ARG:HD2    | 1.92                     | 0.41              |
| 1:3N:236:PHE:CG   | 1:3N:258:GLU:HB2   | 2.56                     | 0.41              |
| 1:3N:239:SER:HB2  | 7:3T:17:SER:O      | 2.20                     | 0.41              |
| 1:3N:290:MET:HE2  | 1:3N:290:MET:HB3   | 1.79                     | 0.41              |
| 2:3O:47:ILE:HD13  | 2:3O:116:ILE:HG21  | 2.03                     | 0.41              |
| 3:3P:173:ALA:HB1  | 3:3P:177:ARG:NH1   | 2.36                     | 0.41              |
| 3:3P:327:MET:HE3  | 3:3P:327:MET:HB2   | 1.90                     | 0.41              |
| 4:3Q:117:VAL:HG12 | 4:3Q:191:ARG:HH21  | 1.84                     | 0.41              |
| 5:3R:128:ALA:HB1  | 12:3R:302:3PE:H392 | 2.03                     | 0.41              |
| 5:3R:244:ASP:CB   | 5:3R:248:ARG:HG2   | 2.51                     | 0.41              |
| 6:3S:96:GLU:HA    | 6:3S:99:ARG:NH1    | 2.35                     | 0.41              |
| 9:3W:9:LEU:HD22   | 9:3W:13:LEU:HD11   | 2.02                     | 0.41              |
| 1:3A:27:SER:HA    | 1:3A:199:ALA:O     | 2.21                     | 0.41              |
| 1:3A:320:LEU:HD21 | 1:3A:415:PHE:CZ    | 2.56                     | 0.41              |
| 3:3C:77:TRP:CD1   | 4:3D:286:GLU:HG3   | 2.55                     | 0.41              |
| 5:3E:111:LYS:HZ2  | 5:3E:111:LYS:HG3   | 1.69                     | 0.41              |
| 6:3F:54:ASP:OD1   | 6:3F:54:ASP:C      | 2.64                     | 0.41              |
| 8:3H:43:THR:HG22  | 8:3H:47:GLU:OE1    | 2.20                     | 0.41              |
| 9:3J:31:PHE:HE1   | 10:3Y:48:ILE:HD11  | 1.86                     | 0.41              |
| 1:3N:431:LEU:HD12 | 1:3N:432:PRO:HD2   | 2.03                     | 0.41              |
| 2:3O:71:LEU:HD11  | 2:3O:147:ASP:OD2   | 2.21                     | 0.41              |
| 4:3Q:216:LEU:HD23 | 4:3Q:216:LEU:HA    | 1.80                     | 0.41              |
| 5:3R:265:PHE:HB2  | 5:3R:271:VAL:HA    | 2.02                     | 0.41              |
| 1:3A:280:TYR:HA   | 1:3A:284:TYR:CE2   | 2.56                     | 0.40              |
| 1:3A:305:GLN:NE2  | 5:3I:42:VAL:HG12   | 2.36                     | 0.40              |
| 2:3B:95:LYS:HE3   | 2:3B:95:LYS:HB3    | 1.80                     | 0.40              |
| 2:3B:109:VAL:HG11 | 2:3B:119:LEU:HB3   | 2.02                     | 0.40              |
| 2:3B:201:SER:HB2  | 2:3B:228:GLY:HA2   | 2.03                     | 0.40              |
| 3:3C:357:LEU:HD23 | 3:3C:361:ILE:HG13  | 2.01                     | 0.40              |
| 4:3D:315:LYS:HD3  | 4:3D:315:LYS:HA    | 1.96                     | 0.40              |
| 7:3G:15:VAL:O     | 7:3G:16:ILE:HD13   | 2.21                     | 0.40              |
| 3:3P:113:TRP:NE1  | 3:3P:301:LEU:O     | 2.32                     | 0.40              |
| 4:3Q:113:LEU:HD12 | 4:3Q:116:ILE:HG21  | 2.01                     | 0.40              |
| 4:3Q:208:MET:HA   | 12:3R:302:3PE:H341 | 2.03                     | 0.40              |
| 5:3R:160:PRO:O    | 5:3R:178:HIS:HB3   | 2.21                     | 0.40              |
| 8:3U:47:ARG:HB3   | 8:3U:50:THR:HB     | 2.02                     | 0.40              |
| 1:3A:68:LYS:HE3   | 1:3A:121:SER:HA    | 2.01                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:3A:219:LEU:HG    | 1:3A:220:SER:H    | 1.86                     | 0.40              |
| 3:3C:132:VAL:HA    | 3:3C:139:SER:OG   | 2.21                     | 0.40              |
| 4:3D:142:VAL:HG11  | 4:3D:281:TRP:CE2  | 2.56                     | 0.40              |
| 5:3E:125:VAL:HG21  | 17:3E:303:PC1:C36 | 2.51                     | 0.40              |
| 6:3F:30:LYS:HA     | 6:3F:30:LYS:HE2   | 2.02                     | 0.40              |
| 2:3O:65:THR:HG23   | 2:3O:191:LEU:HD23 | 2.02                     | 0.40              |
| 3:3P:180:ALA:O     | 3:3P:184:ILE:HG22 | 2.22                     | 0.40              |
| 5:3R:143:SER:O     | 5:3R:147:LEU:HG   | 2.21                     | 0.40              |
| 1:3A:148:VAL:HG22  | 5:3E:80:HIS:CG    | 2.55                     | 0.40              |
| 3:3C:150:LEU:HD23  | 3:3C:150:LEU:HA   | 1.84                     | 0.40              |
| 3:3C:216:ASP:OD1   | 6:3F:75:LYS:NZ    | 2.53                     | 0.40              |
| 4:3D:146:GLU:HG2   | 4:3D:147:GLU:N    | 2.36                     | 0.40              |
| 5:3E:176:VAL:HB    | 5:3E:212:ILE:HG23 | 2.02                     | 0.40              |
| 5:3E:239:HIS:HE2   | 5:3E:241:SER:HB2  | 1.86                     | 0.40              |
| 6:3F:61:ARG:HD3    | 2:3O:135:TRP:CE2  | 2.56                     | 0.40              |
| 2:3O:264:THR:HB    | 2:3O:315:SER:HB2  | 2.03                     | 0.40              |
| 4:3Q:134:TYR:HE1   | 4:3Q:150:ASN:HD22 | 1.68                     | 0.40              |
| 17:3X:101:PC1:H232 | 17:3X:101:PC1:O32 | 2.21                     | 0.40              |
| 1:3A:45:SER:OG     | 1:3A:167:VAL:HA   | 2.21                     | 0.40              |
| 3:3C:91:PHE:CD2    | 3:3C:273:TYR:CG   | 3.10                     | 0.40              |
| 1:3N:208:LEU:HD12  | 1:3N:208:LEU:HA   | 1.91                     | 0.40              |
| 3:3P:223:TYR:CZ    | 4:3Q:230:LEU:HD23 | 2.56                     | 0.40              |
| 6:3S:80:TRP:O      | 6:3S:82:LYS:HD3   | 2.22                     | 0.40              |
| 3:3C:50:PHE:HA     | 3:3C:53:MET:SD    | 2.62                     | 0.40              |
| 3:3C:157:GLY:HA2   | 3:3C:160:LEU:HD12 | 2.04                     | 0.40              |
| 3:3C:234:PHE:CE1   | 3:3C:237:LEU:HD23 | 2.56                     | 0.40              |
| 14:3C:504:U10:O2   | 14:3C:504:U10:C3M | 2.70                     | 0.40              |
| 4:3D:286:GLU:O     | 4:3D:290:ARG:HB2  | 2.22                     | 0.40              |
| 1:3N:122:LEU:HD23  | 1:3N:122:LEU:HA   | 1.93                     | 0.40              |
| 1:3N:224:VAL:HG13  | 1:3N:225:GLU:N    | 2.36                     | 0.40              |
| 1:3N:251:ALA:HB1   | 1:3N:428:ILE:HG22 | 2.03                     | 0.40              |
| 2:3O:26:PHE:CE1    | 2:3O:36:ALA:HB2   | 2.56                     | 0.40              |
| 3:3P:240:LEU:HB3   | 4:3Q:208:MET:HG3  | 2.03                     | 0.40              |
| 14:3P:504:U10:O5   | 14:3P:504:U10:C4M | 2.70                     | 0.40              |
| 5:3V:77:ARG:HD2    | 5:3V:77:ARG:O     | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | 3A    | 436/480 (91%)   | 408 (94%)  | 27 (6%)  | 1 (0%)   | 43          | 72  |
| 1   | 3N    | 444/480 (92%)   | 409 (92%)  | 34 (8%)  | 1 (0%)   | 43          | 72  |
| 2   | 3B    | 414/453 (91%)   | 393 (95%)  | 21 (5%)  | 0        | 100         | 100 |
| 2   | 3O    | 413/453 (91%)   | 384 (93%)  | 29 (7%)  | 0        | 100         | 100 |
| 3   | 3C    | 377/379 (100%)  | 356 (94%)  | 21 (6%)  | 0        | 100         | 100 |
| 3   | 3P    | 377/379 (100%)  | 358 (95%)  | 17 (4%)  | 2 (0%)   | 24          | 57  |
| 4   | 3D    | 235/325 (72%)   | 217 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 4   | 3Q    | 237/325 (73%)   | 221 (93%)  | 16 (7%)  | 0        | 100         | 100 |
| 5   | 3E    | 194/274 (71%)   | 170 (88%)  | 22 (11%) | 2 (1%)   | 12          | 45  |
| 5   | 3I    | 45/274 (16%)    | 36 (80%)   | 9 (20%)  | 0        | 100         | 100 |
| 5   | 3R    | 194/274 (71%)   | 166 (86%)  | 26 (13%) | 2 (1%)   | 12          | 45  |
| 5   | 3V    | 29/274 (11%)    | 28 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 6   | 3F    | 96/111 (86%)    | 95 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 6   | 3S    | 96/111 (86%)    | 95 (99%)   | 0        | 1 (1%)   | 12          | 45  |
| 7   | 3G    | 70/82 (85%)     | 69 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 7   | 3T    | 72/82 (88%)     | 68 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 8   | 3H    | 63/91 (69%)     | 60 (95%)   | 3 (5%)   | 0        | 100         | 100 |
| 8   | 3U    | 63/91 (69%)     | 59 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 9   | 3J    | 54/64 (84%)     | 50 (93%)   | 4 (7%)   | 0        | 100         | 100 |
| 9   | 3W    | 54/64 (84%)     | 53 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 10  | 3X    | 50/56 (89%)     | 44 (88%)   | 4 (8%)   | 2 (4%)   | 2           | 20  |
| 10  | 3Y    | 49/56 (88%)     | 43 (88%)   | 6 (12%)  | 0        | 100         | 100 |
| All | All   | 4062/5178 (78%) | 3782 (93%) | 269 (7%) | 11 (0%)  | 37          | 65  |

All (11) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3A    | 350 | THR  |
| 5   | 3E    | 271 | VAL  |
| 3   | 3P    | 224 | TYR  |
| 5   | 3R    | 158 | ASP  |
| 6   | 3S    | 33  | ARG  |
| 10  | 3X    | 47  | TYR  |
| 3   | 3P    | 110 | LEU  |
| 5   | 3R    | 241 | SER  |
| 1   | 3N    | 224 | VAL  |
| 10  | 3X    | 46  | PRO  |
| 5   | 3E    | 154 | 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   | 3A    | 367/397 (92%)  | 365 (100%) | 2 (0%)   | 81          | 80  |
| 1   | 3N    | 372/397 (94%)  | 357 (96%)  | 15 (4%)  | 28          | 54  |
| 2   | 3B    | 328/355 (92%)  | 327 (100%) | 1 (0%)   | 86          | 83  |
| 2   | 3O    | 327/355 (92%)  | 324 (99%)  | 3 (1%)   | 70          | 76  |
| 3   | 3C    | 332/332 (100%) | 329 (99%)  | 3 (1%)   | 70          | 76  |
| 3   | 3P    | 332/332 (100%) | 327 (98%)  | 5 (2%)   | 57          | 70  |
| 4   | 3D    | 202/258 (78%)  | 202 (100%) | 0        | 100         | 100 |
| 4   | 3Q    | 204/258 (79%)  | 201 (98%)  | 3 (2%)   | 57          | 70  |
| 5   | 3E    | 166/225 (74%)  | 165 (99%)  | 1 (1%)   | 78          | 79  |
| 5   | 3I    | 36/225 (16%)   | 34 (94%)   | 2 (6%)   | 19          | 47  |
| 5   | 3R    | 166/225 (74%)  | 164 (99%)  | 2 (1%)   | 63          | 73  |
| 5   | 3V    | 24/225 (11%)   | 24 (100%)  | 0        | 100         | 100 |
| 6   | 3F    | 90/99 (91%)    | 89 (99%)   | 1 (1%)   | 65          | 74  |
| 6   | 3S    | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 7   | 3G    | 67/73 (92%)    | 66 (98%)   | 1 (2%)   | 57          | 70  |
| 7   | 3T    | 67/73 (92%)    | 67 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 8   | 3H    | 62/85 (73%)     | 61 (98%)   | 1 (2%)   | 55          | 69  |
| 8   | 3U    | 62/85 (73%)     | 62 (100%)  | 0        | 100         | 100 |
| 9   | 3J    | 46/52 (88%)     | 46 (100%)  | 0        | 100         | 100 |
| 9   | 3W    | 46/52 (88%)     | 46 (100%)  | 0        | 100         | 100 |
| 10  | 3X    | 42/46 (91%)     | 42 (100%)  | 0        | 100         | 100 |
| 10  | 3Y    | 41/46 (89%)     | 40 (98%)   | 1 (2%)   | 43          | 63  |
| All | All   | 3469/4294 (81%) | 3428 (99%) | 41 (1%)  | 61          | 73  |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 3A    | 16     | VAL  |
| 1   | 3A    | 195    | MET  |
| 2   | 3B    | 253    | VAL  |
| 3   | 3C    | 229    | ILE  |
| 3   | 3C    | 268    | ILE  |
| 3   | 3C    | 271    | GLU  |
| 5   | 3E    | 120    | THR  |
| 6   | 3F    | 52     | ASP  |
| 7   | 3G    | 69     | GLU  |
| 8   | 3H    | 62     | LEU  |
| 5   | 3I    | 34     | LEU  |
| 5   | 3I    | 37     | THR  |
| 1   | 3N    | 9      | GLN  |
| 1   | 3N    | 28     | GLU  |
| 1   | 3N    | 112    | LEU  |
| 1   | 3N    | 116    | ILE  |
| 1   | 3N    | 117    | VAL  |
| 1   | 3N    | 121    | SER  |
| 1   | 3N    | 132    | ASP  |
| 1   | 3N    | 134    | ILE  |
| 1   | 3N    | 177    | LEU  |
| 1   | 3N    | 181    | ASP  |
| 1   | 3N    | 184    | GLU  |
| 1   | 3N    | 195    | MET  |
| 1   | 3N    | 207[A] | GLN  |
| 1   | 3N    | 207[B] | GLN  |
| 1   | 3N    | 219    | LEU  |
| 2   | 3O    | 109    | VAL  |
| 2   | 3O    | 154    | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 3O    | 183 | ILE  |
| 3   | 3P    | 43  | LEU  |
| 3   | 3P    | 89  | MET  |
| 3   | 3P    | 91  | PHE  |
| 3   | 3P    | 311 | LYS  |
| 3   | 3P    | 373 | GLU  |
| 4   | 3Q    | 21  | LEU  |
| 4   | 3Q    | 71  | GLN  |
| 4   | 3Q    | 113 | LEU  |
| 5   | 3R    | 176 | VAL  |
| 5   | 3R    | 180 | THR  |
| 10  | 3Y    | 40  | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3A    | 21  | ASN  |
| 1   | 3A    | 94  | HIS  |
| 1   | 3A    | 252 | HIS  |
| 1   | 3A    | 271 | GLN  |
| 1   | 3A    | 305 | GLN  |
| 2   | 3B    | 153 | GLN  |
| 2   | 3B    | 162 | ASN  |
| 2   | 3B    | 174 | ASN  |
| 2   | 3B    | 297 | GLN  |
| 3   | 3C    | 137 | GLN  |
| 3   | 3C    | 201 | HIS  |
| 4   | 3D    | 193 | ASN  |
| 4   | 3D    | 245 | GLN  |
| 5   | 3E    | 80  | HIS  |
| 5   | 3E    | 194 | GLN  |
| 5   | 3E    | 199 | GLN  |
| 7   | 3G    | 75  | ASN  |
| 8   | 3H    | 100 | ASN  |
| 1   | 3N    | 126 | GLN  |
| 1   | 3N    | 271 | GLN  |
| 1   | 3N    | 359 | ASN  |
| 2   | 3O    | 125 | ASN  |
| 2   | 3O    | 141 | GLN  |
| 2   | 3O    | 276 | GLN  |
| 2   | 3O    | 394 | GLN  |
| 3   | 3P    | 15  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 3P    | 26  | ASN  |
| 3   | 3P    | 352 | GLN  |
| 3   | 3P    | 374 | ASN  |
| 4   | 3Q    | 71  | GLN  |
| 4   | 3Q    | 106 | ASN  |
| 4   | 3Q    | 121 | HIS  |
| 4   | 3Q    | 166 | ASN  |
| 5   | 3R    | 131 | ASN  |
| 5   | 3R    | 135 | GLN  |
| 5   | 3R    | 242 | HIS  |
| 8   | 3U    | 23  | 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](#)

32 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 16  | FES  | 3R    | 301 | 5    | 0,4,4        | -    | -           | -           |      |             |
| 12  | 3PE  | 3A    | 503 | -    | 31,31,50     | 0.33 | 0           | 34,36,55    | 0.50 | 0           |
| 11  | CDL  | 3G    | 102 | -    | 55,55,99     | 0.35 | 0           | 61,67,111   | 0.60 | 1 (1%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | 3PE  | 3P    | 505 | -    | 32,32,50     | 0.33 | 0        | 35,37,55    | 0.38 | 0        |
| 11  | CDL  | 3T    | 102 | -    | 55,55,99     | 0.36 | 0        | 61,67,111   | 0.52 | 1 (1%)   |
| 12  | 3PE  | 3E    | 302 | -    | 32,32,50     | 0.34 | 0        | 35,37,55    | 0.45 | 0        |
| 12  | 3PE  | 3Y    | 101 | -    | 29,29,50     | 0.35 | 0        | 32,34,55    | 0.42 | 0        |
| 14  | U10  | 3P    | 504 | -    | 32,32,63     | 0.76 | 1 (3%)   | 40,41,79    | 1.01 | 5 (12%)  |
| 11  | CDL  | 3C    | 505 | -    | 51,51,99     | 0.36 | 0        | 57,63,111   | 0.45 | 0        |
| 14  | U10  | 3C    | 503 | -    | 28,28,63     | 0.95 | 2 (7%)   | 36,37,79    | 1.12 | 6 (16%)  |
| 14  | U10  | 3C    | 504 | -    | 23,23,63     | 0.93 | 2 (8%)   | 30,31,79    | 1.21 | 5 (16%)  |
| 15  | HEC  | 3Q    | 501 | 4    | 50,50,50     | 2.84 | 26 (52%) | 68,82,82    | 2.51 | 26 (38%) |
| 17  | PC1  | 3X    | 101 | -    | 28,28,53     | 0.37 | 0        | 34,36,61    | 0.40 | 0        |
| 12  | 3PE  | 3C    | 507 | -    | 33,33,50     | 0.33 | 0        | 36,38,55    | 0.40 | 0        |
| 11  | CDL  | 3N    | 502 | -    | 42,42,99     | 0.39 | 0        | 48,54,111   | 0.57 | 1 (2%)   |
| 12  | 3PE  | 3C    | 506 | -    | 34,34,50     | 0.32 | 0        | 37,39,55    | 0.45 | 0        |
| 13  | HEM  | 3P    | 502 | 3    | 50,50,50     | 1.60 | 9 (18%)  | 67,82,82    | 1.61 | 12 (17%) |
| 13  | HEM  | 3C    | 502 | 3    | 50,50,50     | 1.60 | 9 (18%)  | 67,82,82    | 1.65 | 12 (17%) |
| 16  | FES  | 3E    | 301 | 5    | 0,4,4        | -    | -        | -           | -    | -        |
| 11  | CDL  | 3A    | 501 | -    | 57,57,99     | 0.35 | 0        | 63,69,111   | 0.52 | 0        |
| 13  | HEM  | 3C    | 501 | 3    | 50,50,50     | 1.60 | 9 (18%)  | 67,82,82    | 1.70 | 12 (17%) |
| 11  | CDL  | 3T    | 101 | 7    | 56,56,99     | 0.35 | 0        | 62,68,111   | 0.42 | 0        |
| 12  | 3PE  | 3N    | 501 | -    | 31,31,50     | 0.34 | 0        | 34,36,55    | 0.40 | 0        |
| 17  | PC1  | 3R    | 303 | -    | 44,44,53     | 0.30 | 0        | 50,52,61    | 0.33 | 0        |
| 17  | PC1  | 3E    | 303 | -    | 46,46,53     | 0.29 | 0        | 52,54,61    | 0.29 | 0        |
| 12  | 3PE  | 3G    | 101 | -    | 28,28,50     | 0.34 | 0        | 31,33,55    | 0.42 | 0        |
| 14  | U10  | 3P    | 503 | -    | 32,32,63     | 0.86 | 3 (9%)   | 40,41,79    | 1.31 | 5 (12%)  |
| 15  | HEC  | 3D    | 501 | 4    | 48,49,50     | 2.93 | 25 (52%) | 66,80,82    | 2.37 | 23 (34%) |
| 12  | 3PE  | 3R    | 302 | -    | 46,46,50     | 0.28 | 0        | 49,51,55    | 0.42 | 0        |
| 12  | 3PE  | 3N    | 503 | -    | 24,24,50     | 0.38 | 0        | 27,29,55    | 0.60 | 0        |
| 12  | 3PE  | 3A    | 502 | -    | 26,26,50     | 0.36 | 0        | 29,31,55    | 0.71 | 1 (3%)   |
| 13  | HEM  | 3P    | 501 | 3    | 50,50,50     | 1.61 | 9 (18%)  | 67,82,82    | 1.67 | 11 (16%) |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 16  | FES  | 3R    | 301 | 5    | -       | -            | 0/1/1/1 |
| 12  | 3PE  | 3A    | 503 | -    | -       | 7/35/35/54   | -       |
| 11  | CDL  | 3G    | 102 | -    | -       | 14/66/66/110 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 12  | 3PE  | 3P    | 505 | -    | -       | 5/36/36/54   | -       |
| 11  | CDL  | 3T    | 102 | -    | -       | 17/66/66/110 | -       |
| 12  | 3PE  | 3E    | 302 | -    | -       | 2/36/36/54   | -       |
| 12  | 3PE  | 3Y    | 101 | -    | -       | 8/33/33/54   | -       |
| 14  | U10  | 3P    | 504 | -    | -       | 8/26/50/87   | 0/1/1/1 |
| 11  | CDL  | 3C    | 505 | -    | -       | 11/62/62/110 | -       |
| 14  | U10  | 3C    | 503 | -    | -       | 4/21/45/87   | 0/1/1/1 |
| 14  | U10  | 3C    | 504 | -    | -       | 3/15/39/87   | 0/1/1/1 |
| 15  | HEC  | 3Q    | 501 | 4    | 1/1/3/7 | 7/14/54/54   | -       |
| 17  | PC1  | 3X    | 101 | -    | -       | 9/32/32/57   | -       |
| 12  | 3PE  | 3C    | 507 | -    | -       | 12/37/37/54  | -       |
| 11  | CDL  | 3N    | 502 | -    | -       | 14/53/53/110 | -       |
| 12  | 3PE  | 3C    | 506 | -    | -       | 5/38/38/54   | -       |
| 13  | HEM  | 3P    | 502 | 3    | -       | 8/14/54/54   | -       |
| 13  | HEM  | 3C    | 502 | 3    | -       | 6/14/54/54   | -       |
| 16  | FES  | 3E    | 301 | 5    | -       | -            | 0/1/1/1 |
| 11  | CDL  | 3A    | 501 | -    | -       | 10/68/68/110 | -       |
| 13  | HEM  | 3C    | 501 | 3    | -       | 5/14/54/54   | -       |
| 11  | CDL  | 3T    | 101 | 7    | -       | 16/67/67/110 | -       |
| 12  | 3PE  | 3N    | 501 | -    | -       | 7/35/35/54   | -       |
| 17  | PC1  | 3R    | 303 | -    | -       | 8/48/48/57   | -       |
| 17  | PC1  | 3E    | 303 | -    | -       | 5/50/50/57   | -       |
| 12  | 3PE  | 3G    | 101 | -    | -       | 6/32/32/54   | -       |
| 14  | U10  | 3P    | 503 | -    | -       | 6/26/50/87   | 0/1/1/1 |
| 15  | HEC  | 3D    | 501 | 4    | 1/1/2/7 | 6/13/53/54   | -       |
| 12  | 3PE  | 3R    | 302 | -    | -       | 12/50/50/54  | -       |
| 12  | 3PE  | 3N    | 503 | -    | -       | 7/28/28/54   | -       |
| 12  | 3PE  | 3A    | 502 | -    | -       | 2/30/30/54   | -       |
| 13  | HEM  | 3P    | 501 | 3    | -       | 5/14/54/54   | -       |

All (95) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 15  | 3Q    | 501 | HEC  | C3B-C2B | 5.19 | 1.48        | 1.36     |
| 15  | 3D    | 501 | HEC  | C3B-C2B | 5.15 | 1.47        | 1.36     |
| 15  | 3D    | 501 | HEC  | C3D-C2D | 5.11 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 15  | 3D    | 501 | HEC  | C2A-C3A | 5.10  | 1.47        | 1.36     |
| 13  | 3P    | 501 | HEM  | FE-NB   | 5.05  | 2.10        | 1.94     |
| 13  | 3C    | 501 | HEM  | FE-NB   | 5.04  | 2.10        | 1.94     |
| 13  | 3C    | 502 | HEM  | FE-NB   | 5.00  | 2.10        | 1.94     |
| 15  | 3D    | 501 | HEC  | CHA-C1A | 4.98  | 1.48        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C2A-C3A | 4.96  | 1.47        | 1.36     |
| 13  | 3P    | 502 | HEM  | FE-NB   | 4.93  | 2.10        | 1.94     |
| 15  | 3Q    | 501 | HEC  | FE-NB   | 4.88  | 2.09        | 1.94     |
| 15  | 3Q    | 501 | HEC  | FE-ND   | 4.87  | 2.09        | 1.94     |
| 15  | 3D    | 501 | HEC  | CHD-C1D | 4.87  | 1.48        | 1.38     |
| 15  | 3D    | 501 | HEC  | CHB-C4A | 4.86  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | CHB-C4A | 4.82  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | CHA-C1A | 4.76  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C3D-C2D | 4.73  | 1.47        | 1.36     |
| 15  | 3D    | 501 | HEC  | FE-ND   | 4.67  | 2.09        | 1.94     |
| 15  | 3D    | 501 | HEC  | FE-NB   | 4.62  | 2.09        | 1.94     |
| 15  | 3D    | 501 | HEC  | CHC-C4B | 4.54  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | FE-NC   | 4.51  | 2.10        | 1.95     |
| 15  | 3Q    | 501 | HEC  | FE-NA   | 4.48  | 2.09        | 1.95     |
| 15  | 3Q    | 501 | HEC  | CHD-C1D | 4.46  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | CHC-C4B | 4.43  | 1.47        | 1.38     |
| 15  | 3D    | 501 | HEC  | FE-NC   | 4.28  | 2.09        | 1.95     |
| 15  | 3D    | 501 | HEC  | FE-NA   | 4.27  | 2.09        | 1.95     |
| 13  | 3C    | 501 | HEM  | FE-NC   | 4.10  | 2.08        | 1.95     |
| 13  | 3C    | 502 | HEM  | FE-NC   | 4.04  | 2.08        | 1.95     |
| 13  | 3P    | 502 | HEM  | FE-NC   | 4.04  | 2.08        | 1.95     |
| 13  | 3P    | 501 | HEM  | FE-NC   | 4.00  | 2.08        | 1.95     |
| 15  | 3D    | 501 | HEC  | CHD-C4C | 3.92  | 1.48        | 1.39     |
| 15  | 3D    | 501 | HEC  | CHA-C4D | 3.83  | 1.47        | 1.39     |
| 15  | 3Q    | 501 | HEC  | CHB-C1B | 3.79  | 1.47        | 1.39     |
| 15  | 3Q    | 501 | HEC  | CHA-C4D | 3.73  | 1.47        | 1.39     |
| 15  | 3D    | 501 | HEC  | CHB-C1B | 3.70  | 1.47        | 1.39     |
| 13  | 3P    | 502 | HEM  | C1B-NB  | -3.56 | 1.34        | 1.40     |
| 15  | 3D    | 501 | HEC  | C3C-C2C | 3.55  | 1.48        | 1.38     |
| 13  | 3P    | 501 | HEM  | C1B-NB  | -3.55 | 1.34        | 1.40     |
| 13  | 3C    | 502 | HEM  | C1B-NB  | -3.53 | 1.34        | 1.40     |
| 13  | 3P    | 502 | HEM  | C4D-ND  | -3.50 | 1.34        | 1.40     |
| 15  | 3Q    | 501 | HEC  | CHD-C4C | 3.49  | 1.47        | 1.39     |
| 15  | 3Q    | 501 | HEC  | CHC-C1C | 3.47  | 1.47        | 1.39     |
| 15  | 3D    | 501 | HEC  | CHC-C1C | 3.44  | 1.47        | 1.39     |
| 13  | 3C    | 501 | HEM  | C4D-ND  | -3.42 | 1.34        | 1.40     |
| 13  | 3C    | 501 | HEM  | C1B-NB  | -3.41 | 1.34        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | 3P    | 501 | HEM  | C4D-ND  | -3.40 | 1.34        | 1.40     |
| 13  | 3C    | 502 | HEM  | C4D-ND  | -3.38 | 1.34        | 1.40     |
| 15  | 3D    | 501 | HEC  | C1D-ND  | -3.33 | 1.34        | 1.40     |
| 15  | 3D    | 501 | HEC  | C4B-NB  | -3.29 | 1.34        | 1.40     |
| 15  | 3Q    | 501 | HEC  | C3C-C2C | 3.22  | 1.47        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C4B-NB  | -3.19 | 1.34        | 1.40     |
| 15  | 3Q    | 501 | HEC  | C1D-ND  | -3.09 | 1.34        | 1.40     |
| 14  | 3C    | 503 | U10  | C3-C2   | -2.86 | 1.40        | 1.48     |
| 15  | 3D    | 501 | HEC  | C4A-NA  | -2.79 | 1.34        | 1.39     |
| 13  | 3C    | 502 | HEM  | FE-ND   | -2.72 | 1.86        | 1.94     |
| 15  | 3D    | 501 | HEC  | C4C-NC  | -2.72 | 1.34        | 1.39     |
| 13  | 3P    | 502 | HEM  | FE-ND   | -2.69 | 1.86        | 1.94     |
| 13  | 3P    | 501 | HEM  | FE-ND   | -2.68 | 1.86        | 1.94     |
| 14  | 3P    | 504 | U10  | C3-C2   | -2.67 | 1.41        | 1.48     |
| 14  | 3C    | 504 | U10  | C4-C5   | -2.66 | 1.41        | 1.48     |
| 13  | 3C    | 501 | HEM  | FE-ND   | -2.61 | 1.86        | 1.94     |
| 15  | 3Q    | 501 | HEC  | C4C-NC  | -2.58 | 1.34        | 1.39     |
| 13  | 3P    | 501 | HEM  | C1C-C2C | -2.57 | 1.40        | 1.45     |
| 13  | 3P    | 502 | HEM  | C1C-C2C | -2.57 | 1.40        | 1.45     |
| 13  | 3C    | 501 | HEM  | C1C-C2C | -2.55 | 1.40        | 1.45     |
| 14  | 3P    | 503 | U10  | C3-C2   | -2.53 | 1.41        | 1.48     |
| 14  | 3C    | 503 | U10  | C4-C5   | -2.50 | 1.41        | 1.48     |
| 13  | 3C    | 502 | HEM  | C1C-C2C | -2.49 | 1.40        | 1.45     |
| 15  | 3Q    | 501 | HEC  | C4A-NA  | -2.47 | 1.35        | 1.39     |
| 15  | 3Q    | 501 | HEC  | C1C-C2C | 2.45  | 1.48        | 1.43     |
| 13  | 3C    | 502 | HEM  | C1D-ND  | -2.45 | 1.34        | 1.38     |
| 15  | 3D    | 501 | HEC  | C1A-NA  | -2.41 | 1.35        | 1.39     |
| 15  | 3D    | 501 | HEC  | C1C-NC  | -2.41 | 1.35        | 1.39     |
| 13  | 3P    | 502 | HEM  | C1D-ND  | -2.39 | 1.34        | 1.38     |
| 14  | 3P    | 503 | U10  | C4-C5   | -2.36 | 1.42        | 1.48     |
| 15  | 3D    | 501 | HEC  | C1C-C2C | 2.35  | 1.48        | 1.43     |
| 13  | 3C    | 501 | HEM  | C1D-ND  | -2.31 | 1.34        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C1C-NC  | -2.30 | 1.35        | 1.39     |
| 15  | 3Q    | 501 | HEC  | C1A-NA  | -2.29 | 1.35        | 1.39     |
| 13  | 3P    | 501 | HEM  | C3C-C4C | -2.28 | 1.42        | 1.46     |
| 13  | 3P    | 501 | HEM  | C1D-ND  | -2.27 | 1.34        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C1B-C2B | 2.27  | 1.49        | 1.44     |
| 13  | 3C    | 502 | HEM  | C4B-NB  | -2.25 | 1.34        | 1.38     |
| 15  | 3D    | 501 | HEC  | C1B-C2B | 2.24  | 1.49        | 1.44     |
| 15  | 3Q    | 501 | HEC  | C4D-C3D | 2.23  | 1.48        | 1.45     |
| 13  | 3P    | 502 | HEM  | C3C-C4C | -2.23 | 1.42        | 1.46     |
| 13  | 3C    | 501 | HEM  | C3C-C4C | -2.22 | 1.42        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 13  | 3C    | 502 | HEM  | C3C-C4C | -2.22 | 1.42        | 1.46     |
| 13  | 3P    | 502 | HEM  | C4B-NB  | -2.22 | 1.34        | 1.38     |
| 14  | 3P    | 503 | U10  | C4-C3   | 2.20  | 1.44        | 1.36     |
| 13  | 3C    | 501 | HEM  | C4B-NB  | -2.19 | 1.34        | 1.38     |
| 15  | 3D    | 501 | HEC  | C4D-C3D | 2.13  | 1.48        | 1.45     |
| 13  | 3P    | 501 | HEM  | C4B-NB  | -2.11 | 1.34        | 1.38     |
| 15  | 3Q    | 501 | HEC  | C1A-C2A | 2.03  | 1.48        | 1.45     |
| 14  | 3C    | 504 | U10  | C4-C3   | 2.01  | 1.43        | 1.36     |

All (121) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 3Q    | 501 | HEC  | C1B-C2B-C3B | -5.97 | 100.70      | 106.98   |
| 15  | 3D    | 501 | HEC  | C1B-C2B-C3B | -5.84 | 100.84      | 106.98   |
| 13  | 3C    | 501 | HEM  | CHC-C4B-NB  | 5.56  | 130.40      | 124.42   |
| 15  | 3D    | 501 | HEC  | C1C-C2C-C3C | -5.51 | 100.50      | 106.82   |
| 13  | 3P    | 501 | HEM  | CHC-C4B-NB  | 5.48  | 130.32      | 124.42   |
| 15  | 3Q    | 501 | HEC  | C2A-C1A-NA  | 5.38  | 115.52      | 110.32   |
| 15  | 3Q    | 501 | HEC  | C2B-C1B-NB  | 5.31  | 116.04      | 109.90   |
| 15  | 3Q    | 501 | HEC  | C1C-C2C-C3C | -5.31 | 100.73      | 106.82   |
| 13  | 3C    | 502 | HEM  | CHC-C4B-NB  | 5.27  | 130.09      | 124.42   |
| 15  | 3D    | 501 | HEC  | C2B-C1B-NB  | 5.16  | 115.87      | 109.90   |
| 15  | 3Q    | 501 | HEC  | C3D-C4D-ND  | 5.12  | 115.30      | 110.35   |
| 13  | 3P    | 502 | HEM  | CHC-C4B-NB  | 5.03  | 129.83      | 124.42   |
| 15  | 3Q    | 501 | HEC  | C2D-C1D-ND  | 4.86  | 115.42      | 109.84   |
| 15  | 3D    | 501 | HEC  | C3D-C4D-ND  | 4.66  | 114.86      | 110.35   |
| 13  | 3C    | 501 | HEM  | CHD-C1D-ND  | 4.65  | 129.43      | 124.42   |
| 13  | 3P    | 501 | HEM  | CHD-C1D-ND  | 4.65  | 129.43      | 124.42   |
| 15  | 3D    | 501 | HEC  | C2A-C1A-NA  | 4.60  | 114.76      | 110.32   |
| 15  | 3D    | 501 | HEC  | CBB-CAB-C3B | 4.43  | 124.42      | 112.42   |
| 15  | 3Q    | 501 | HEC  | CBC-CAC-C3C | 4.42  | 124.41      | 112.42   |
| 15  | 3D    | 501 | HEC  | CBC-CAC-C3C | 4.40  | 124.36      | 112.42   |
| 15  | 3Q    | 501 | HEC  | CBB-CAB-C3B | 4.33  | 124.17      | 112.42   |
| 13  | 3C    | 502 | HEM  | CHD-C1D-ND  | 4.25  | 128.99      | 124.42   |
| 15  | 3D    | 501 | HEC  | C2D-C1D-ND  | 4.12  | 114.58      | 109.84   |
| 15  | 3Q    | 501 | HEC  | C2C-C1C-NC  | 3.96  | 116.49      | 110.14   |
| 15  | 3Q    | 501 | HEC  | C1D-C2D-C3D | -3.95 | 102.83      | 106.98   |
| 15  | 3Q    | 501 | HEC  | C3C-C4C-NC  | 3.83  | 114.41      | 110.15   |
| 13  | 3P    | 502 | HEM  | CHD-C1D-ND  | 3.81  | 128.52      | 124.42   |
| 15  | 3D    | 501 | HEC  | C2C-C1C-NC  | 3.76  | 116.17      | 110.14   |
| 13  | 3C    | 501 | HEM  | CHA-C4D-ND  | 3.65  | 128.88      | 124.37   |
| 15  | 3Q    | 501 | HEC  | C3B-C4B-NB  | 3.64  | 114.16      | 110.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15  | 3Q    | 501 | HEC  | C1A-C2A-C3A | -3.59 | 102.38      | 107.11   |
| 13  | 3C    | 502 | HEM  | C1B-NB-C4B  | 3.52  | 109.37      | 105.21   |
| 15  | 3D    | 501 | HEC  | C1D-C2D-C3D | -3.50 | 103.30      | 106.98   |
| 15  | 3D    | 501 | HEC  | C1A-C2A-C3A | -3.49 | 102.51      | 107.11   |
| 13  | 3P    | 502 | HEM  | C1B-NB-C4B  | 3.49  | 109.33      | 105.21   |
| 13  | 3C    | 502 | HEM  | CHA-C4D-ND  | 3.48  | 128.68      | 124.37   |
| 13  | 3C    | 501 | HEM  | CHB-C1B-NB  | 3.45  | 128.63      | 124.37   |
| 13  | 3P    | 502 | HEM  | CHA-C4D-ND  | 3.42  | 128.60      | 124.37   |
| 13  | 3P    | 501 | HEM  | CHA-C4D-ND  | 3.37  | 128.54      | 124.37   |
| 13  | 3P    | 501 | HEM  | CHB-C1B-NB  | 3.37  | 128.53      | 124.37   |
| 14  | 3P    | 503 | U10  | O4-C4-C3    | 3.35  | 136.32      | 123.64   |
| 14  | 3P    | 503 | U10  | O3-C3-C4    | 3.35  | 136.31      | 123.64   |
| 14  | 3P    | 503 | U10  | O4-C4-C5    | -3.30 | 105.50      | 116.64   |
| 15  | 3D    | 501 | HEC  | C3B-C4B-NB  | 3.28  | 113.77      | 110.17   |
| 13  | 3C    | 501 | HEM  | C1B-NB-C4B  | 3.27  | 109.08      | 105.21   |
| 15  | 3D    | 501 | HEC  | CMC-C2C-C3C | 3.23  | 132.47      | 125.62   |
| 13  | 3P    | 501 | HEM  | C1B-NB-C4B  | 3.17  | 108.96      | 105.21   |
| 15  | 3D    | 501 | HEC  | C4D-C3D-C2D | -3.12 | 102.35      | 106.89   |
| 13  | 3P    | 502 | HEM  | CHB-C1B-NB  | 3.10  | 128.20      | 124.37   |
| 14  | 3P    | 503 | U10  | O3-C3-C2    | -3.09 | 106.20      | 116.64   |
| 13  | 3C    | 502 | HEM  | CHB-C1B-NB  | 3.07  | 128.16      | 124.37   |
| 15  | 3Q    | 501 | HEC  | C3A-C4A-NA  | 3.01  | 115.20      | 109.64   |
| 15  | 3Q    | 501 | HEC  | C4D-C3D-C2D | -2.94 | 102.61      | 106.89   |
| 11  | 3G    | 102 | CDL  | OA6-CA5-C11 | 2.94  | 117.83      | 111.48   |
| 15  | 3Q    | 501 | HEC  | CMC-C2C-C3C | 2.92  | 131.82      | 125.62   |
| 15  | 3D    | 501 | HEC  | C3C-C4C-NC  | 2.89  | 113.36      | 110.15   |
| 13  | 3P    | 502 | HEM  | C3B-C4B-NB  | -2.85 | 107.42      | 109.47   |
| 13  | 3C    | 502 | HEM  | C3B-C4B-NB  | -2.85 | 107.42      | 109.47   |
| 13  | 3P    | 501 | HEM  | CHD-C4C-NC  | 2.83  | 127.54      | 124.45   |
| 14  | 3C    | 503 | U10  | O3-C3-C4    | 2.83  | 134.36      | 123.64   |
| 13  | 3C    | 501 | HEM  | CHD-C1D-C2D | -2.82 | 120.57      | 125.03   |
| 15  | 3D    | 501 | HEC  | C3A-C4A-NA  | 2.79  | 114.80      | 109.64   |
| 13  | 3P    | 501 | HEM  | CHD-C1D-C2D | -2.78 | 120.64      | 125.03   |
| 13  | 3C    | 501 | HEM  | CHD-C4C-NC  | 2.75  | 127.44      | 124.45   |
| 13  | 3P    | 502 | HEM  | C4C-CHD-C1D | -2.74 | 120.20      | 126.02   |
| 12  | 3A    | 502 | 3PE  | O21-C21-C22 | 2.73  | 117.39      | 111.48   |
| 14  | 3C    | 504 | U10  | O3-C3-C2    | 2.73  | 125.84      | 116.64   |
| 15  | 3Q    | 501 | HEC  | CAD-C3D-C4D | 2.72  | 129.44      | 124.70   |
| 15  | 3Q    | 501 | HEC  | C4A-C3A-C2A | -2.69 | 102.98      | 106.97   |
| 15  | 3D    | 501 | HEC  | C4A-C3A-C2A | -2.63 | 103.08      | 106.97   |
| 14  | 3C    | 504 | U10  | O4-C4-C5    | -2.57 | 107.97      | 116.64   |
| 13  | 3C    | 502 | HEM  | C4A-CHB-C1B | -2.57 | 120.21      | 126.25   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | 3C    | 502 | HEM  | C4C-CHD-C1D | -2.56 | 120.58      | 126.02   |
| 13  | 3C    | 501 | HEM  | C3B-C4B-NB  | -2.55 | 107.64      | 109.47   |
| 14  | 3P    | 504 | U10  | C7-C6-C1    | -2.53 | 120.55      | 124.89   |
| 13  | 3P    | 502 | HEM  | C4A-CHB-C1B | -2.51 | 120.35      | 126.25   |
| 14  | 3C    | 504 | U10  | C4-C3-C2    | -2.49 | 116.11      | 120.69   |
| 13  | 3P    | 501 | HEM  | C3B-C4B-NB  | -2.49 | 107.68      | 109.47   |
| 15  | 3Q    | 501 | HEC  | CAD-CBD-CGD | -2.49 | 107.06      | 113.67   |
| 13  | 3C    | 502 | HEM  | CHD-C1D-C2D | -2.49 | 121.10      | 125.03   |
| 15  | 3Q    | 501 | HEC  | CAC-C3C-C2C | 2.46  | 130.78      | 126.89   |
| 14  | 3C    | 503 | U10  | C4-C3-C2    | -2.45 | 116.19      | 120.69   |
| 15  | 3D    | 501 | HEC  | CAC-C3C-C2C | 2.44  | 130.75      | 126.89   |
| 15  | 3D    | 501 | HEC  | CHB-C1B-NB  | -2.40 | 121.83      | 124.42   |
| 11  | 3T    | 102 | CDL  | OA6-CA5-C11 | 2.39  | 116.65      | 111.48   |
| 14  | 3P    | 504 | U10  | O3-C3-C2    | -2.39 | 108.58      | 116.64   |
| 14  | 3C    | 503 | U10  | O4-C4-C3    | 2.38  | 132.66      | 123.64   |
| 14  | 3C    | 503 | U10  | O3-C3-C2    | -2.38 | 108.62      | 116.64   |
| 14  | 3P    | 503 | U10  | C7-C6-C1    | -2.34 | 120.88      | 124.89   |
| 15  | 3Q    | 501 | HEC  | CMB-C2B-C3B | 2.32  | 132.43      | 126.15   |
| 13  | 3C    | 502 | HEM  | C1A-CHA-C4D | -2.32 | 120.80      | 126.25   |
| 15  | 3Q    | 501 | HEC  | CAB-C3B-C2B | 2.30  | 131.79      | 127.56   |
| 13  | 3C    | 502 | HEM  | CHD-C4C-NC  | 2.28  | 126.94      | 124.45   |
| 14  | 3P    | 504 | U10  | C3-C4-C5    | -2.28 | 116.50      | 120.69   |
| 15  | 3D    | 501 | HEC  | CAD-C3D-C4D | 2.26  | 128.64      | 124.70   |
| 14  | 3P    | 504 | U10  | O4-C4-C5    | 2.24  | 124.18      | 116.64   |
| 15  | 3Q    | 501 | HEC  | CHC-C1C-C2C | -2.22 | 120.98      | 127.43   |
| 13  | 3C    | 501 | HEM  | CHA-C4D-C3D | -2.22 | 121.13      | 125.23   |
| 14  | 3P    | 504 | U10  | O3-C3-C4    | 2.22  | 132.04      | 123.64   |
| 15  | 3D    | 501 | HEC  | CMB-C2B-C3B | 2.21  | 132.13      | 126.15   |
| 14  | 3C    | 504 | U10  | C7-C6-C1    | -2.20 | 121.12      | 124.89   |
| 13  | 3P    | 502 | HEM  | C1A-CHA-C4D | -2.19 | 121.10      | 126.25   |
| 13  | 3P    | 502 | HEM  | CHD-C1D-C2D | -2.18 | 121.59      | 125.03   |
| 13  | 3P    | 502 | HEM  | CHD-C4C-NC  | 2.18  | 126.82      | 124.45   |
| 15  | 3Q    | 501 | HEC  | CHB-C1B-C2B | -2.17 | 121.61      | 125.03   |
| 13  | 3C    | 502 | HEM  | C4D-ND-C1D  | 2.15  | 107.75      | 105.21   |
| 14  | 3C    | 503 | U10  | O4-C4-C5    | -2.15 | 109.39      | 116.64   |
| 13  | 3P    | 502 | HEM  | C4D-ND-C1D  | 2.15  | 107.75      | 105.21   |
| 15  | 3Q    | 501 | HEC  | CMD-C2D-C1D | 2.14  | 128.38      | 125.03   |
| 13  | 3P    | 501 | HEM  | C1A-CHA-C4D | -2.13 | 121.23      | 126.25   |
| 13  | 3C    | 501 | HEM  | C1A-CHA-C4D | -2.12 | 121.27      | 126.25   |
| 14  | 3C    | 503 | U10  | C7-C6-C1    | -2.11 | 121.27      | 124.89   |
| 13  | 3P    | 501 | HEM  | CHA-C4D-C3D | -2.09 | 121.38      | 125.23   |
| 15  | 3D    | 501 | HEC  | CHA-C4D-ND  | -2.09 | 122.18      | 124.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 13  | 3C    | 501 | HEM  | C4C-CHD-C1D | -2.08 | 121.59      | 126.02   |
| 14  | 3C    | 504 | U10  | O4-C4-C3    | 2.07  | 131.49      | 123.64   |
| 13  | 3C    | 501 | HEM  | CHA-C1A-NA  | 2.06  | 127.59      | 123.86   |
| 15  | 3D    | 501 | HEC  | CHA-C1A-NA  | -2.05 | 122.22      | 124.45   |
| 15  | 3Q    | 501 | HEC  | CAA-CBA-CGA | -2.04 | 108.25      | 113.67   |
| 13  | 3P    | 501 | HEM  | C4C-CHD-C1D | -2.02 | 121.72      | 126.02   |
| 11  | 3N    | 502 | CDL  | OB6-CB4-CB3 | 2.01  | 115.56      | 108.34   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 15  | 3D    | 501 | HEC  | NA   |
| 15  | 3Q    | 501 | HEC  | NA   |

All (235) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | 3A    | 501 | CDL  | C1-CA2-OA2-PA1  |
| 11  | 3A    | 501 | CDL  | C1-CB2-OB2-PB2  |
| 11  | 3C    | 505 | CDL  | CA3-OA5-PA1-OA2 |
| 11  | 3C    | 505 | CDL  | CA3-OA5-PA1-OA3 |
| 11  | 3C    | 505 | CDL  | CB2-OB2-PB2-OB3 |
| 11  | 3C    | 505 | CDL  | OB9-CB7-OB8-CB6 |
| 11  | 3C    | 505 | CDL  | C71-CB7-OB8-CB6 |
| 11  | 3G    | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 11  | 3G    | 102 | CDL  | CA3-OA5-PA1-OA3 |
| 11  | 3G    | 102 | CDL  | CA4-CA3-OA5-PA1 |
| 11  | 3G    | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 11  | 3G    | 102 | CDL  | C11-CA5-OA6-CA4 |
| 11  | 3G    | 102 | CDL  | C1-CB2-OB2-PB2  |
| 11  | 3G    | 102 | CDL  | CB4-CB3-OB5-PB2 |
| 11  | 3N    | 502 | CDL  | C1-CA2-OA2-PA1  |
| 11  | 3N    | 502 | CDL  | CA2-OA2-PA1-OA4 |
| 11  | 3N    | 502 | CDL  | CA2-OA2-PA1-OA5 |
| 11  | 3N    | 502 | CDL  | CB2-OB2-PB2-OB3 |
| 11  | 3N    | 502 | CDL  | CB2-OB2-PB2-OB4 |
| 11  | 3N    | 502 | CDL  | CB2-OB2-PB2-OB5 |
| 11  | 3N    | 502 | CDL  | CB3-OB5-PB2-OB3 |
| 11  | 3T    | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 11  | 3T    | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 11  | 3T    | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 11  | 3T    | 101 | CDL  | OB9-CB7-OB8-CB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | 3T    | 101 | CDL  | C71-CB7-OB8-CB6 |
| 11  | 3T    | 102 | CDL  | C1-CA2-OA2-PA1  |
| 11  | 3T    | 102 | CDL  | CA2-OA2-PA1-OA3 |
| 11  | 3T    | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 11  | 3T    | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 11  | 3T    | 102 | CDL  | CB3-OB5-PB2-OB3 |
| 11  | 3T    | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 11  | 3T    | 102 | CDL  | C71-CB7-OB8-CB6 |
| 12  | 3A    | 502 | 3PE  | O22-C21-O21-C2  |
| 12  | 3A    | 502 | 3PE  | C22-C21-O21-C2  |
| 12  | 3A    | 503 | 3PE  | C2-C1-O11-P     |
| 12  | 3A    | 503 | 3PE  | O22-C21-O21-C2  |
| 12  | 3A    | 503 | 3PE  | C22-C21-O21-C2  |
| 12  | 3C    | 506 | 3PE  | C11-O13-P-O14   |
| 12  | 3C    | 507 | 3PE  | C1-O11-P-O14    |
| 12  | 3C    | 507 | 3PE  | C2-C1-O11-P     |
| 12  | 3C    | 507 | 3PE  | O21-C2-C3-O31   |
| 12  | 3G    | 101 | 3PE  | O32-C31-O31-C3  |
| 12  | 3G    | 101 | 3PE  | C32-C31-O31-C3  |
| 12  | 3N    | 503 | 3PE  | O22-C21-O21-C2  |
| 12  | 3N    | 503 | 3PE  | C22-C21-O21-C2  |
| 12  | 3R    | 302 | 3PE  | C1-O11-P-O12    |
| 12  | 3R    | 302 | 3PE  | C11-O13-P-O14   |
| 12  | 3Y    | 101 | 3PE  | C2-C1-O11-P     |
| 12  | 3Y    | 101 | 3PE  | O32-C31-O31-C3  |
| 12  | 3Y    | 101 | 3PE  | C32-C31-O31-C3  |
| 13  | 3C    | 501 | HEM  | C2B-C3B-CAB-CBB |
| 13  | 3C    | 501 | HEM  | C4B-C3B-CAB-CBB |
| 13  | 3C    | 502 | HEM  | C2B-C3B-CAB-CBB |
| 13  | 3C    | 502 | HEM  | C4B-C3B-CAB-CBB |
| 13  | 3C    | 502 | HEM  | C2C-C3C-CAC-CBC |
| 13  | 3P    | 501 | HEM  | C2B-C3B-CAB-CBB |
| 13  | 3P    | 501 | HEM  | C4B-C3B-CAB-CBB |
| 13  | 3P    | 502 | HEM  | C2B-C3B-CAB-CBB |
| 13  | 3P    | 502 | HEM  | C2C-C3C-CAC-CBC |
| 17  | 3R    | 303 | PC1  | C1-O11-P-O12    |
| 17  | 3R    | 303 | PC1  | C2-C1-O11-P     |
| 17  | 3X    | 101 | PC1  | C1-O11-P-O12    |
| 17  | 3X    | 101 | PC1  | C1-O11-P-O14    |
| 17  | 3X    | 101 | PC1  | C1-O11-P-O13    |
| 15  | 3D    | 501 | HEC  | C4B-C3B-CAB-CBB |
| 15  | 3Q    | 501 | HEC  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | 3D    | 501 | HEC  | C4C-C3C-CAC-CBC |
| 15  | 3Q    | 501 | HEC  | C4C-C3C-CAC-CBC |
| 15  | 3D    | 501 | HEC  | C2B-C3B-CAB-CBB |
| 15  | 3Q    | 501 | HEC  | C2B-C3B-CAB-CBB |
| 15  | 3D    | 501 | HEC  | C2C-C3C-CAC-CBC |
| 15  | 3Q    | 501 | HEC  | C2C-C3C-CAC-CBC |
| 11  | 3T    | 101 | CDL  | CB4-CB3-OB5-PB2 |
| 14  | 3C    | 503 | U10  | C15-C14-C16-C17 |
| 14  | 3C    | 503 | U10  | C13-C14-C16-C17 |
| 14  | 3C    | 504 | U10  | C4-C3-O3-C3M    |
| 14  | 3P    | 504 | U10  | C3-C4-O4-C4M    |
| 11  | 3C    | 505 | CDL  | CB4-CB3-OB5-PB2 |
| 17  | 3X    | 101 | PC1  | C21-C22-C23-C24 |
| 11  | 3T    | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 12  | 3P    | 505 | 3PE  | C31-C32-C33-C34 |
| 12  | 3N    | 503 | 3PE  | C21-C22-C23-C24 |
| 12  | 3R    | 302 | 3PE  | C3A-C3B-C3C-C3D |
| 12  | 3N    | 501 | 3PE  | C21-C22-C23-C24 |
| 12  | 3Y    | 101 | 3PE  | C1-C2-C3-O31    |
| 12  | 3A    | 503 | 3PE  | C32-C33-C34-C35 |
| 11  | 3T    | 101 | CDL  | CA7-C31-C32-C33 |
| 12  | 3R    | 302 | 3PE  | C35-C36-C37-C38 |
| 13  | 3C    | 501 | HEM  | C3D-CAD-CBD-CGD |
| 14  | 3P    | 504 | U10  | C6-C7-C8-C9     |
| 11  | 3T    | 102 | CDL  | C33-C34-C35-C36 |
| 13  | 3C    | 502 | HEM  | C4C-C3C-CAC-CBC |
| 13  | 3P    | 502 | HEM  | C4B-C3B-CAB-CBB |
| 13  | 3P    | 502 | HEM  | C4C-C3C-CAC-CBC |
| 11  | 3T    | 101 | CDL  | OA6-CA4-CA6-OA8 |
| 12  | 3Y    | 101 | 3PE  | O21-C2-C3-O31   |
| 11  | 3T    | 102 | CDL  | OA5-CA3-CA4-CA6 |
| 11  | 3G    | 102 | CDL  | C53-C54-C55-C56 |
| 12  | 3C    | 507 | 3PE  | C1-C2-C3-O31    |
| 12  | 3E    | 302 | 3PE  | C1-C2-C3-O31    |
| 11  | 3G    | 102 | CDL  | C51-C52-C53-C54 |
| 14  | 3C    | 504 | U10  | C2-C3-O3-C3M    |
| 17  | 3E    | 303 | PC1  | C35-C36-C37-C38 |
| 12  | 3R    | 302 | 3PE  | C21-C22-C23-C24 |
| 17  | 3R    | 303 | PC1  | C34-C35-C36-C37 |
| 17  | 3X    | 101 | PC1  | O21-C21-C22-C23 |
| 11  | 3G    | 102 | CDL  | C71-C72-C73-C74 |
| 17  | 3E    | 303 | PC1  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | 3T    | 101 | CDL  | C1-CB2-OB2-PB2  |
| 11  | 3T    | 102 | CDL  | CA4-CA3-OA5-PA1 |
| 12  | 3N    | 501 | 3PE  | C2-C1-O11-P     |
| 12  | 3G    | 101 | 3PE  | O21-C21-C22-C23 |
| 12  | 3A    | 503 | 3PE  | O11-C1-C2-C3    |
| 12  | 3C    | 507 | 3PE  | O11-C1-C2-C3    |
| 12  | 3N    | 501 | 3PE  | O21-C21-C22-C23 |
| 11  | 3G    | 102 | CDL  | CB5-C51-C52-C53 |
| 11  | 3C    | 505 | CDL  | C73-C74-C75-C76 |
| 11  | 3G    | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 17  | 3R    | 303 | PC1  | C1-C2-C3-O31    |
| 11  | 3N    | 502 | CDL  | CA5-C11-C12-C13 |
| 11  | 3T    | 102 | CDL  | OA5-CA3-CA4-OA6 |
| 12  | 3A    | 503 | 3PE  | O11-C1-C2-O21   |
| 11  | 3N    | 502 | CDL  | C52-C51-CB5-OB6 |
| 12  | 3R    | 302 | 3PE  | C2-C1-O11-P     |
| 11  | 3T    | 102 | CDL  | C31-C32-C33-C34 |
| 11  | 3A    | 501 | CDL  | C32-C31-CA7-OA8 |
| 11  | 3T    | 102 | CDL  | C12-C11-CA5-OA6 |
| 15  | 3Q    | 501 | HEC  | C3D-CAD-CBD-CGD |
| 14  | 3P    | 504 | U10  | C1-C6-C7-C8     |
| 13  | 3C    | 501 | HEM  | C2C-C3C-CAC-CBC |
| 11  | 3T    | 101 | CDL  | CA3-CA4-CA6-OA8 |
| 12  | 3P    | 505 | 3PE  | C1-C2-C3-O31    |
| 12  | 3N    | 501 | 3PE  | C27-C28-C29-C2A |
| 12  | 3C    | 507 | 3PE  | C12-C11-O13-P   |
| 12  | 3G    | 101 | 3PE  | C12-C11-O13-P   |
| 12  | 3R    | 302 | 3PE  | C12-C11-O13-P   |
| 12  | 3Y    | 101 | 3PE  | C12-C11-O13-P   |
| 14  | 3P    | 504 | U10  | C5-C6-C7-C8     |
| 17  | 3R    | 303 | PC1  | C12-C11-O13-P   |
| 17  | 3X    | 101 | PC1  | C12-C11-O13-P   |
| 11  | 3A    | 501 | CDL  | OB6-CB4-CB6-OB8 |
| 11  | 3G    | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 12  | 3N    | 503 | 3PE  | O21-C2-C3-O31   |
| 12  | 3C    | 507 | 3PE  | O21-C21-C22-C23 |
| 17  | 3X    | 101 | PC1  | O13-C11-C12-N   |
| 12  | 3Y    | 101 | 3PE  | C32-C33-C34-C35 |
| 14  | 3P    | 503 | U10  | C12-C11-C9-C10  |
| 17  | 3E    | 303 | PC1  | C22-C23-C24-C25 |
| 17  | 3R    | 303 | PC1  | O21-C2-C3-O31   |
| 12  | 3C    | 506 | 3PE  | C25-C26-C27-C28 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 12  | 3N    | 503 | 3PE  | C1-C2-C3-O31    |
| 11  | 3C    | 505 | CDL  | CA2-OA2-PA1-OA3 |
| 11  | 3C    | 505 | CDL  | CB2-OB2-PB2-OB5 |
| 11  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 11  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 11  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 11  | 3T    | 102 | CDL  | CB2-OB2-PB2-OB3 |
| 12  | 3A    | 503 | 3PE  | C1-O11-P-O14    |
| 12  | 3C    | 506 | 3PE  | C1-O11-P-O13    |
| 12  | 3C    | 507 | 3PE  | C11-O13-P-O14   |
| 12  | 3E    | 302 | 3PE  | C1-O11-P-O14    |
| 12  | 3N    | 501 | 3PE  | C11-O13-P-O14   |
| 12  | 3P    | 505 | 3PE  | C11-O13-P-O14   |
| 12  | 3R    | 302 | 3PE  | C1-O11-P-O13    |
| 12  | 3R    | 302 | 3PE  | C1-O11-P-O14    |
| 17  | 3R    | 303 | PC1  | C1-O11-P-O14    |
| 17  | 3R    | 303 | PC1  | C1-O11-P-O13    |
| 11  | 3T    | 101 | CDL  | CB5-C51-C52-C53 |
| 11  | 3A    | 501 | CDL  | C34-C35-C36-C37 |
| 11  | 3C    | 505 | CDL  | CA4-CA3-OA5-PA1 |
| 11  | 3N    | 502 | CDL  | C1-CB2-OB2-PB2  |
| 11  | 3T    | 102 | CDL  | CB4-CB3-OB5-PB2 |
| 17  | 3X    | 101 | PC1  | C2-C1-O11-P     |
| 17  | 3E    | 303 | PC1  | C26-C27-C28-C29 |
| 14  | 3P    | 503 | U10  | C12-C11-C9-C8   |
| 14  | 3P    | 503 | U10  | C21-C22-C23-C24 |
| 14  | 3P    | 504 | U10  | C14-C16-C17-C18 |
| 12  | 3N    | 501 | 3PE  | O22-C21-C22-C23 |
| 17  | 3E    | 303 | PC1  | C33-C34-C35-C36 |
| 14  | 3P    | 504 | U10  | C2-C3-O3-C3M    |
| 14  | 3P    | 504 | U10  | C5-C4-O4-C4M    |
| 12  | 3R    | 302 | 3PE  | C28-C29-C2A-C2B |
| 12  | 3C    | 506 | 3PE  | C1-C2-O21-C21   |
| 13  | 3P    | 501 | HEM  | CAD-CBD-CGD-O1D |
| 13  | 3P    | 502 | HEM  | CAD-CBD-CGD-O1D |
| 12  | 3C    | 507 | 3PE  | C23-C24-C25-C26 |
| 11  | 3A    | 501 | CDL  | CB4-CB3-OB5-PB2 |
| 13  | 3C    | 502 | HEM  | CAA-CBA-CGA-O1A |
| 15  | 3Q    | 501 | HEC  | CAD-CBD-CGD-O1D |
| 11  | 3N    | 502 | CDL  | OA6-CA4-CA6-OA8 |
| 12  | 3G    | 101 | 3PE  | O21-C2-C3-O31   |
| 13  | 3P    | 502 | HEM  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 11  | 3T    | 101 | CDL  | CA5-C11-C12-C13 |
| 14  | 3P    | 503 | U10  | C20-C19-C21-C22 |
| 13  | 3P    | 502 | HEM  | CAD-CBD-CGD-O2D |
| 15  | 3D    | 501 | HEC  | CAA-CBA-CGA-O2A |
| 13  | 3C    | 502 | HEM  | CAA-CBA-CGA-O2A |
| 13  | 3P    | 501 | HEM  | CAD-CBD-CGD-O2D |
| 15  | 3Q    | 501 | HEC  | CAD-CBD-CGD-O2D |
| 13  | 3P    | 502 | HEM  | CAA-CBA-CGA-O2A |
| 12  | 3C    | 507 | 3PE  | O11-C1-C2-O21   |
| 11  | 3T    | 102 | CDL  | C12-C13-C14-C15 |
| 12  | 3G    | 101 | 3PE  | O22-C21-C22-C23 |
| 12  | 3C    | 506 | 3PE  | C23-C24-C25-C26 |
| 12  | 3R    | 302 | 3PE  | C27-C28-C29-C2A |
| 15  | 3D    | 501 | HEC  | CAA-CBA-CGA-O1A |
| 11  | 3A    | 501 | CDL  | CB3-CB4-CB6-OB8 |
| 13  | 3C    | 501 | HEM  | C4C-C3C-CAC-CBC |
| 17  | 3X    | 101 | PC1  | O22-C21-C22-C23 |
| 12  | 3C    | 507 | 3PE  | C22-C23-C24-C25 |
| 12  | 3N    | 501 | 3PE  | C12-C11-O13-P   |
| 14  | 3P    | 504 | U10  | C11-C12-C13-C14 |
| 11  | 3A    | 501 | CDL  | C32-C31-CA7-OA9 |
| 14  | 3C    | 504 | U10  | C5-C4-O4-C4M    |
| 11  | 3T    | 102 | CDL  | C12-C11-CA5-OA7 |
| 11  | 3N    | 502 | CDL  | CA4-CA6-OA8-CA7 |
| 12  | 3N    | 503 | 3PE  | O31-C31-C32-C33 |
| 11  | 3N    | 502 | CDL  | CB3-CB4-OB6-CB5 |
| 11  | 3N    | 502 | CDL  | CB6-CB4-OB6-CB5 |
| 14  | 3P    | 503 | U10  | C6-C7-C8-C9     |
| 11  | 3A    | 501 | CDL  | CA4-CA3-OA5-PA1 |
| 12  | 3C    | 507 | 3PE  | O22-C21-C22-C23 |
| 11  | 3C    | 505 | CDL  | OB6-CB4-CB6-OB8 |
| 12  | 3P    | 505 | 3PE  | O21-C2-C3-O31   |
| 11  | 3G    | 102 | CDL  | C72-C73-C74-C75 |
| 12  | 3P    | 505 | 3PE  | C24-C25-C26-C27 |
| 11  | 3A    | 501 | CDL  | C52-C51-CB5-OB6 |
| 13  | 3P    | 501 | HEM  | C2C-C3C-CAC-CBC |
| 12  | 3Y    | 101 | 3PE  | O31-C31-C32-C33 |
| 14  | 3C    | 503 | U10  | C2-C3-O3-C3M    |
| 14  | 3C    | 503 | U10  | C5-C4-O4-C4M    |
| 14  | 3P    | 503 | U10  | C2-C3-O3-C3M    |
| 12  | 3R    | 302 | 3PE  | O31-C31-C32-C33 |
| 12  | 3N    | 503 | 3PE  | O32-C31-C32-C33 |

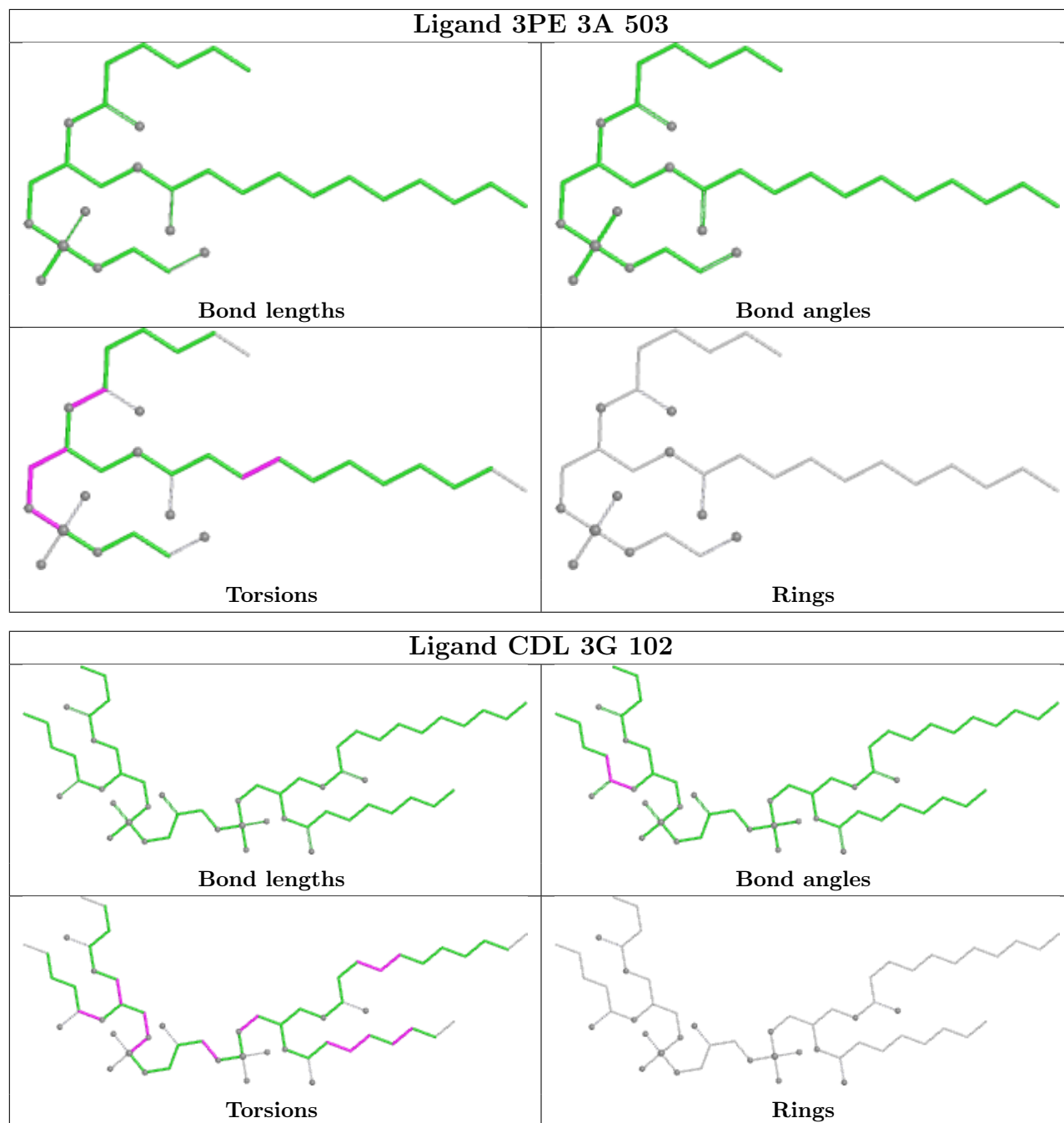
There are no ring outliers.

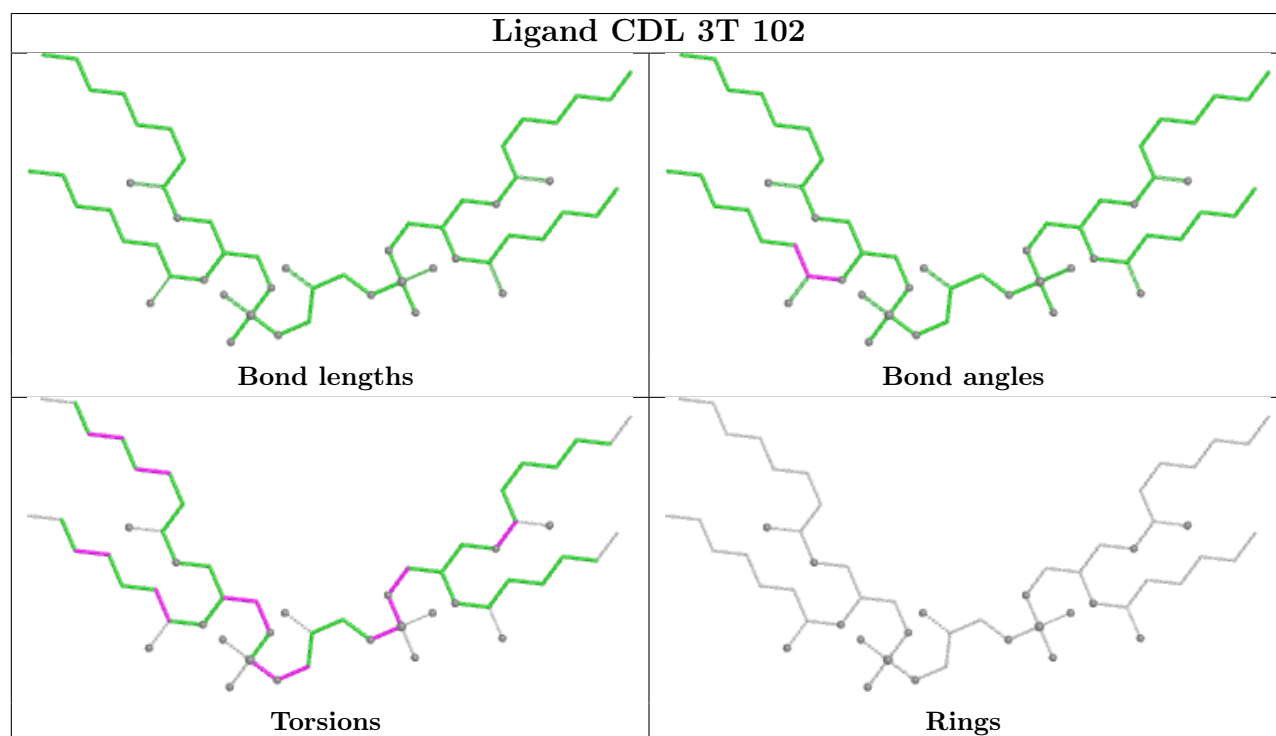
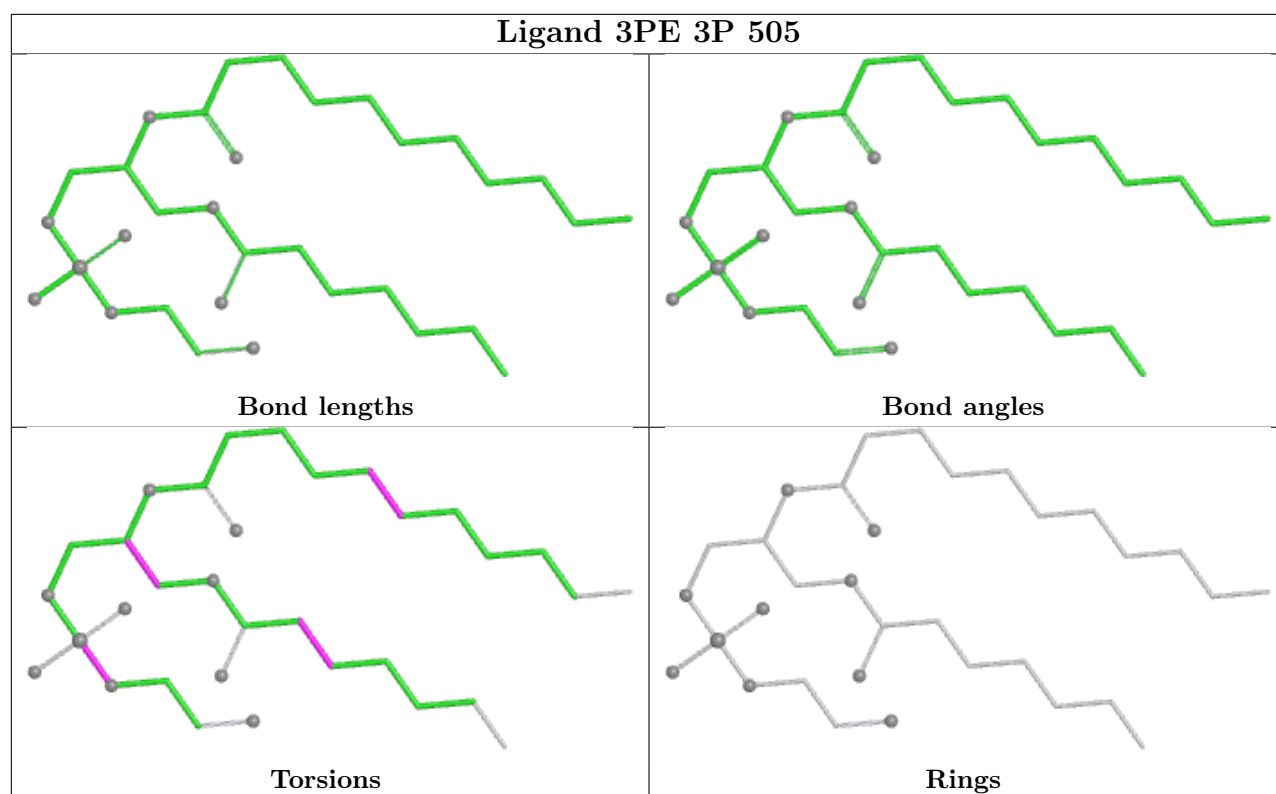
31 monomers are involved in 145 short contacts:

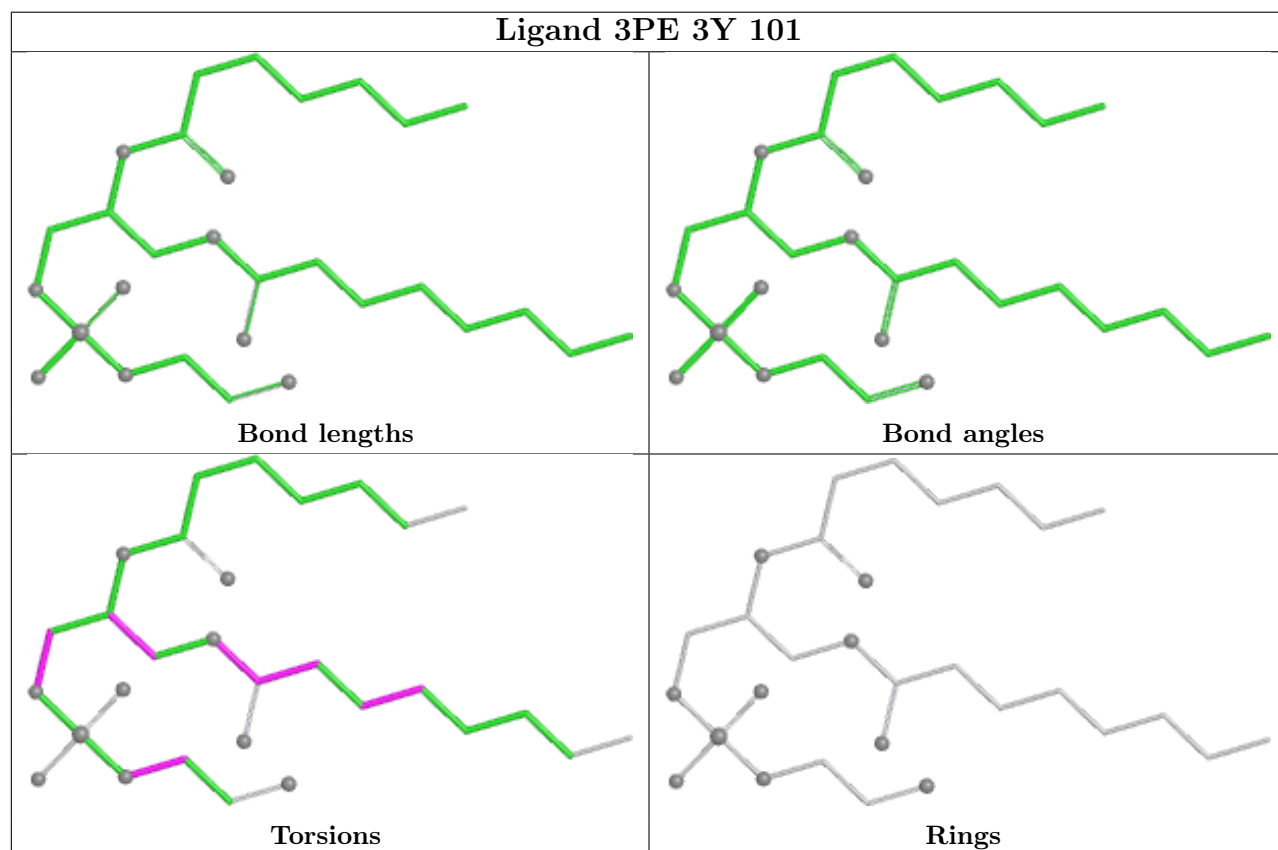
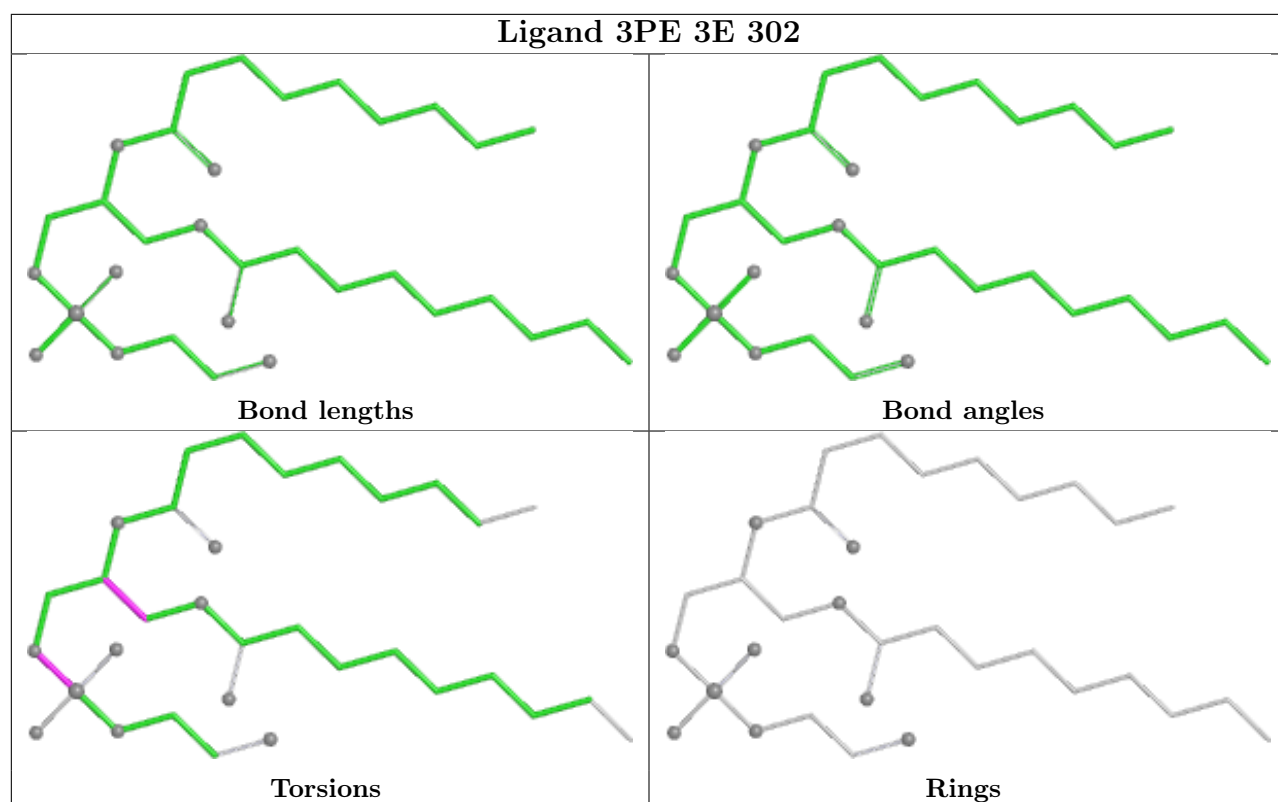
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | 3R    | 301 | FES  | 1       | 0            |
| 12  | 3A    | 503 | 3PE  | 4       | 0            |
| 11  | 3G    | 102 | CDL  | 7       | 0            |
| 11  | 3T    | 102 | CDL  | 8       | 0            |
| 12  | 3E    | 302 | 3PE  | 6       | 0            |
| 12  | 3Y    | 101 | 3PE  | 4       | 0            |
| 14  | 3P    | 504 | U10  | 5       | 0            |
| 11  | 3C    | 505 | CDL  | 5       | 0            |
| 14  | 3C    | 503 | U10  | 6       | 0            |
| 14  | 3C    | 504 | U10  | 4       | 0            |
| 15  | 3Q    | 501 | HEC  | 3       | 0            |
| 17  | 3X    | 101 | PC1  | 4       | 0            |
| 12  | 3C    | 507 | 3PE  | 5       | 0            |
| 11  | 3N    | 502 | CDL  | 5       | 0            |
| 12  | 3C    | 506 | 3PE  | 2       | 0            |
| 13  | 3P    | 502 | HEM  | 4       | 0            |
| 13  | 3C    | 502 | HEM  | 5       | 0            |
| 16  | 3E    | 301 | FES  | 4       | 0            |
| 11  | 3A    | 501 | CDL  | 4       | 0            |
| 13  | 3C    | 501 | HEM  | 5       | 0            |
| 11  | 3T    | 101 | CDL  | 10      | 0            |
| 12  | 3N    | 501 | 3PE  | 6       | 0            |
| 17  | 3R    | 303 | PC1  | 5       | 0            |
| 17  | 3E    | 303 | PC1  | 7       | 0            |
| 12  | 3G    | 101 | 3PE  | 2       | 0            |
| 14  | 3P    | 503 | U10  | 7       | 0            |
| 15  | 3D    | 501 | HEC  | 1       | 0            |
| 12  | 3R    | 302 | 3PE  | 8       | 0            |
| 12  | 3N    | 503 | 3PE  | 9       | 0            |
| 12  | 3A    | 502 | 3PE  | 5       | 0            |
| 13  | 3P    | 501 | HEM  | 3       | 0            |

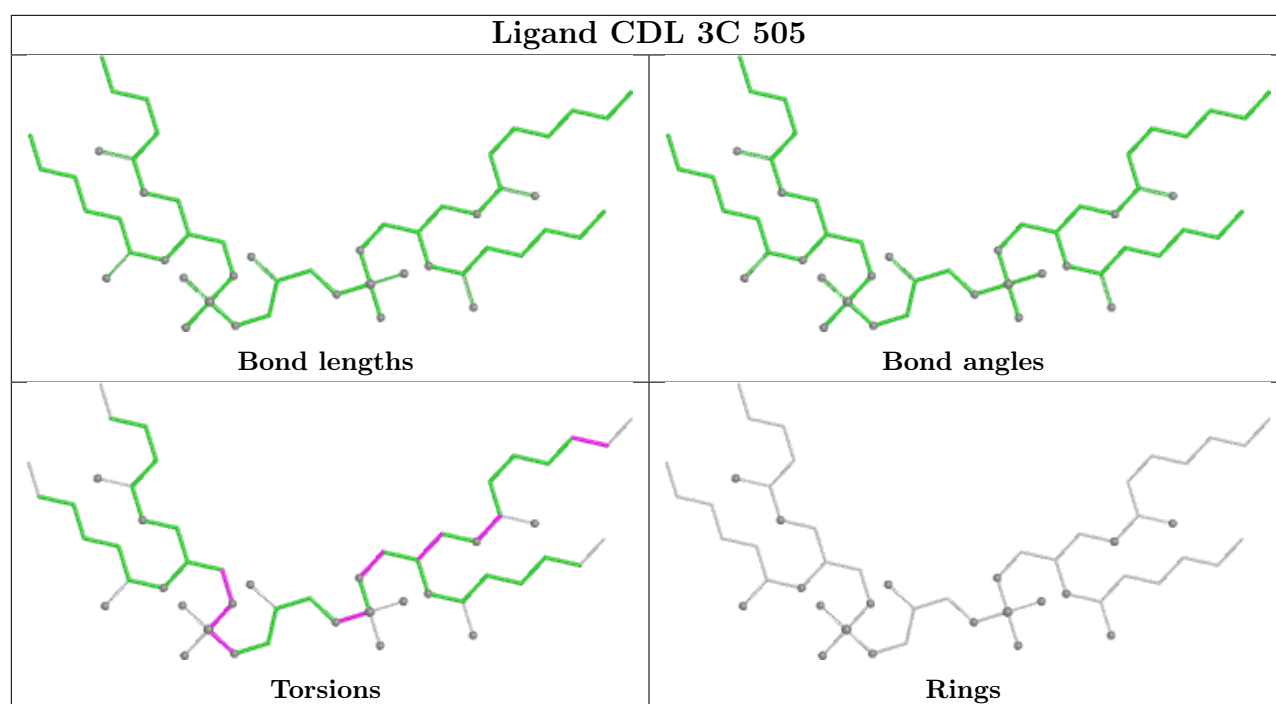
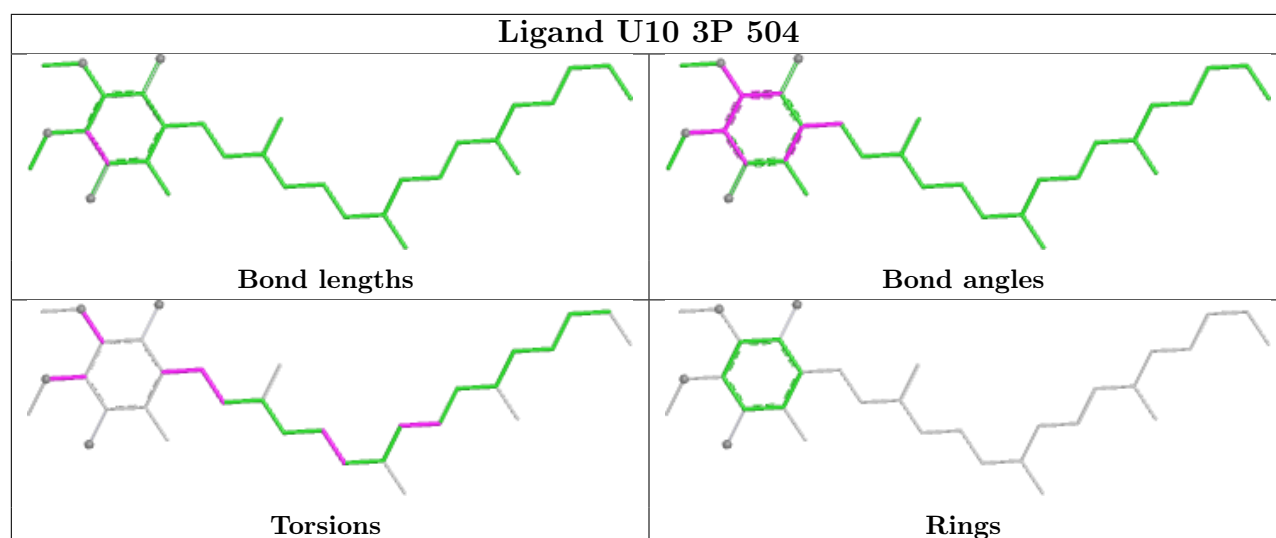
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

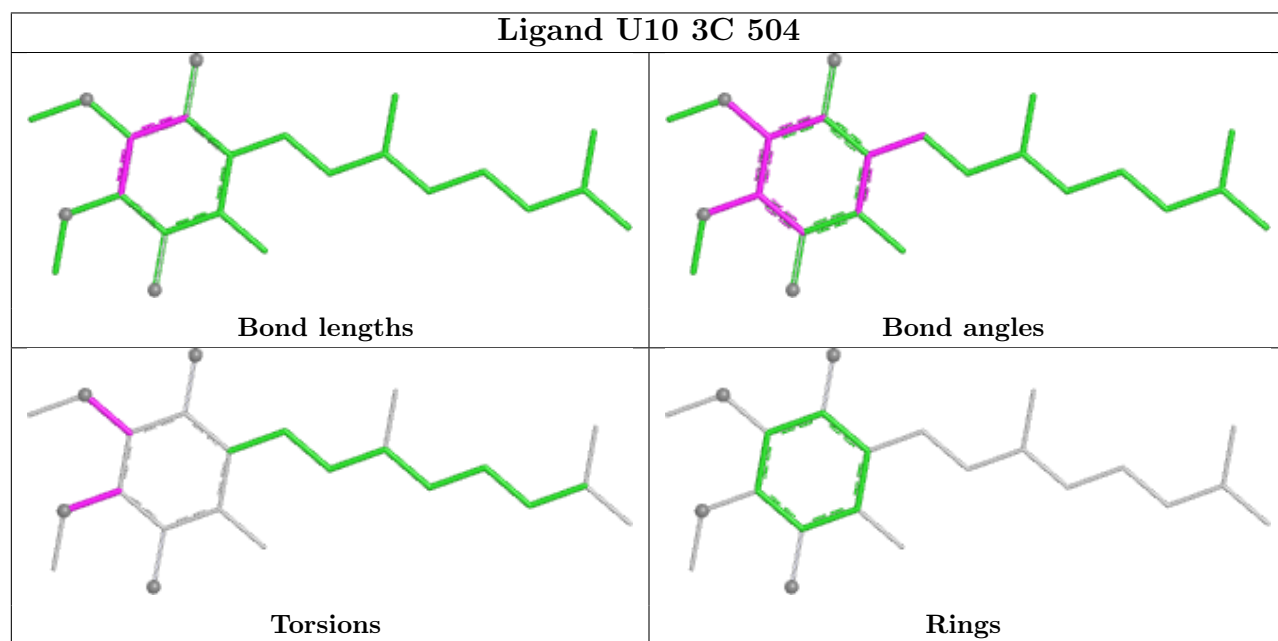
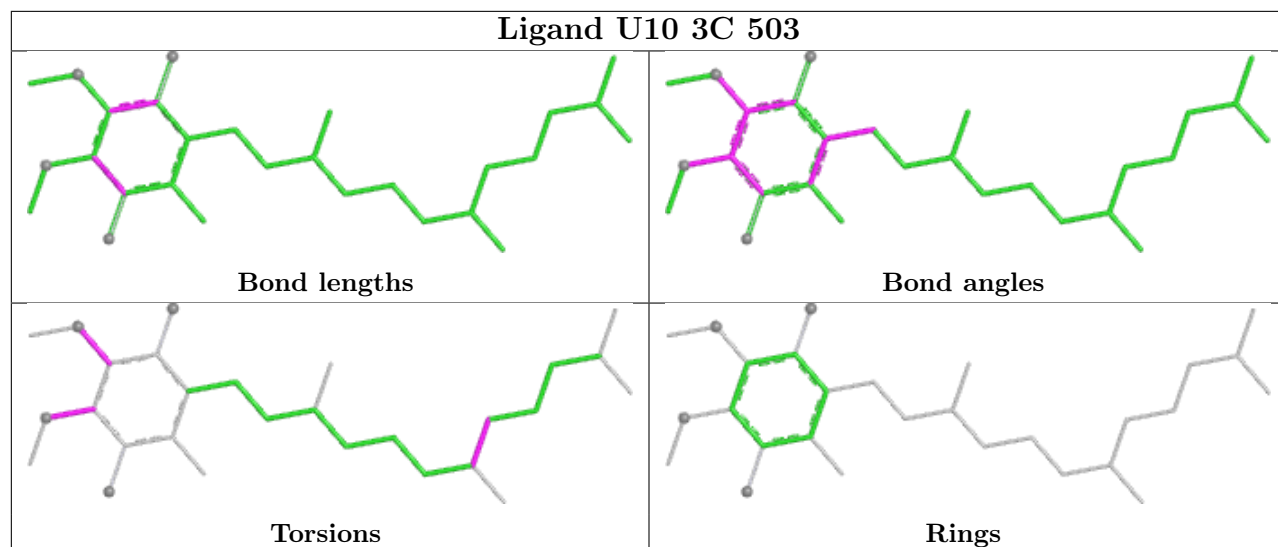
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



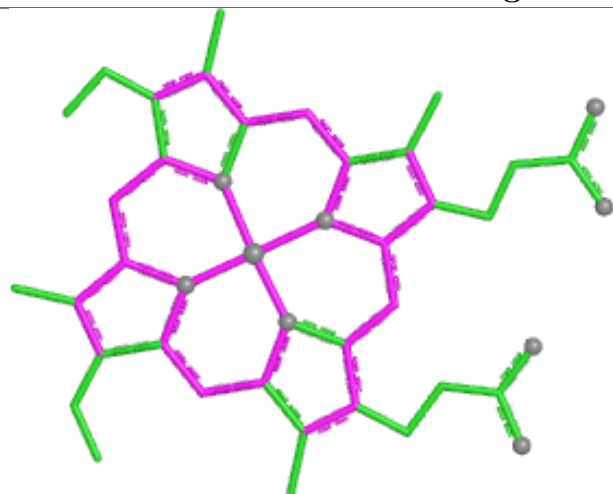




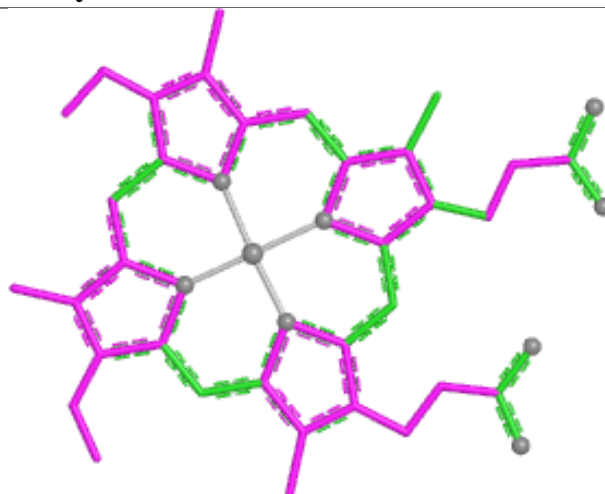




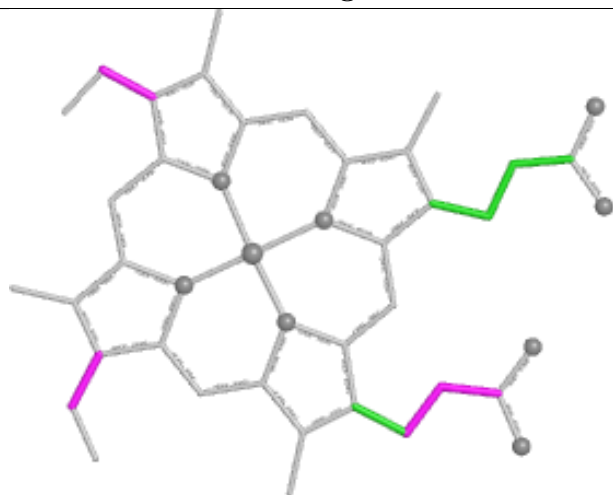
## Ligand HEC 3Q 501



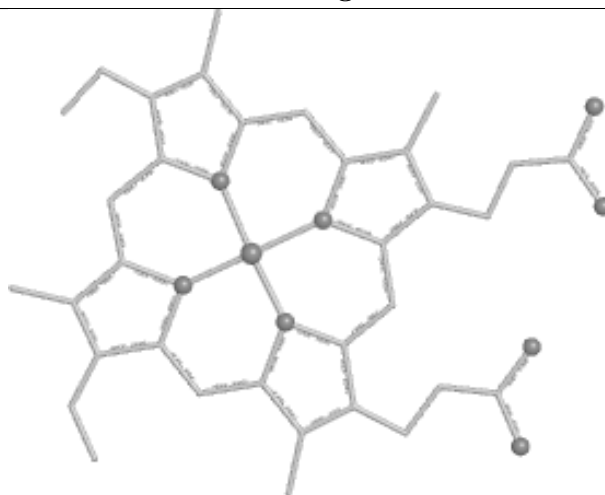
Bond lengths



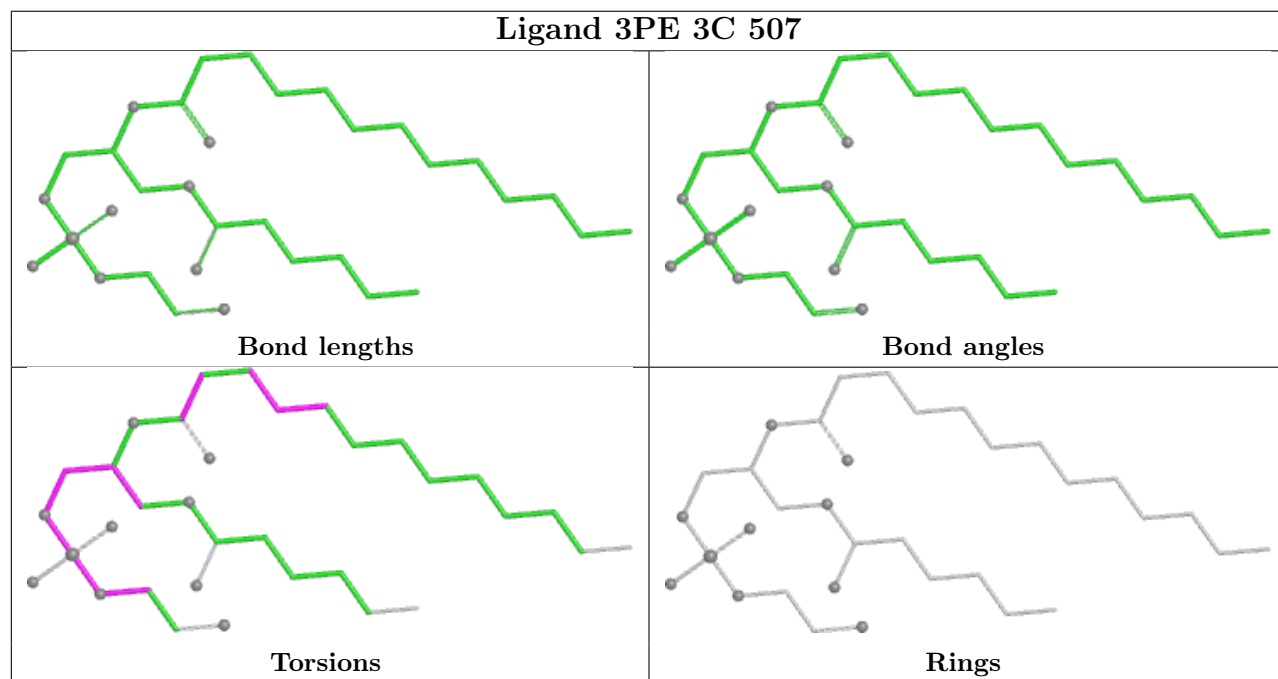
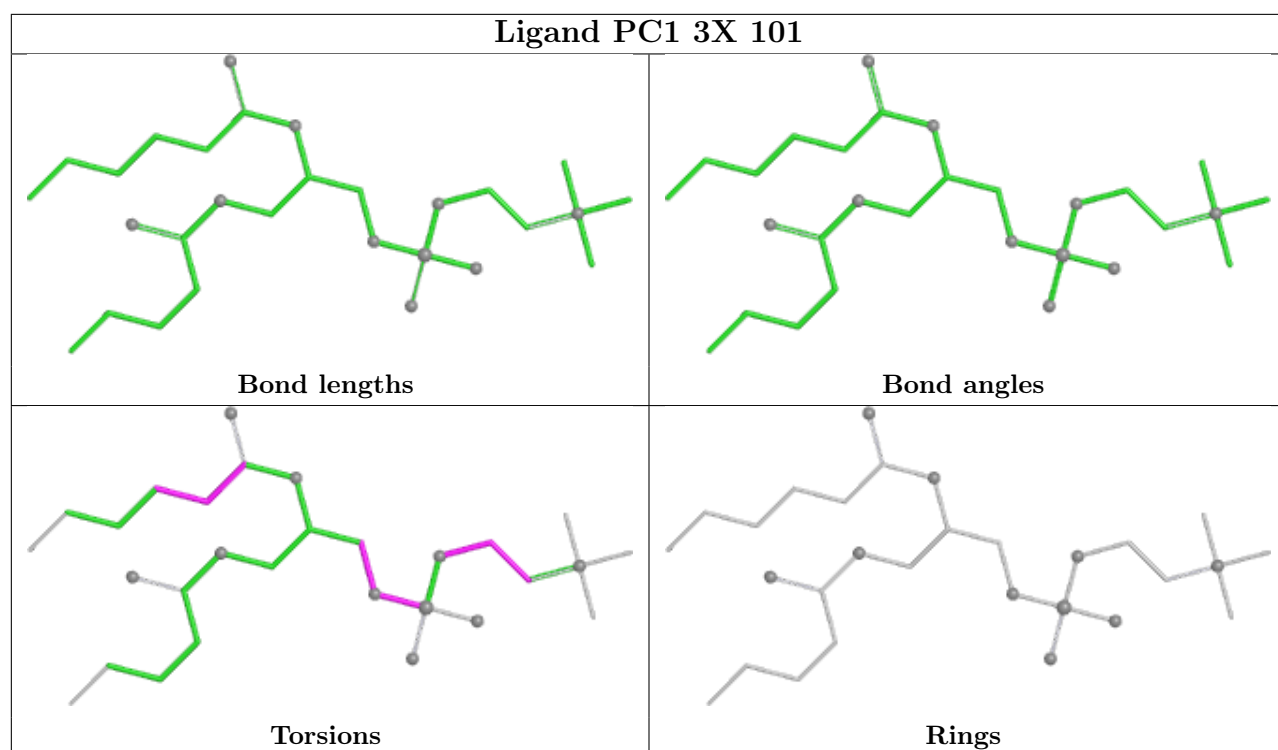
Bond angles

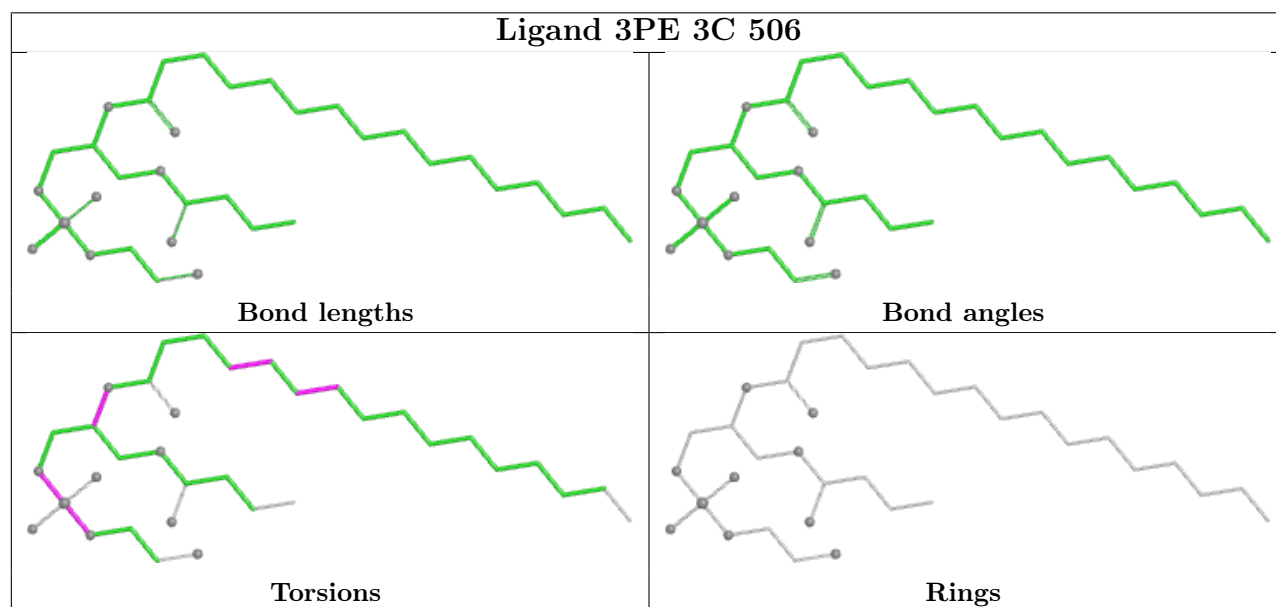
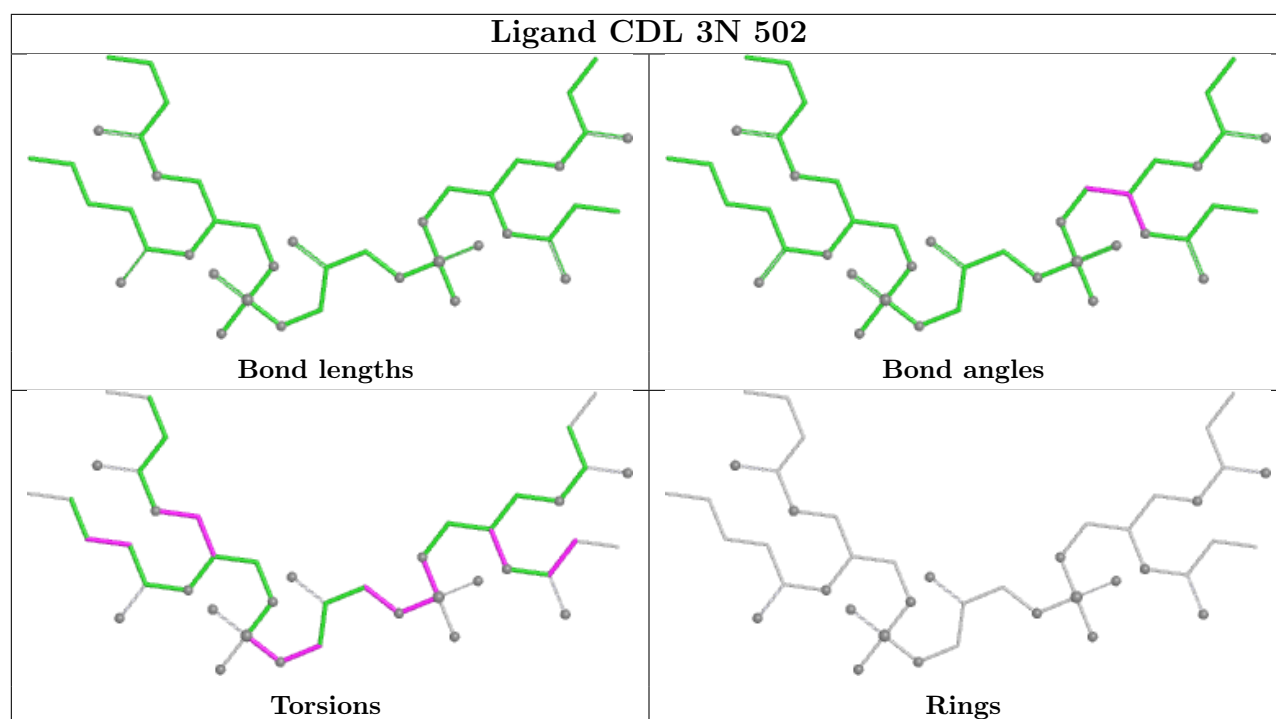


Torsions

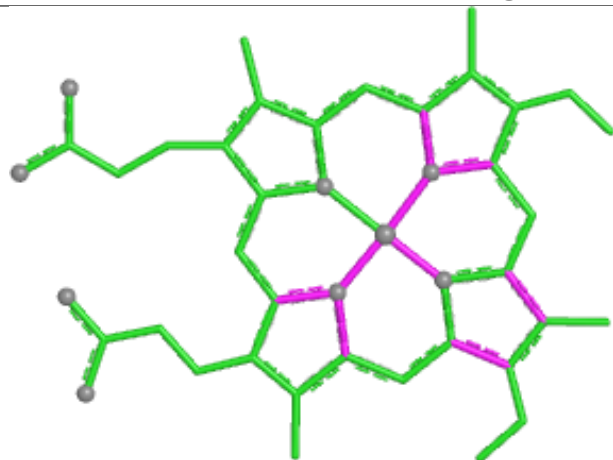


Rings

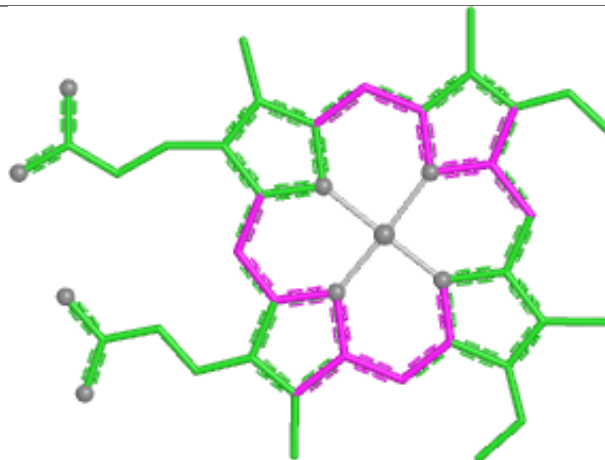




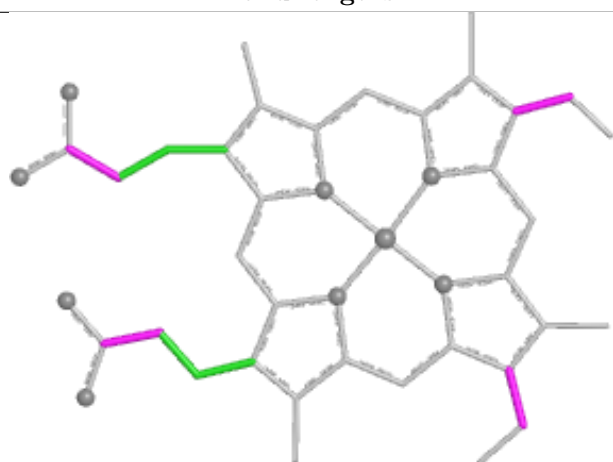
## Ligand HEM 3P 502



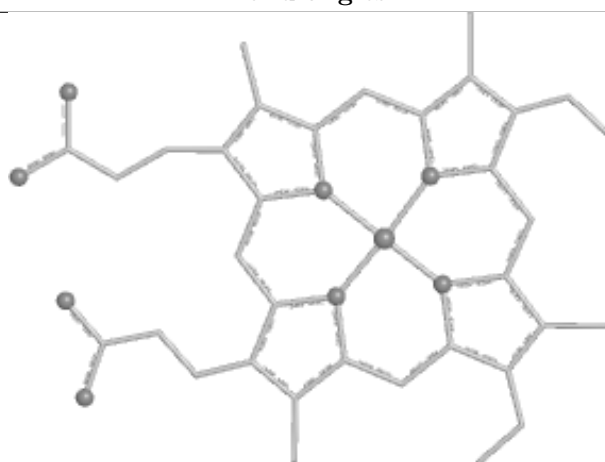
Bond lengths



Bond angles

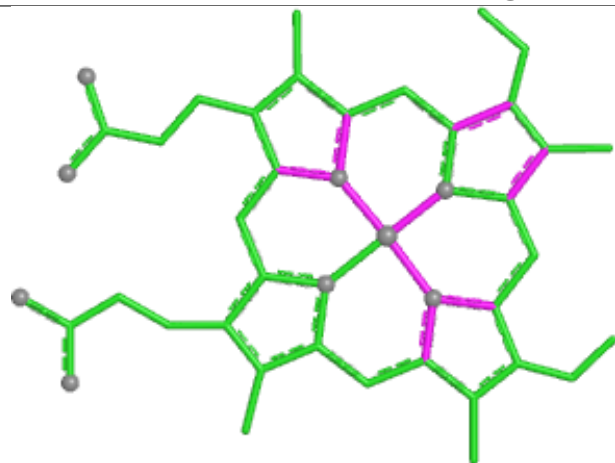


Torsions

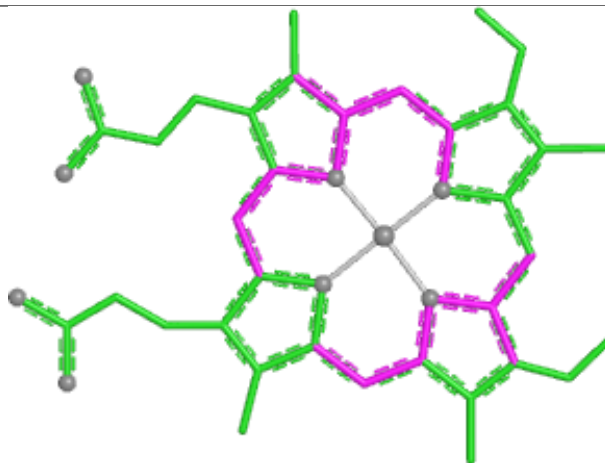


Rings

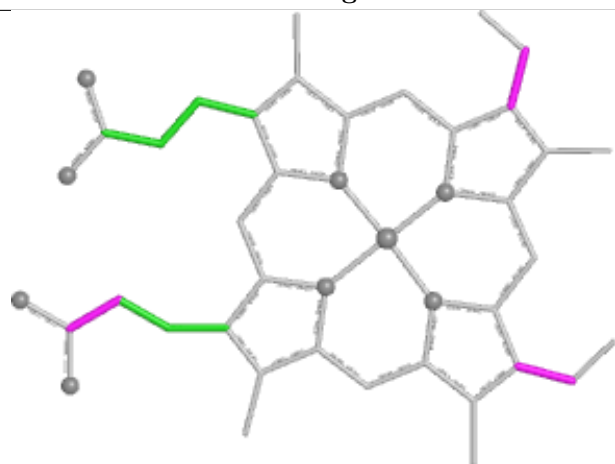
## Ligand HEM 3C 502



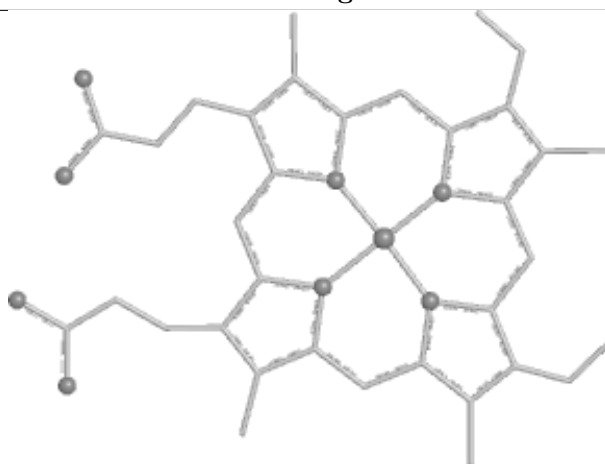
Bond lengths



Bond angles

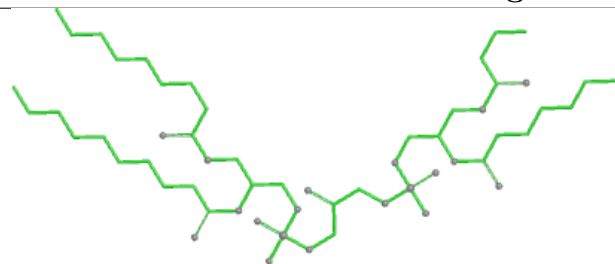


Torsions

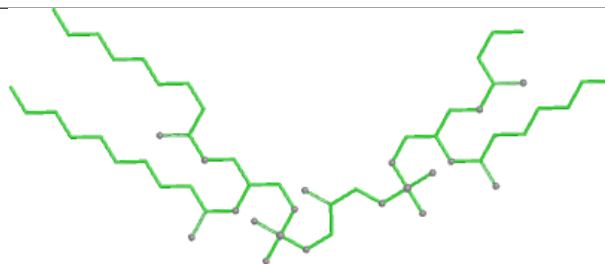


Rings

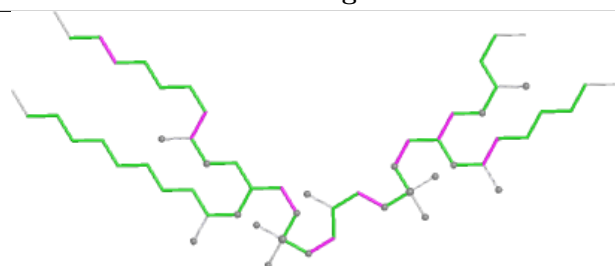
## Ligand CDL 3A 501



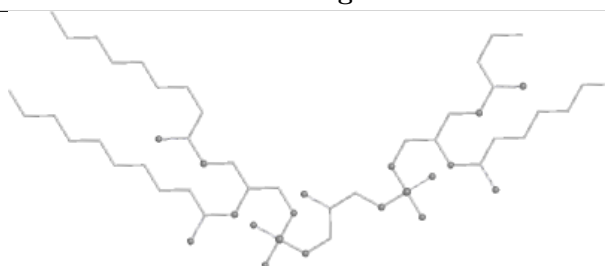
Bond lengths



Bond angles

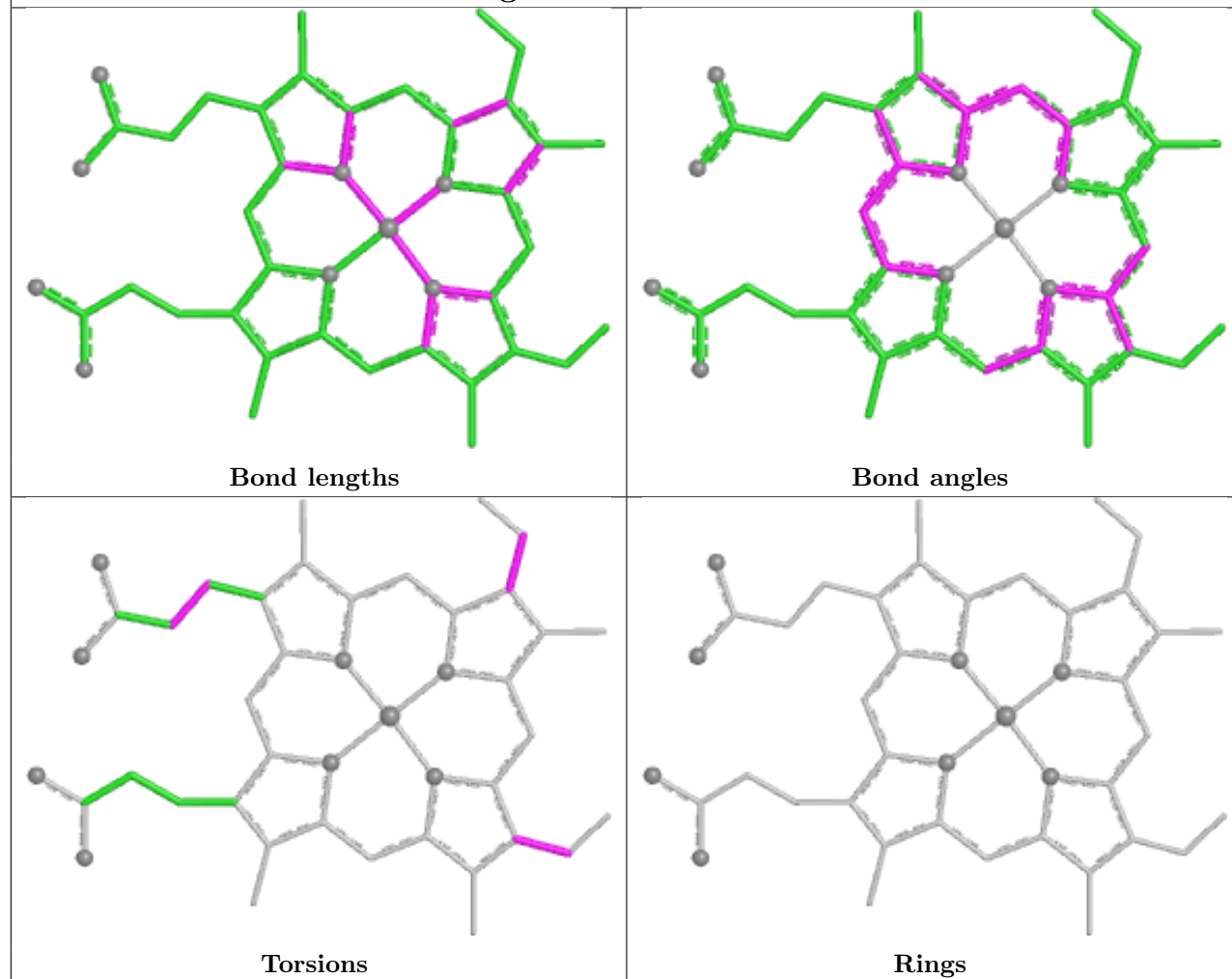


Torsions

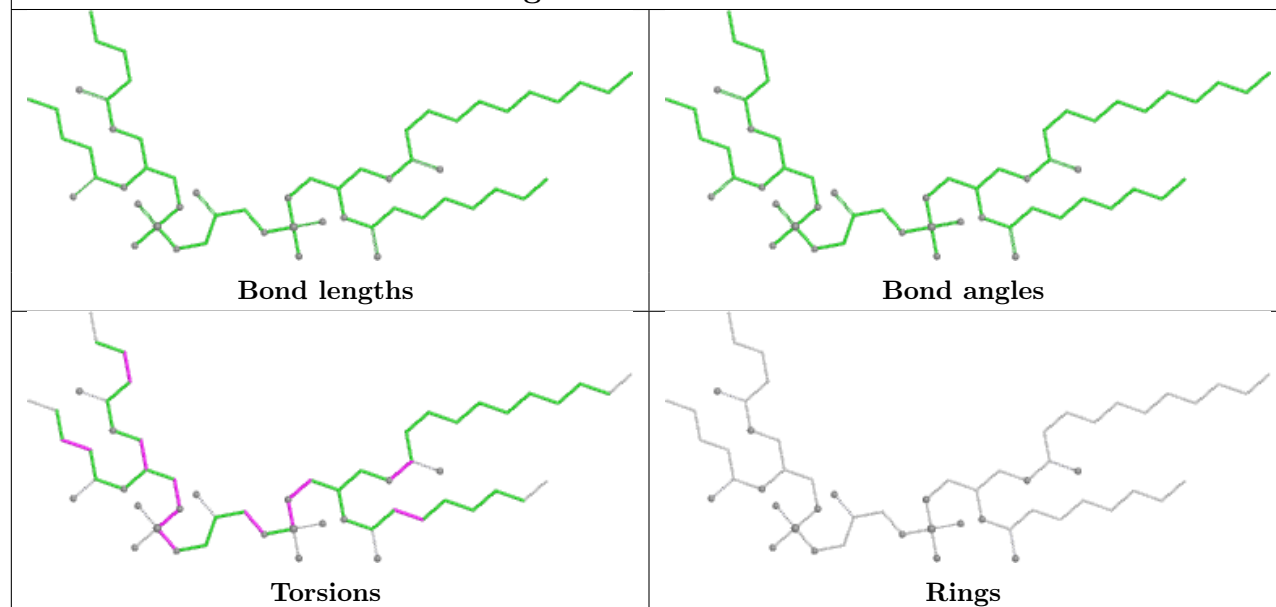


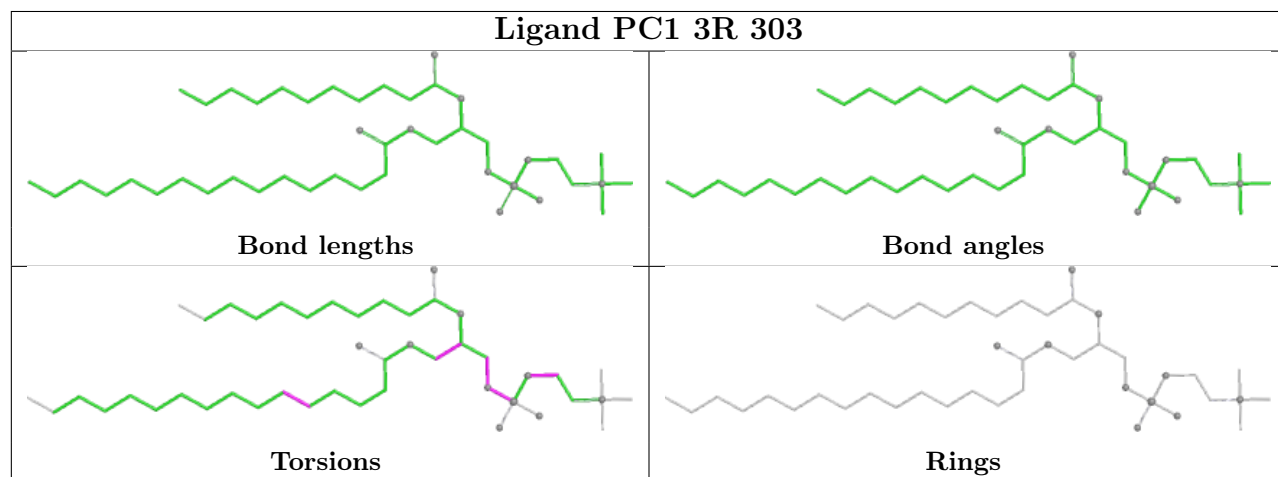
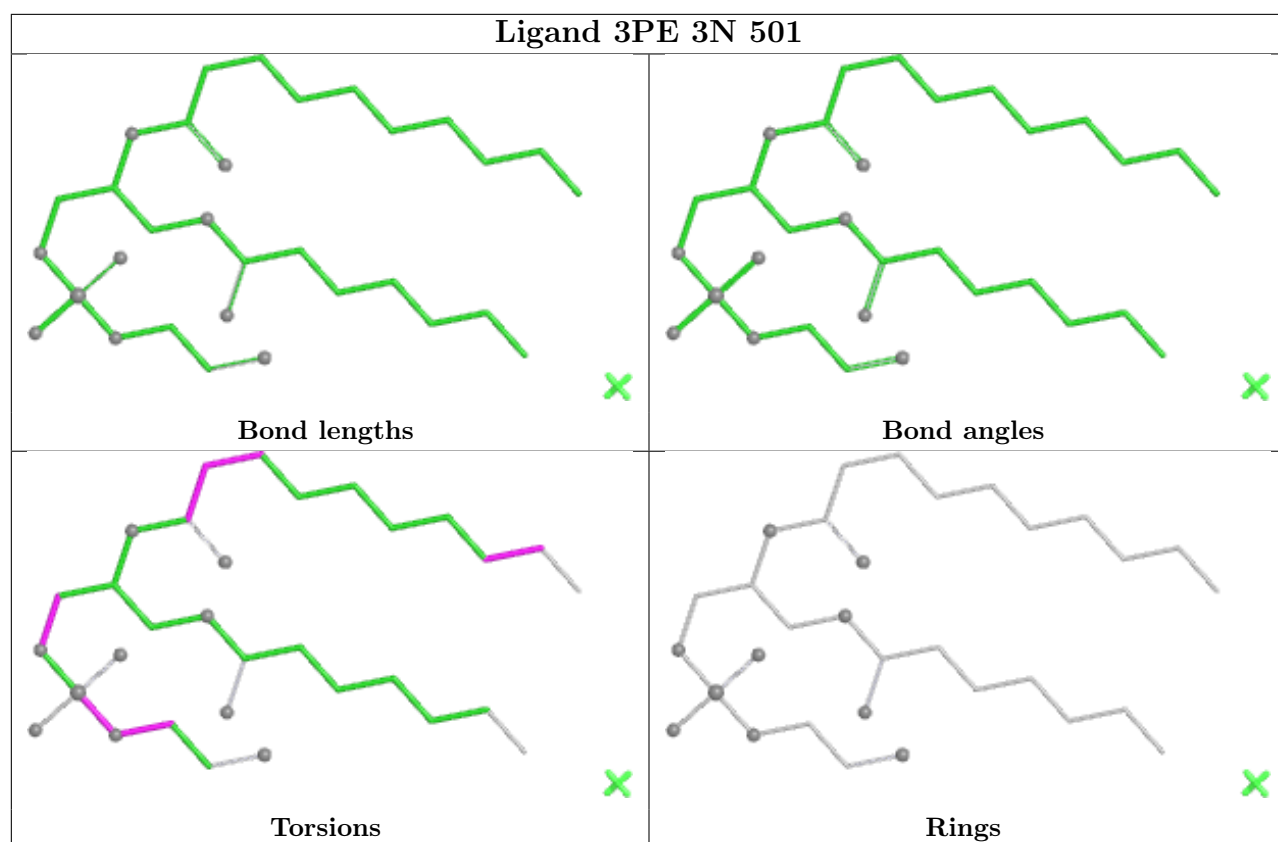
Rings

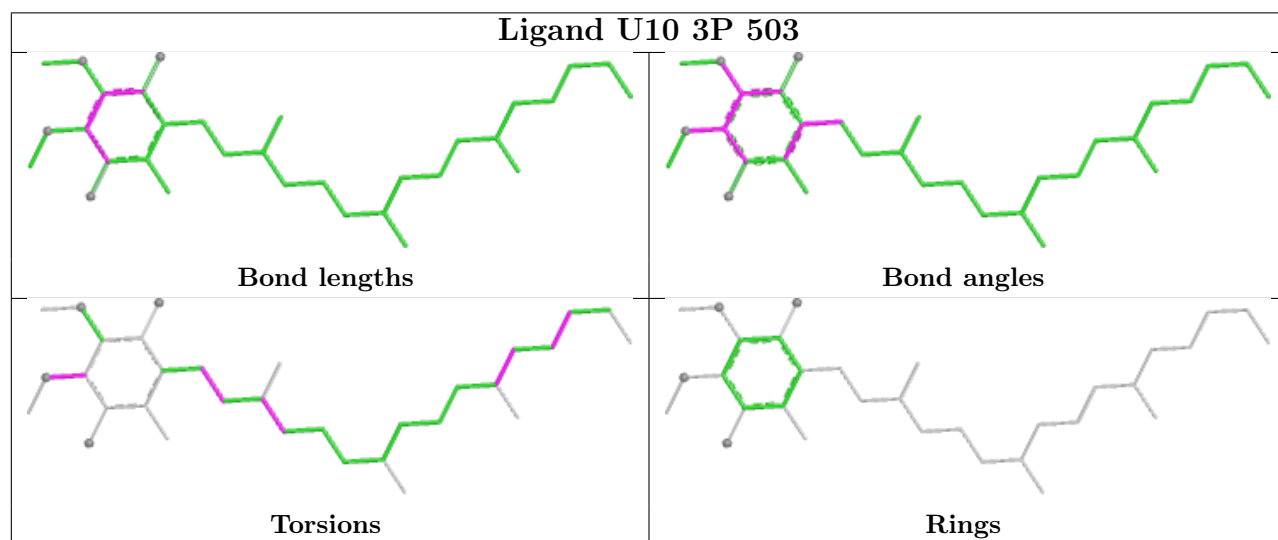
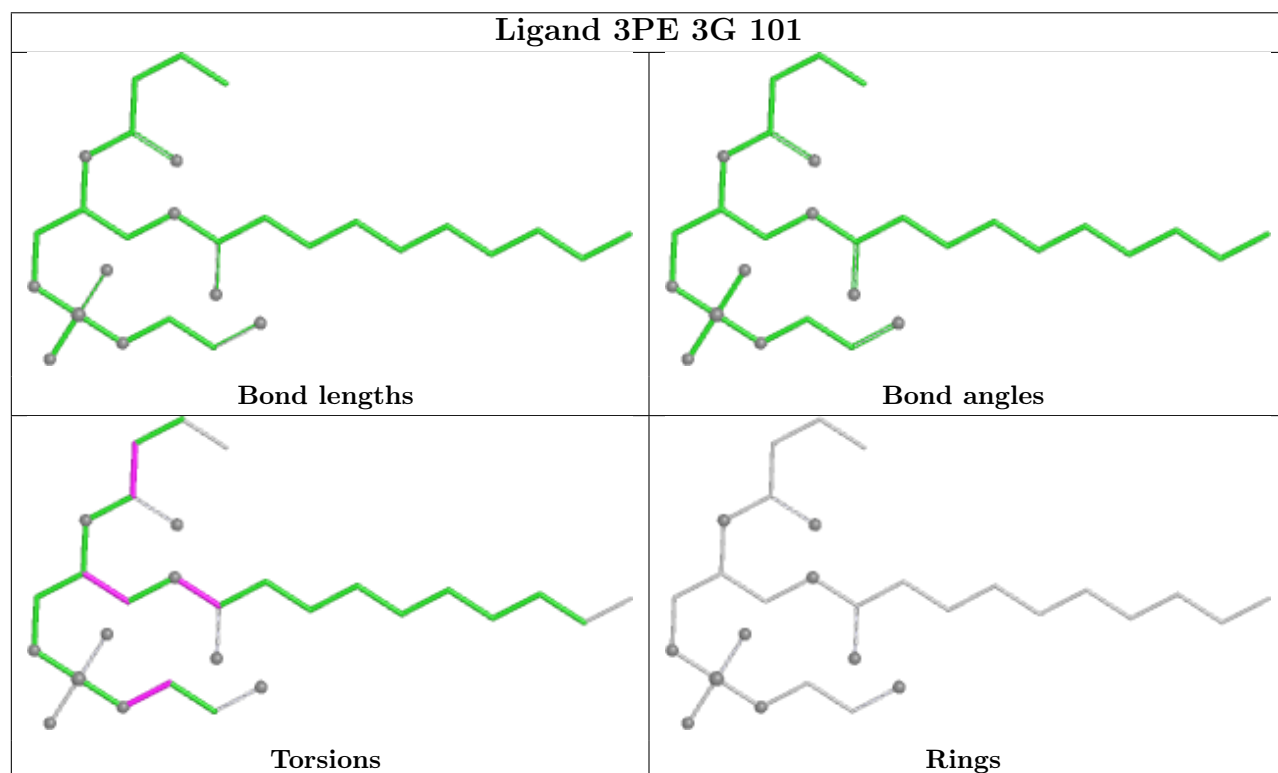
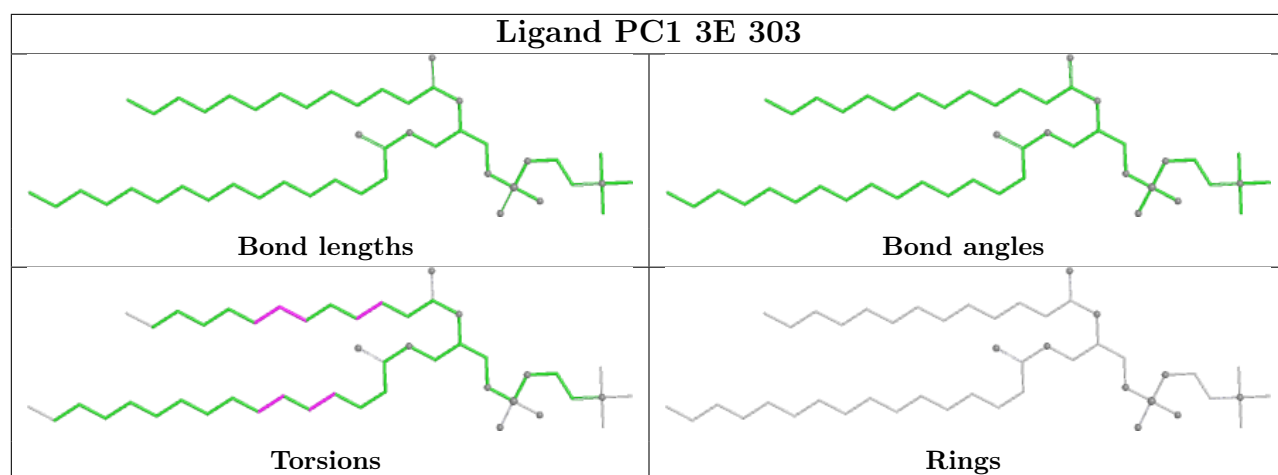
## Ligand HEM 3C 501

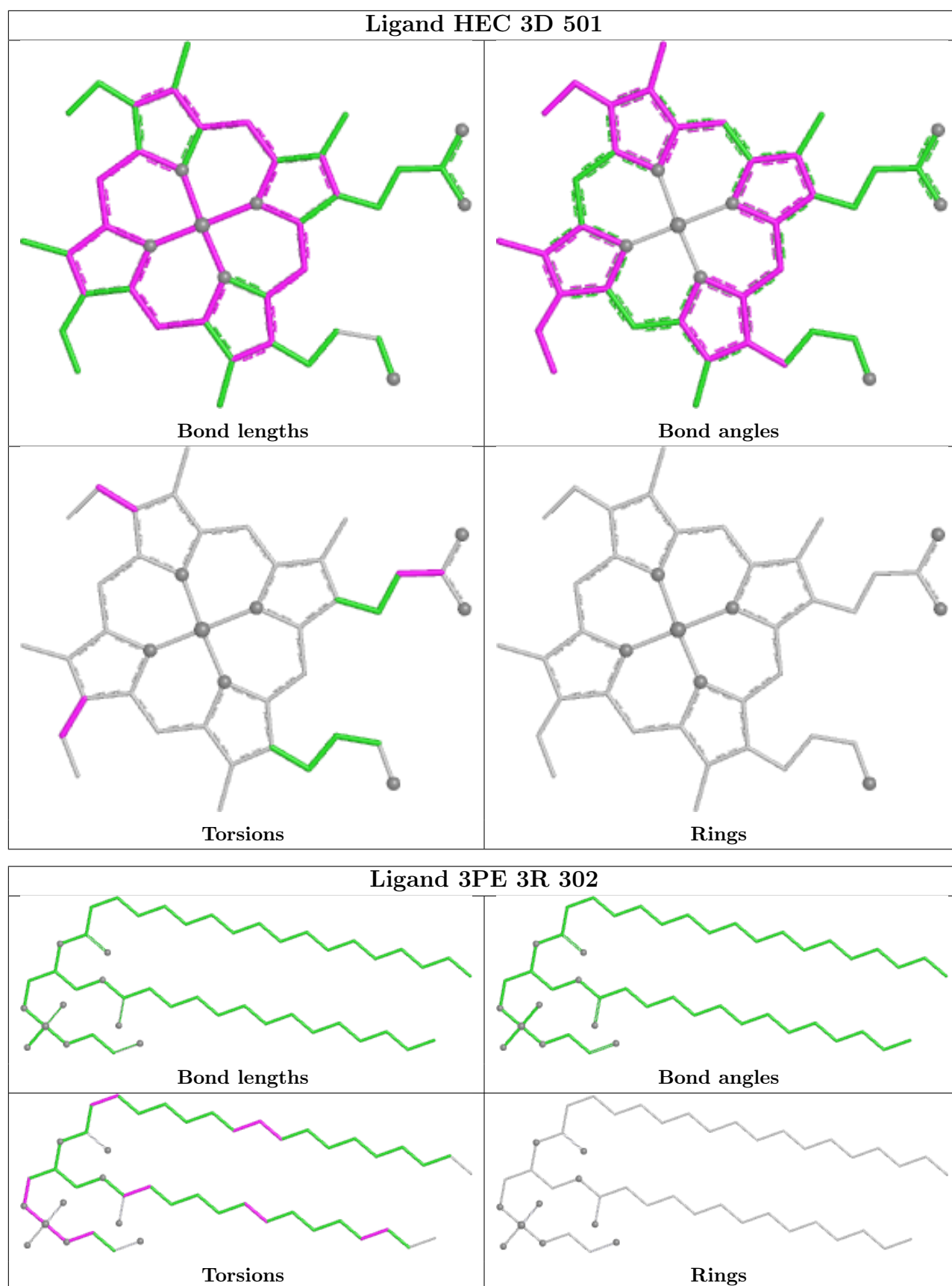


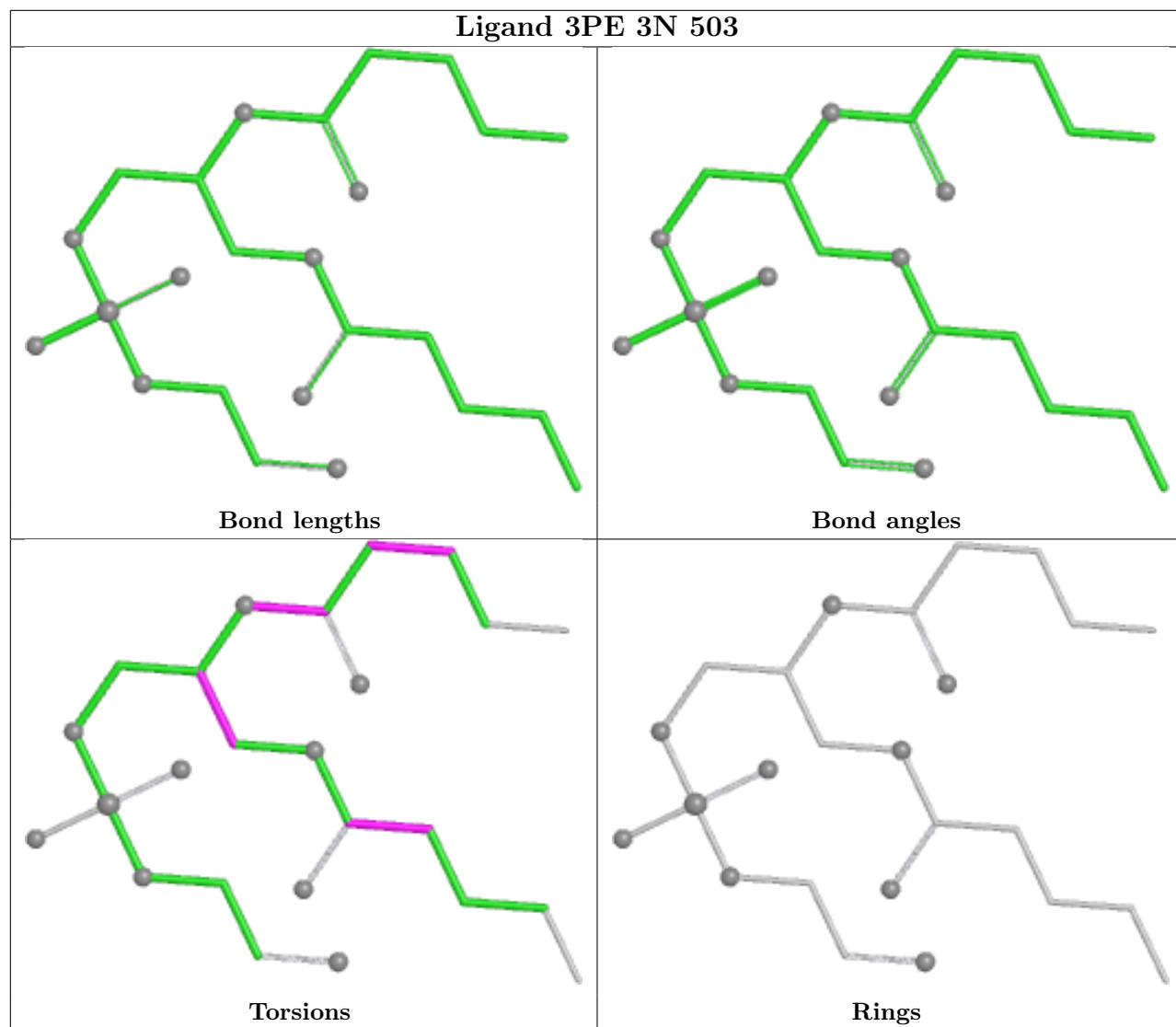
## Ligand CDL 3T 101

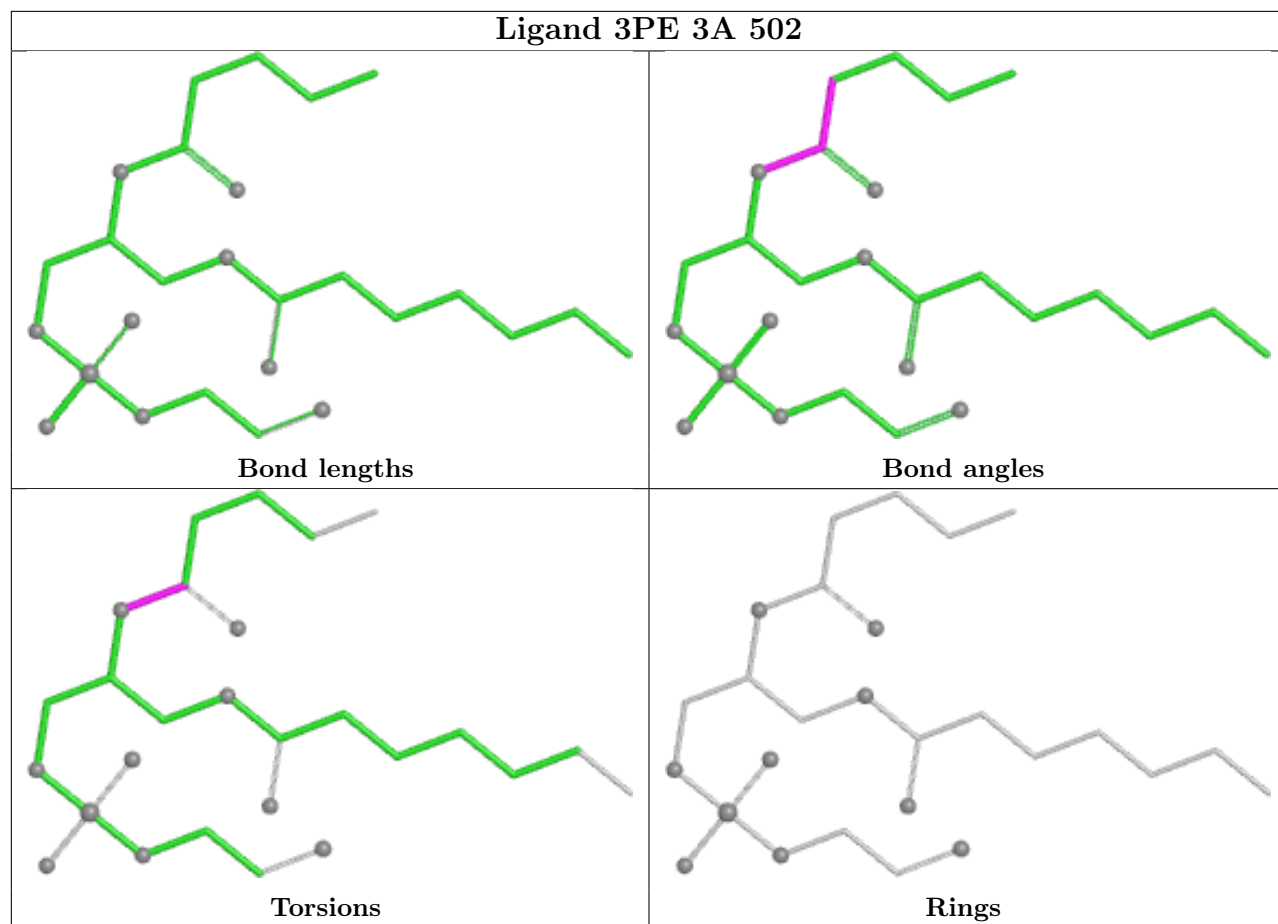


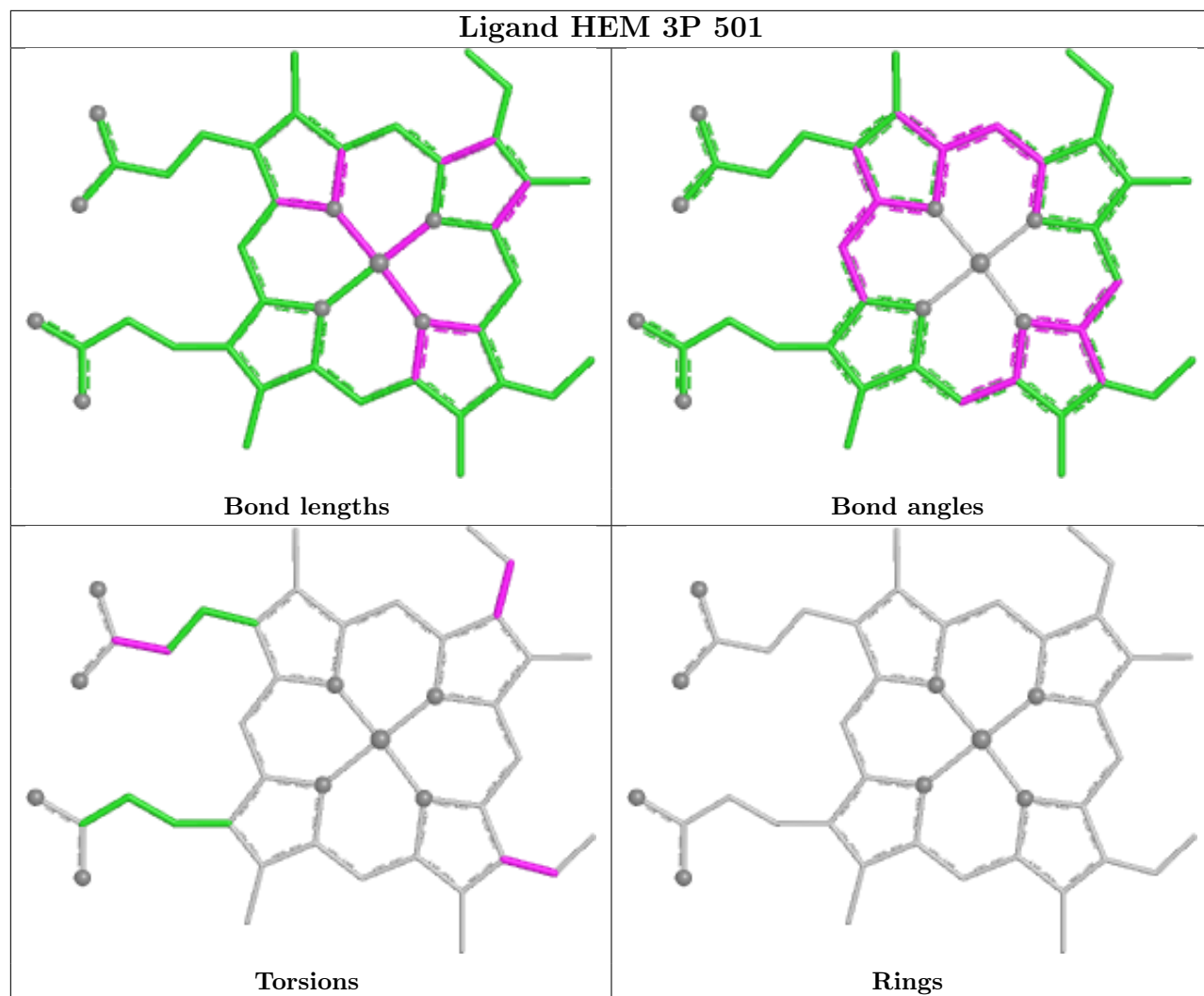












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 7   | 3G    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 3G    | 75:ASN    | C      | 82:PRO    | N      | 4.66         |

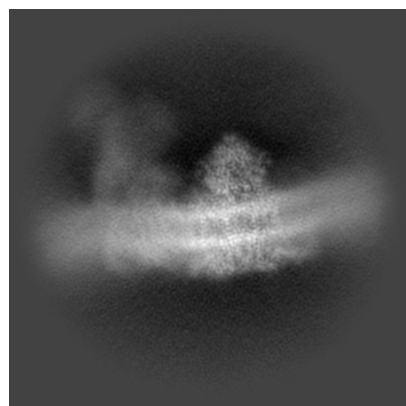
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42223. These allow visual inspection of the internal detail of the map and identification of artifacts.

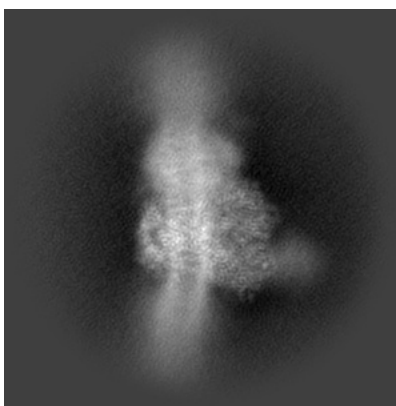
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

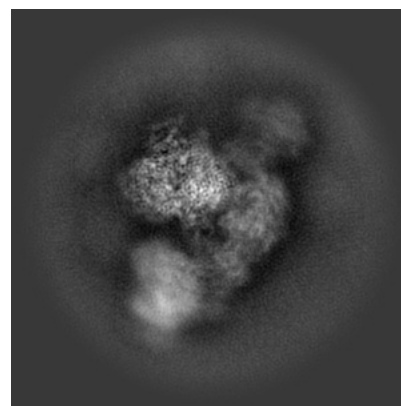
#### 6.1.1 Primary map



X

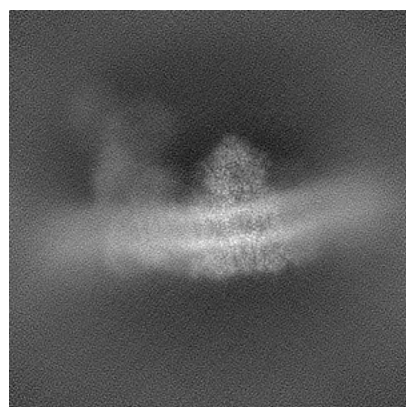


Y

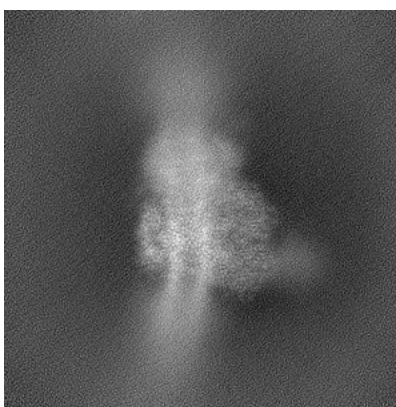


Z

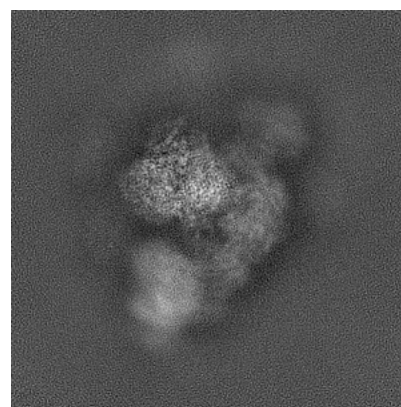
#### 6.1.2 Raw map



X



Y

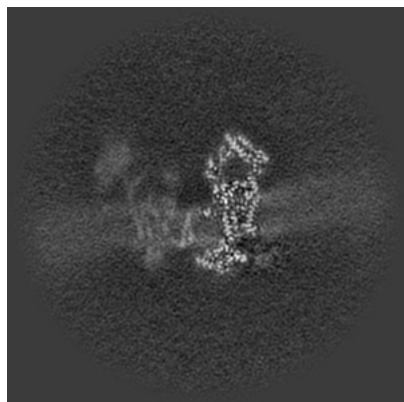


Z

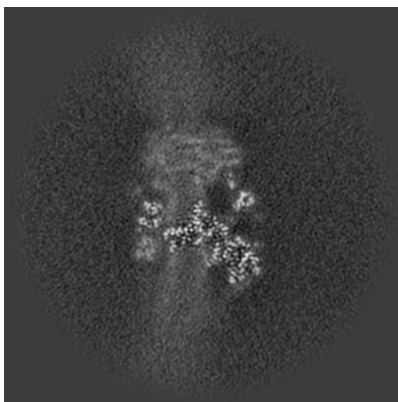
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

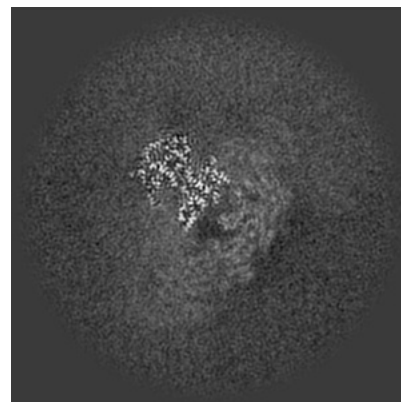
### 6.2.1 Primary map



X Index: 160

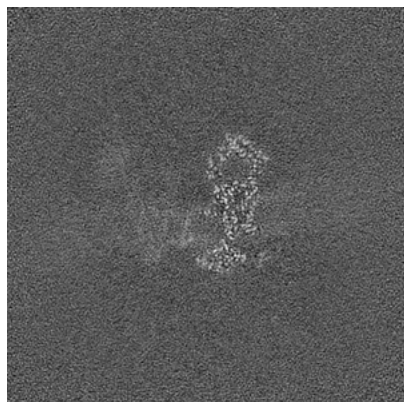


Y Index: 160

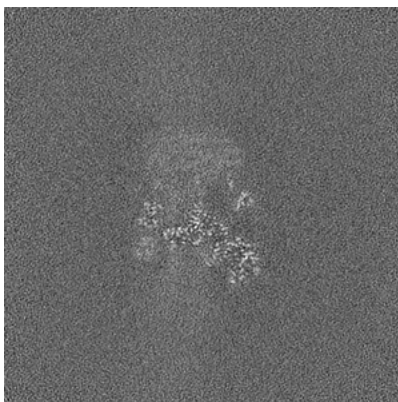


Z Index: 160

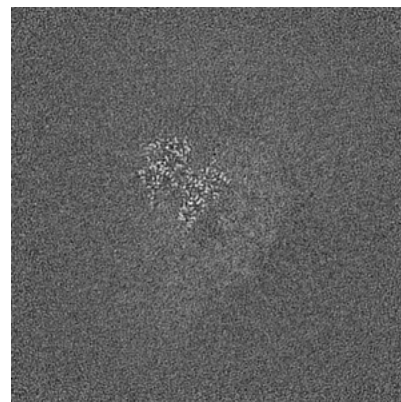
### 6.2.2 Raw map



X Index: 160



Y Index: 160

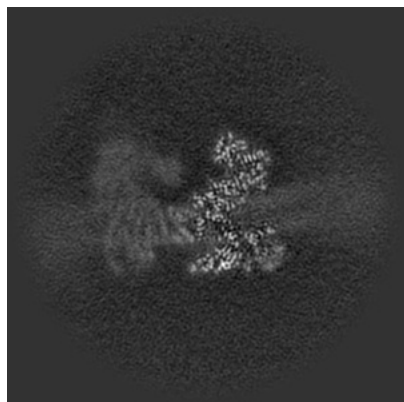


Z Index: 160

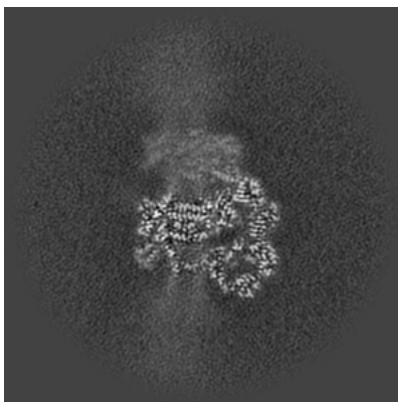
The images above show central slices of the map in three orthogonal directions.

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

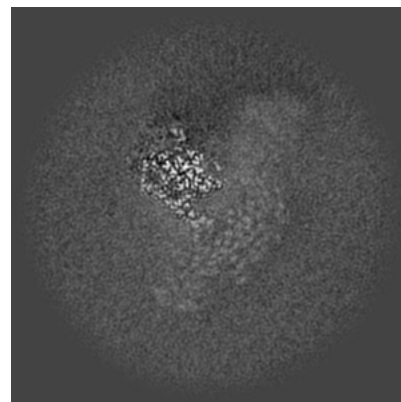
### 6.3.1 Primary map



X Index: 147

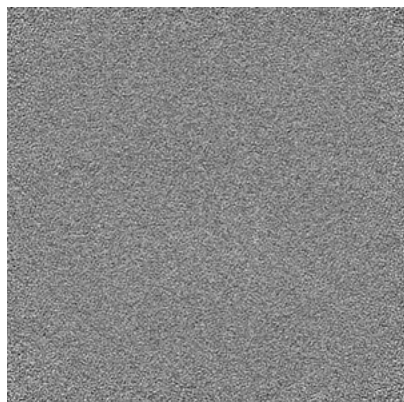


Y Index: 175

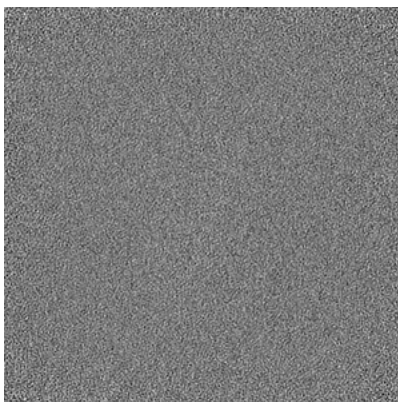


Z Index: 136

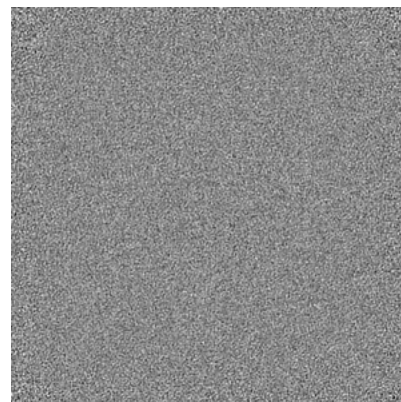
### 6.3.2 Raw map



X Index: 0



Y Index: 0

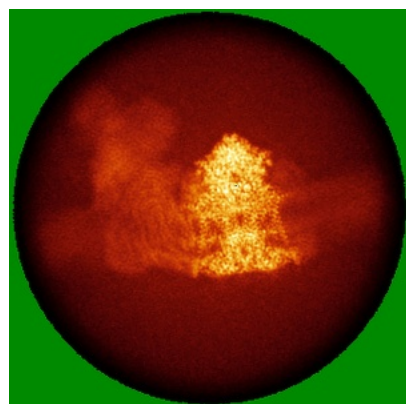


Z Index: 0

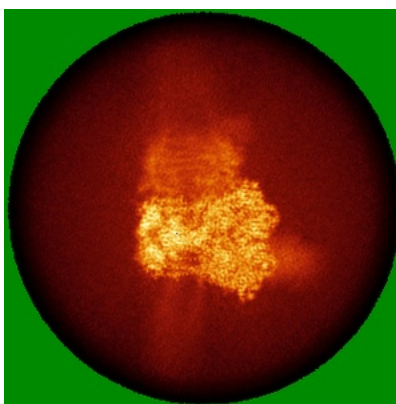
The images above show the largest variance slices of the map in three orthogonal directions.

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

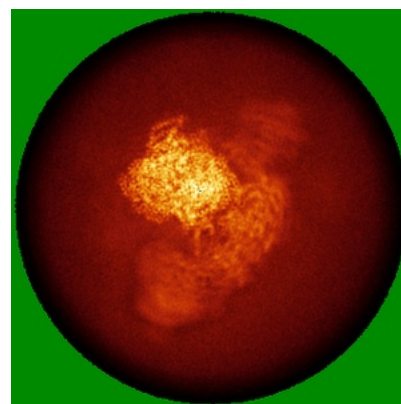
### 6.4.1 Primary map



X

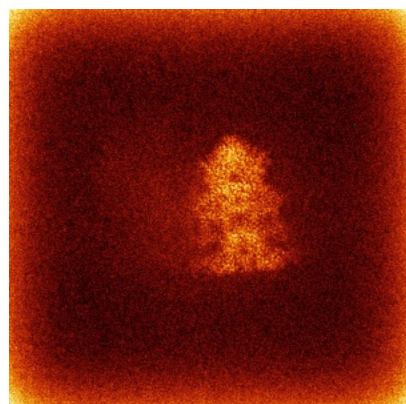


Y

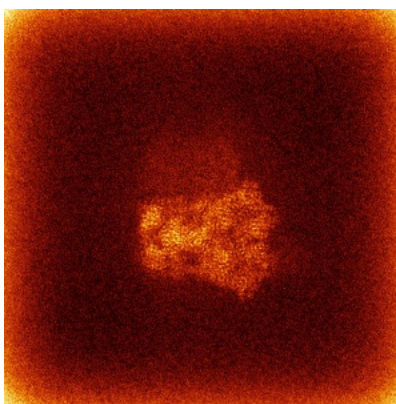


Z

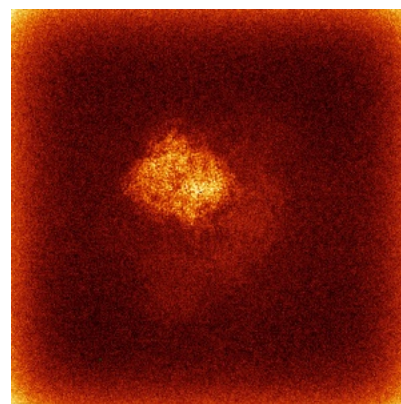
### 6.4.2 Raw map



X



Y

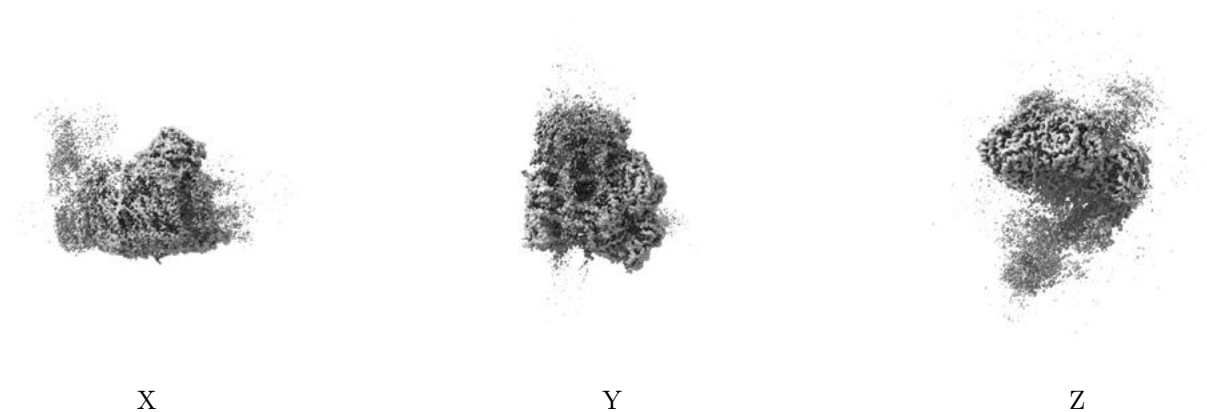


Z

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

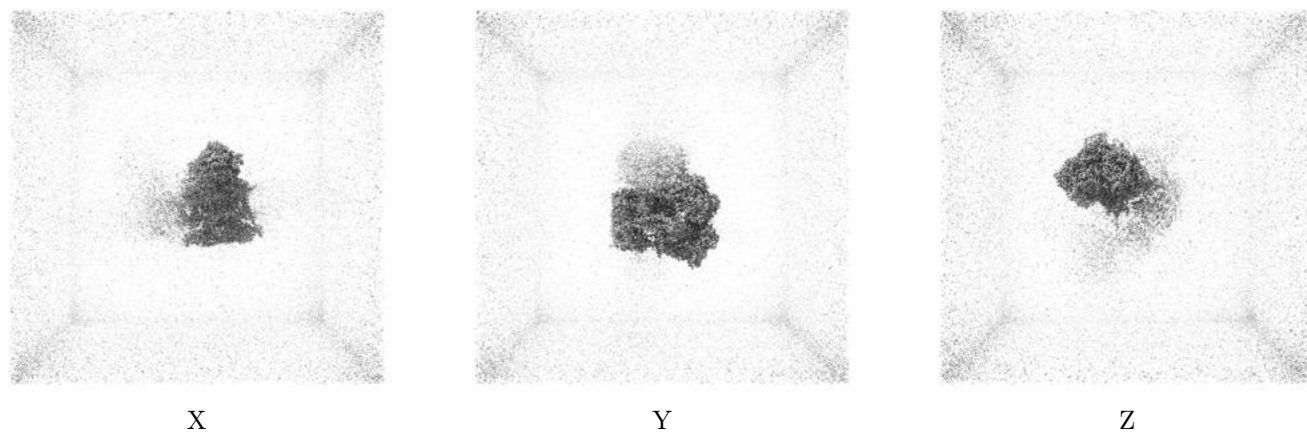
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

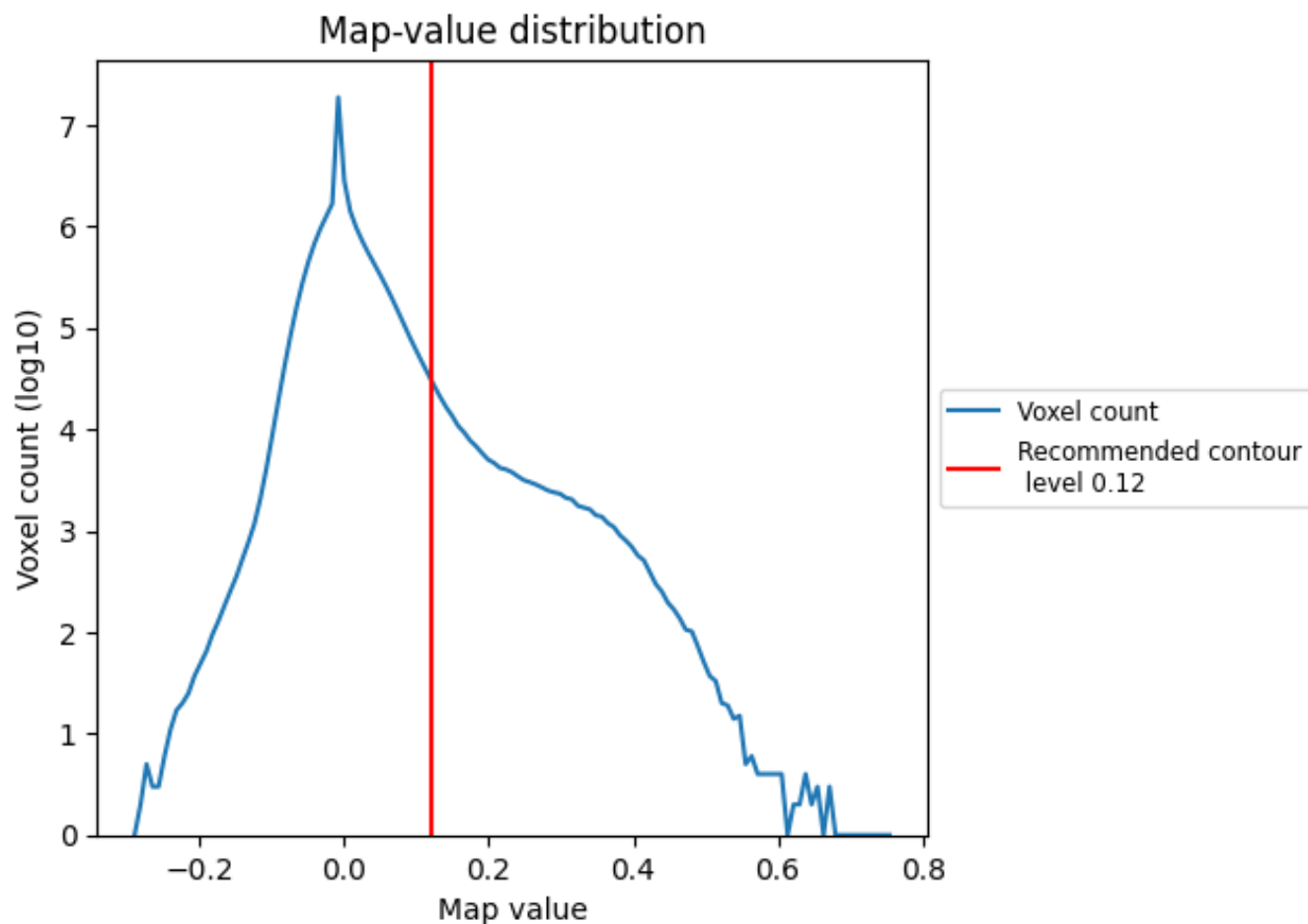
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

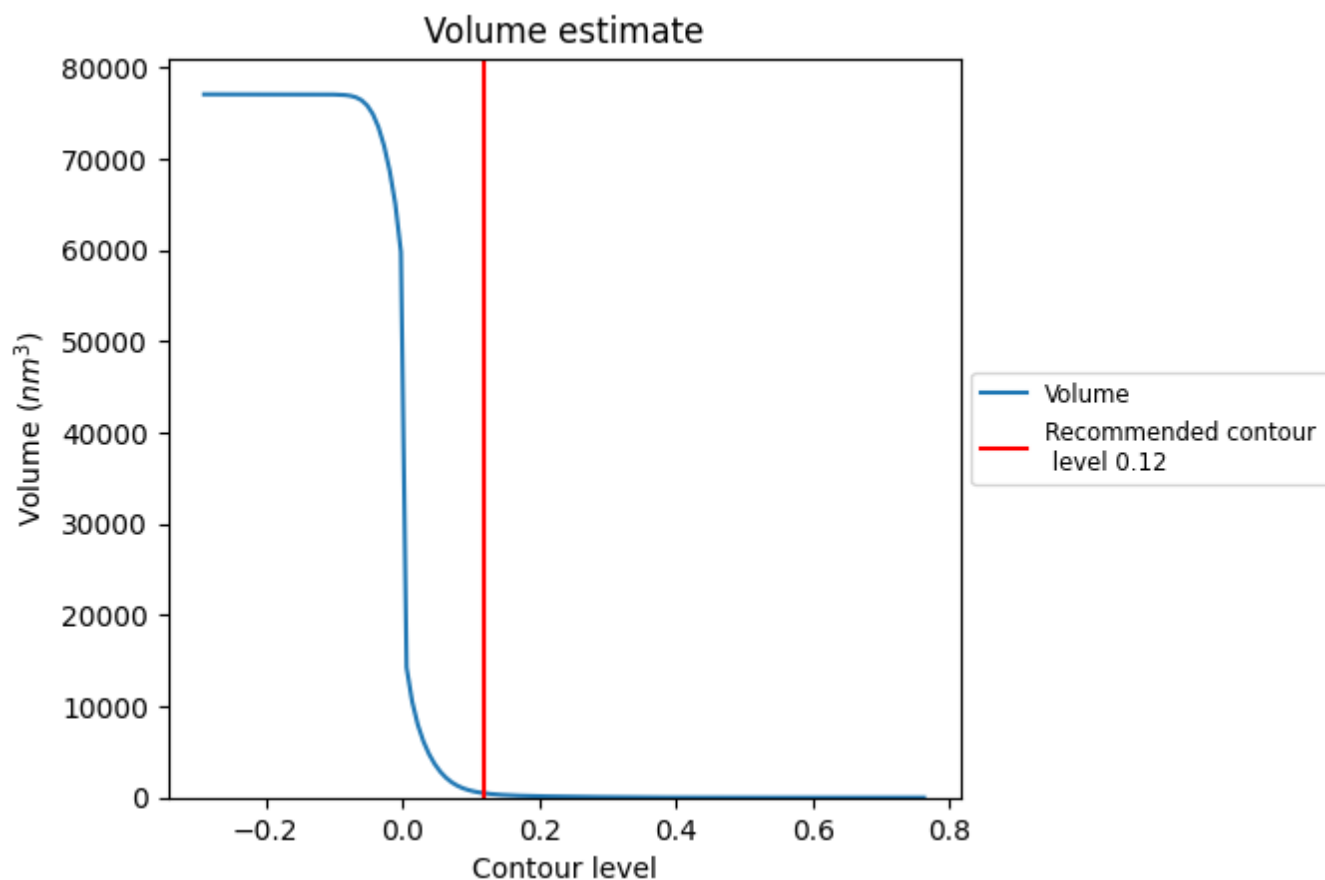
This section contains the results of statistical analysis of the map.

### 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.

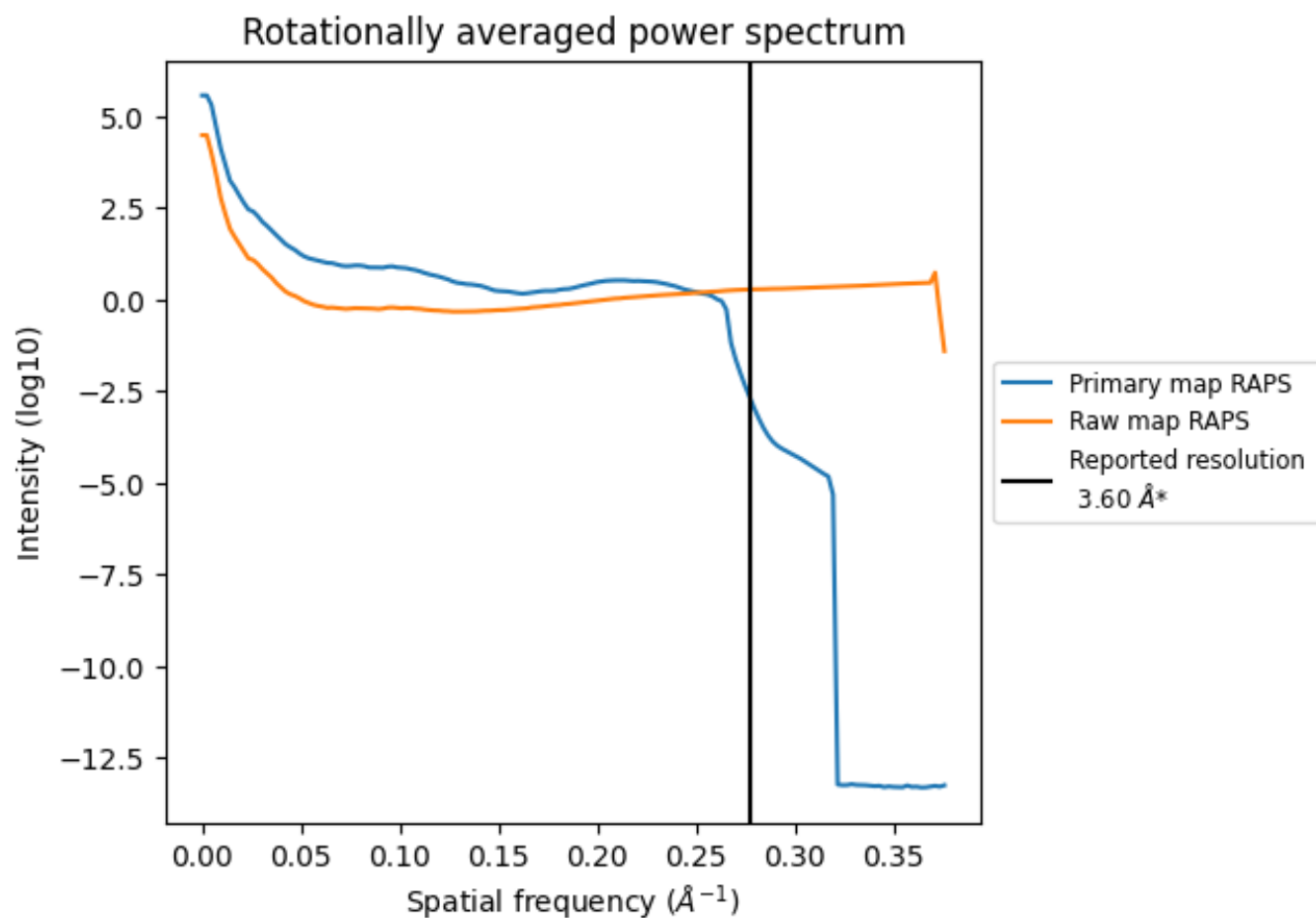
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 472  $\text{nm}^3$ ; this corresponds to an approximate mass of 426 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 ⓘ

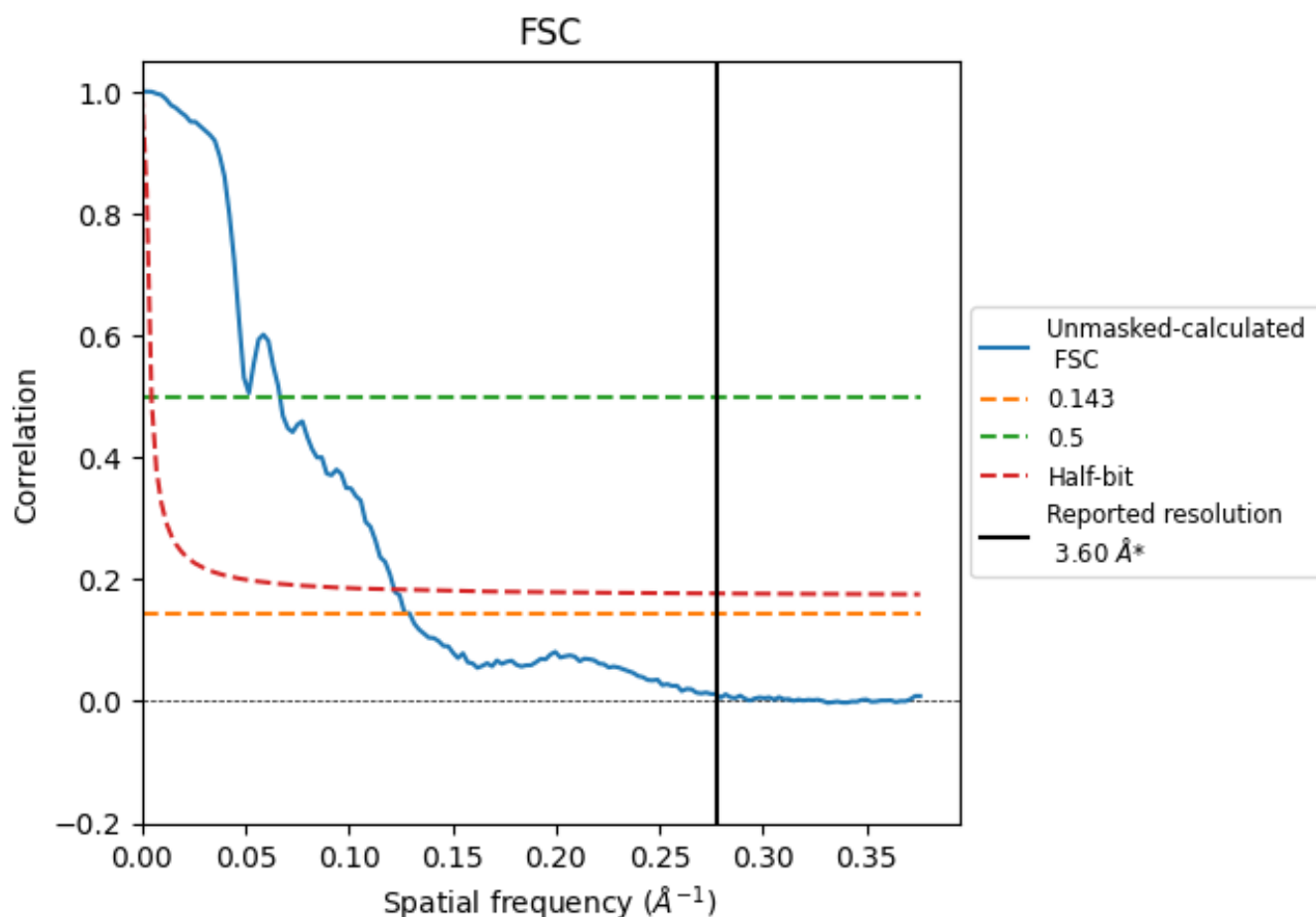


\*Reported resolution corresponds to spatial frequency of 0.278  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

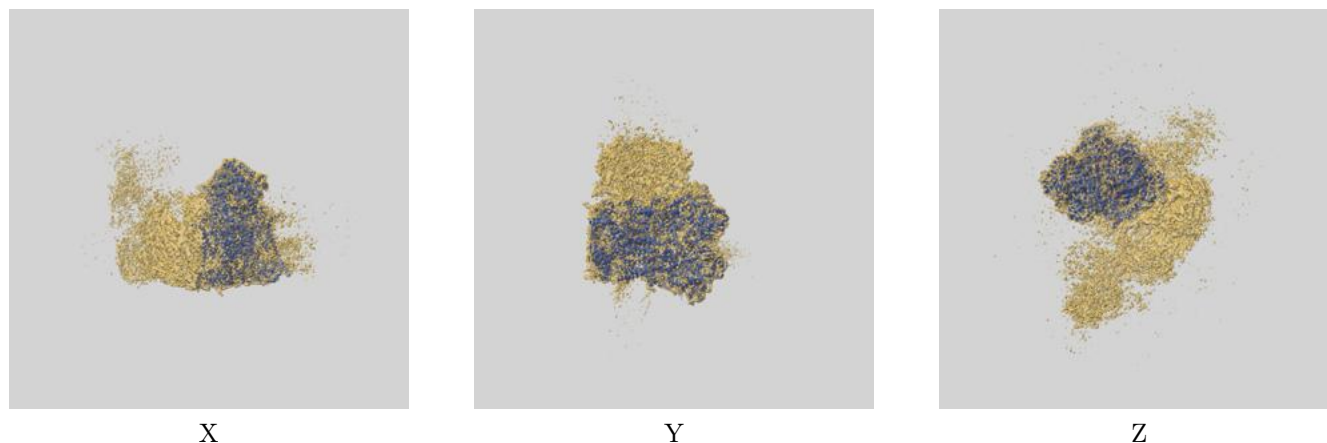
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 3.60                               | -     | -        |
| Author-provided FSC curve | -                                  | -     | -        |
| Unmasked-calculated*      | 7.73                               | 15.02 | 8.20     |

\*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 7.73 differs from the reported value 3.6 by more than 10 %

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

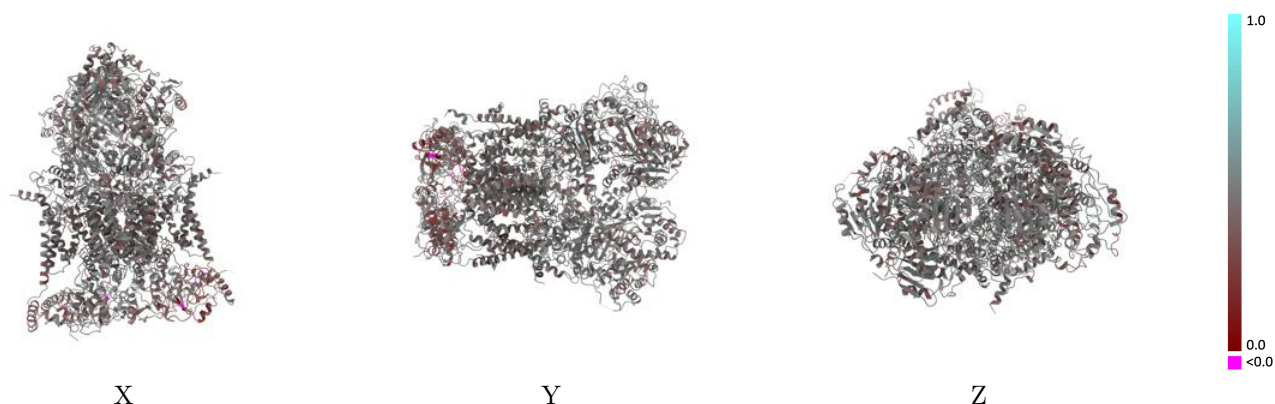
This section contains information regarding the fit between EMDB map EMD-42223 and PDB model 8UGF. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



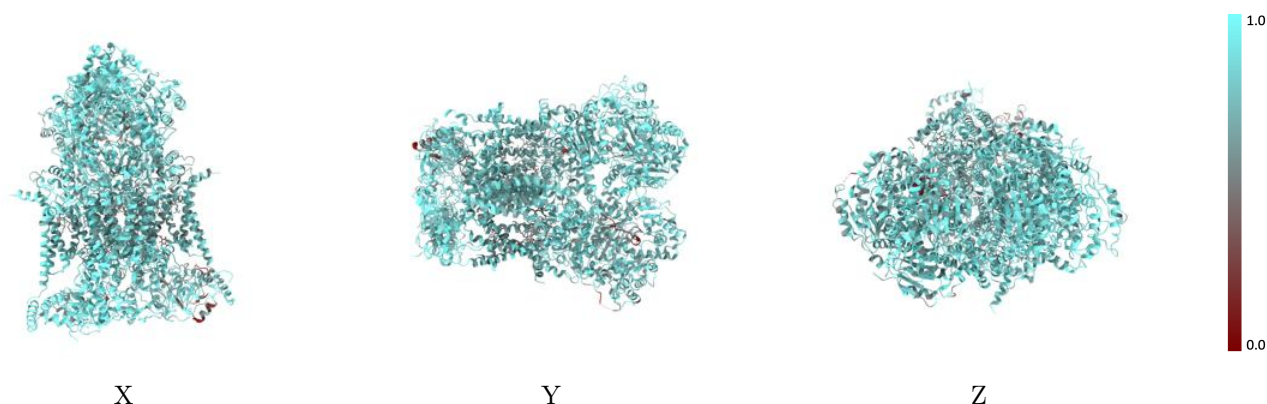
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



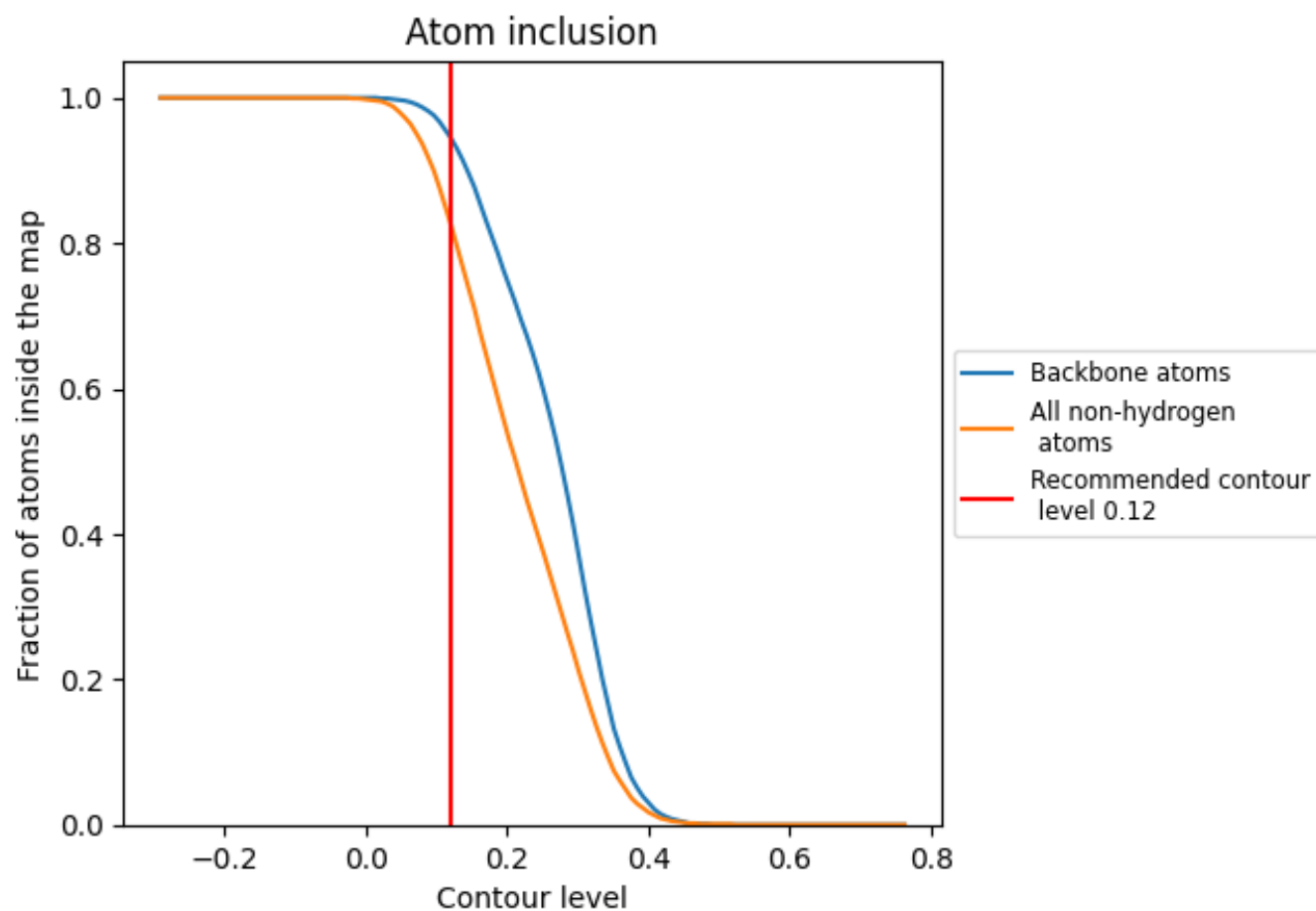
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 83% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8280   |  0.4420   |
| 3A    |  0.7940   |  0.4550   |
| 3B    |  0.8290   |  0.4570   |
| 3C    |  0.8040   |  0.4520   |
| 3D    |  0.8730   |  0.4550   |
| 3E    |  0.7130   |  0.3690   |
| 3F    |  0.8250   |  0.4540   |
| 3G    |  0.7800   |  0.4530   |
| 3H    |  0.8450   |  0.3860   |
| 3I    |  0.3960   |  0.3580   |
| 3J    |  0.8100   |  0.4310   |
| 3N    |  0.8850   |  0.4570   |
| 3O    |  0.8720   |  0.4540   |
| 3P    |  0.8630   |  0.4580   |
| 3Q    |  0.9160  |  0.4610  |
| 3R    |  0.7040 |  0.3430 |
| 3S    |  0.8720 |  0.4600 |
| 3T    |  0.8650 |  0.4460 |
| 3U    |  0.9020 |  0.4190 |
| 3V    |  0.6840 |  0.4260 |
| 3W    |  0.8980 |  0.4620 |
| 3X    |  0.8070 |  0.4310 |
| 3Y    |  0.7470 |  0.4410 |

