



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 01:38 PM UTC

PDB ID : 8RGP / pdb\_00008rgp  
EMDB ID : EMD-19145  
Title : Closed Complex I from murine brain  
Authors : Vercellino, I.; Sazanov, L.A.  
Deposited on : 2023-12-14  
Resolution : 3.00 Å(reported)  
Based on initial model : 6g2j

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

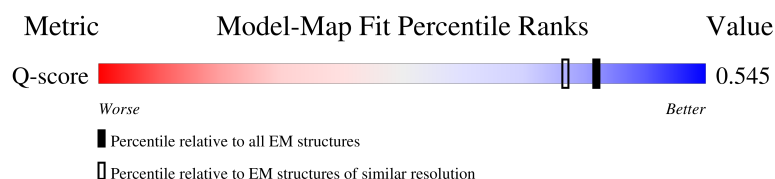
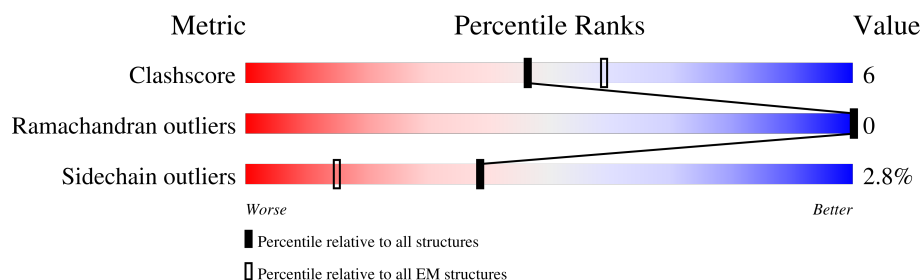
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



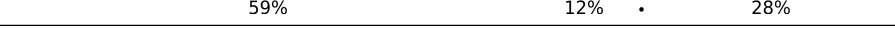
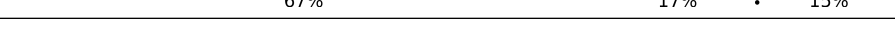
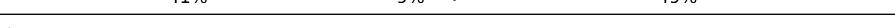
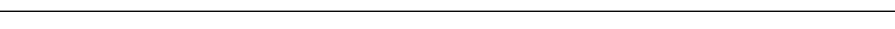
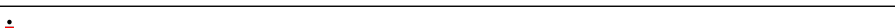
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14081 ( 2.50 - 3.50 )                                    |

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   | 6     | 224    | <br>57% 12% 31%     |
| 2   | C     | 263    | <br>65% 13% 21%     |
| 3   | D     | 463    | <br>5% 72% 19% • 7% |
| 4   | 2     | 248    | <br>68% 18% • 14%   |

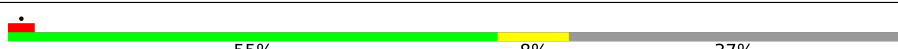
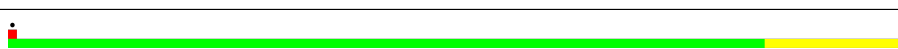
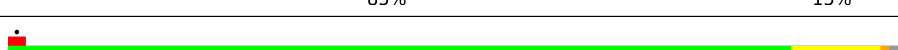
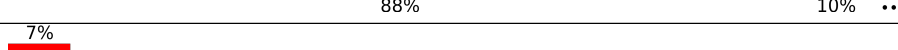
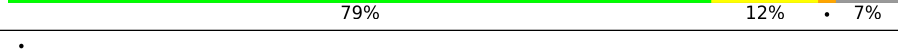
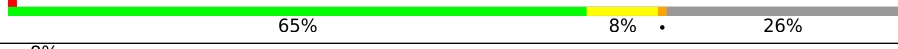
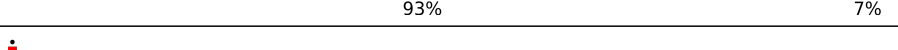
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | 1     | 464    |    |
| 6   | 3     | 727    |    |
| 7   | 9     | 212    |    |
| 8   | P     | 377    |    |
| 9   | Q     | 175    |    |
| 10  | 7     | 116    |    |
| 11  | S     | 99     |    |
| 12  | T     | 156    |    |
| 12  | U     | 156    |    |
| 13  | V     | 116    |    |
| 14  | W     | 131    |    |
| 15  | q     | 145    |  |
| 16  | r     | 113    |  |
| 17  | s     | 104    |  |
| 18  | A     | 115    |  |
| 19  | H     | 318    |  |
| 20  | J     | 172    |  |
| 21  | K     | 98     |  |
| 22  | L     | 607    |  |
| 23  | M     | 459    |  |
| 24  | N     | 345    |  |
| 25  | O     | 355    |  |
| 26  | X     | 172    |  |
| 27  | Y     | 141    |  |
| 28  | Z     | 144    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | a     | 70     |    |
| 30  | b     | 84     |    |
| 31  | c     | 76     |    |
| 32  | d     | 120    |    |
| 33  | e     | 106    |    |
| 34  | f     | 57     |    |
| 35  | g     | 151    |    |
| 36  | h     | 189    |    |
| 37  | i     | 128    |    |
| 38  | j     | 105    |    |
| 39  | k     | 104    |    |
| 40  | l     | 186    |    |
| 41  | m     | 129    |   |
| 42  | n     | 179    |  |
| 43  | o     | 137    |  |
| 44  | p     | 176    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 37  | SAC  | i     | 1   | -         | X        | -       | -                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 67868 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 1   | 6     | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1241  | 793 | 222 | 212 | 14 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | C     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1721  | 1110 | 295 | 313 | 3 |         |       |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | D     | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3464  | 2215 | 595 | 630 | 24 |         |       |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 2     | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1660  | 1056 | 279 | 314 | 11 |         |       |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 1     | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3321  | 2092 | 596 | 611 | 22 |         |       |

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 6   | 3     | 690      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5305  | 3326 | 921 | 1017 | 41 |         |       |

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | 9     | 178      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1431  | 898 | 245 | 276 | 12 |         |       |

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 8   | P     | 342      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1777 | 483 | 481 | 7 |         |       |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | Q     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1022  | 646 | 180 | 192 | 4 |         |       |

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | 7     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 758   | 470 | 141 | 144 | 3 |         |       |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | S     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 421 | 127 | 120 | 3 |         |       |

- Molecule 12 is a protein called Acyl carrier protein, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 12  | T     | 79       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 637   | 410 | 95 | 127 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | U     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 706   | 453 | 104 | 144 | 5 |         |       |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | V     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 915   | 596 | 152 | 164 | 3 |         |       |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | W     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 970   | 619 | 180 | 165 | 6 |         |       |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | q     | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1209  | 777 | 215 | 212 | 5 |         |       |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | r     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 796   | 504 | 148 | 141 | 3 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 17  | s     | 41       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 344   | 215 | 61 | 68 |         |       |

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | A     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 633 | 132 | 160 | 7 |         |       |

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19  | H     | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2540  | 1706 | 384 | 428 | 22 |         |       |

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 20  | J     | 172      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1308  | 878 | 186 | 229 | 15 |         |       |

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 21  | K     | 98       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 737   | 477 | 112 | 137 | 11 |         |       |

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22  | L     | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4800  | 3182 | 746 | 827 | 45 |         |       |

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | M     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2408 | 567 | 617 | 40 |         |       |

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 24  | N     | 345      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2703  | 1795 | 417 | 454 | 37 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 25  | O     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2607  | 1674 | 431 | 492 | 10 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 26  | X     | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1396  | 889 | 250 | 247 | 10 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Y     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1037  | 662 | 175 | 192 | 8 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | Z     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 750 | 207 | 202 | 8 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 29  | a     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 572   | 370 | 101 | 97 | 4 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | b     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 427 | 105 | 115 | 4 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | c     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 398   | 261 | 69 | 67 | 1 |         |       |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | d     | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 651 | 171 | 165 | 9 |         |       |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | e     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 877   | 555 | 162 | 152 | 8 |         |       |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | f     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 456   | 295 | 82 | 77 | 2 |         |       |

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | g     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 850   | 549 | 136 | 161 | 4 |         |       |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | h     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1166  | 764 | 195 | 204 | 3 |         |       |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | i     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 828   | 537 | 146 | 142 | 3 |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | j     | 64       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 555   | 365 | 92 | 97 | 1 |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | k     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 626   | 414 | 106 | 104 | 2 |         |       |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 40  | l     | 157      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1323  | 855 | 220 | 237 | 11 |         |       |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 41  | m     | 126      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1050  | 676 | 189 | 185 |         |       |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 42  | n     | 178      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1541  | 985 | 276 | 269 | 11 |         |       |

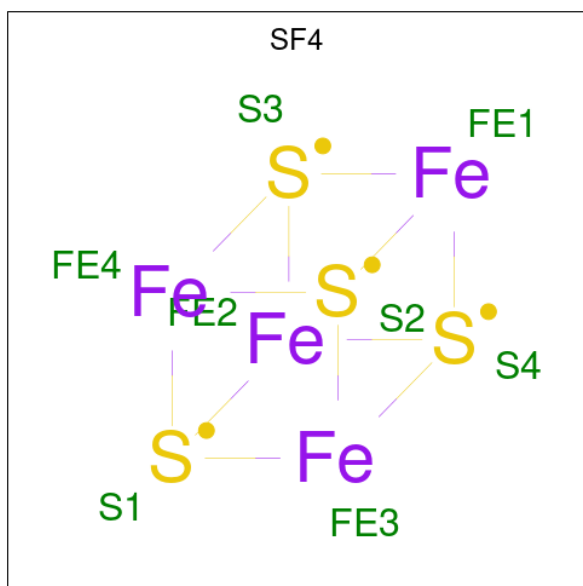
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | o     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1014  | 639 | 190 | 177 | 8 |         |       |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

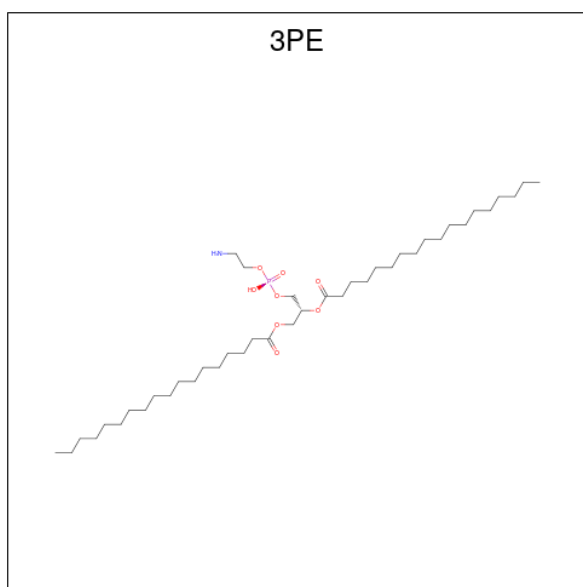
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | p     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1438  | 903 | 258 | 269 | 8 |         |       |

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



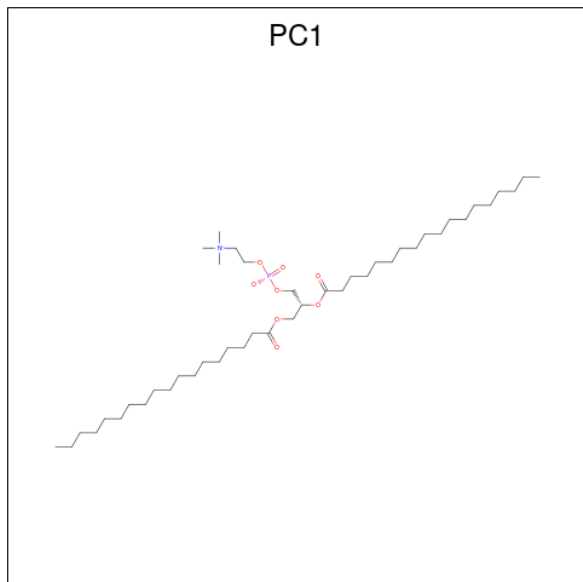
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | 6     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | 1     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | 3     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | 3     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | 9     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | 9     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 46 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $\text{C}_{41}\text{H}_{82}\text{NO}_8\text{P}$ ).



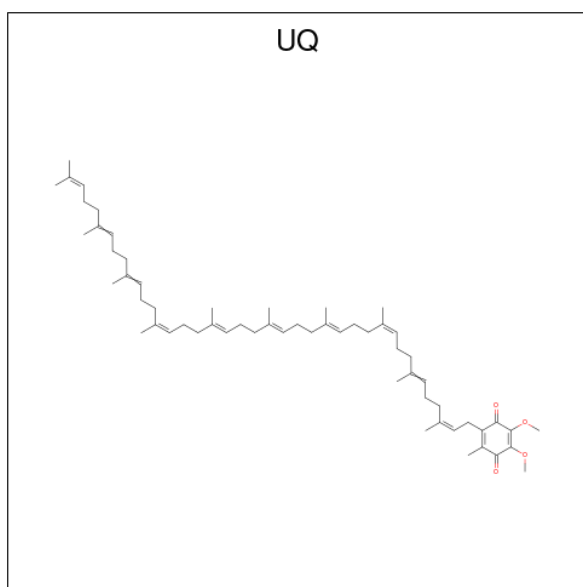
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | 6     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 46  | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 46  | K     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 46  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 46  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 46  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 46  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 46  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 28    | 18 | 1 | 8 | 1 |         |
| 46  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 46  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 46  | h     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 46  | i     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 46  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 30    | 20 | 1 | 8 | 1 |         |

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



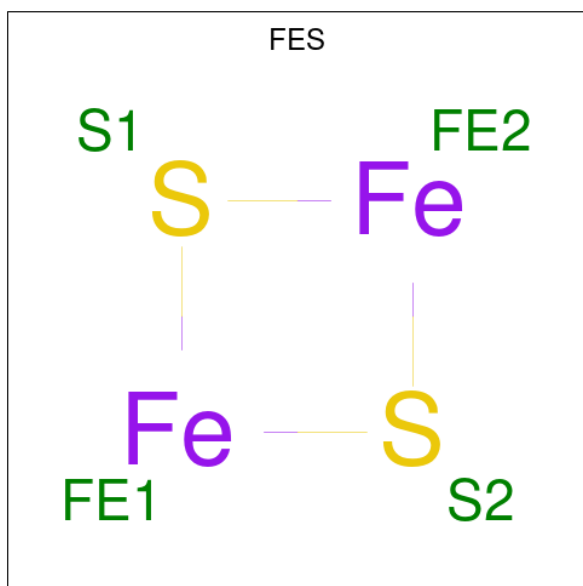
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 47  | 6     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 43    | 33 | 1 | 8 | 1 |         |
| 47  | 9     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 47  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 47  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 47  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |

- Molecule 48 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula:  $C_{59}H_{90}O_4$ ).



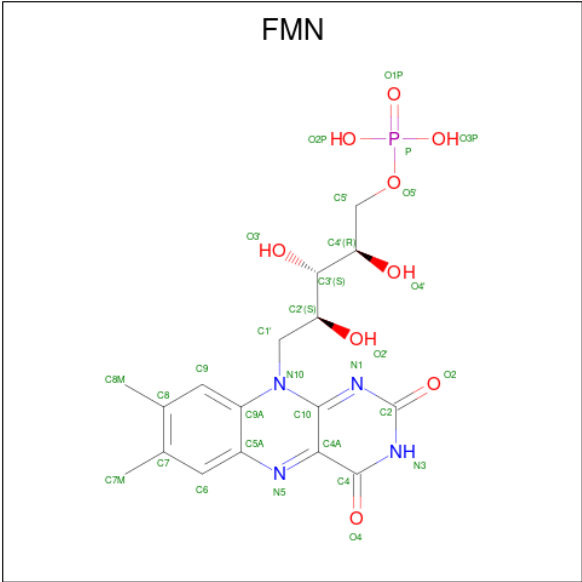
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 48  | D     | 1        | Total | C  | O | 0       |
|     |       |          | 63    | 59 | 4 |         |

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 49  | 2     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 49  | 3     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).

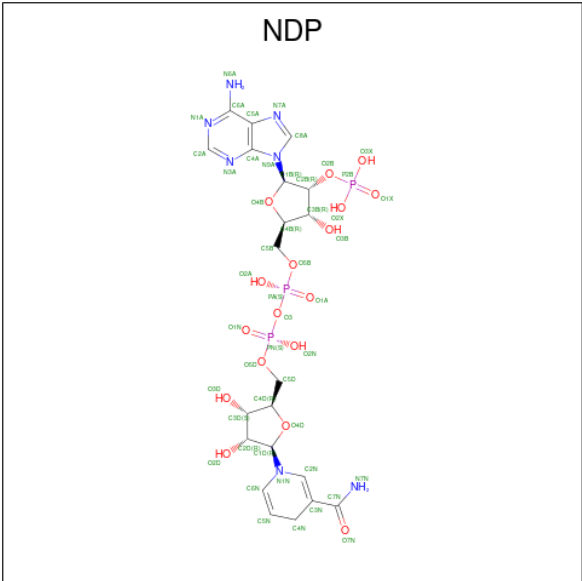


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 50  | 1     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 51  | 3     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



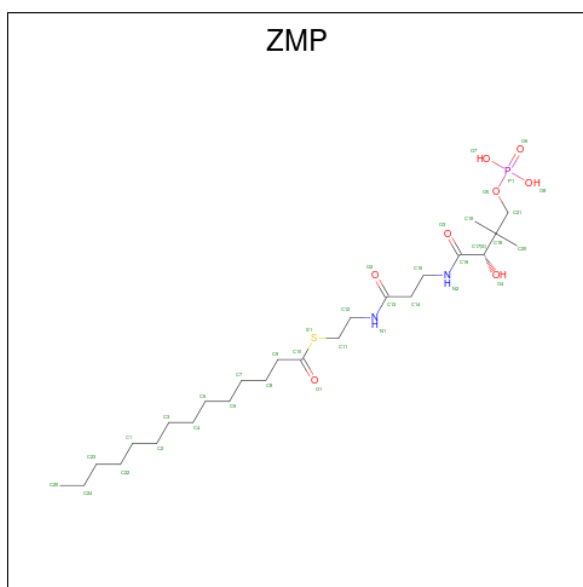


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 52  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

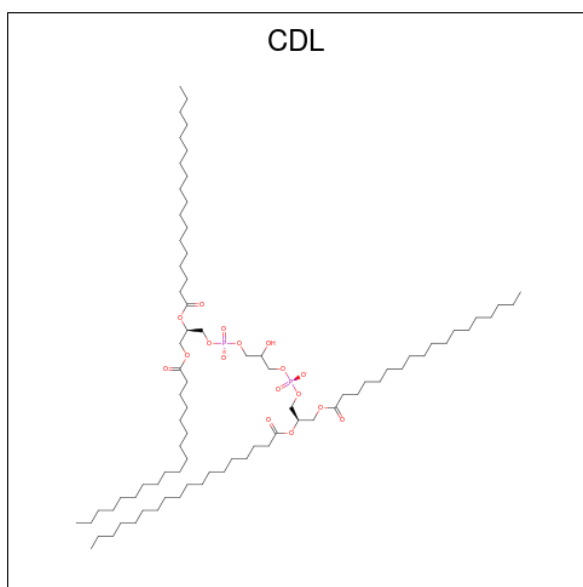
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 53  | 7     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 54 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



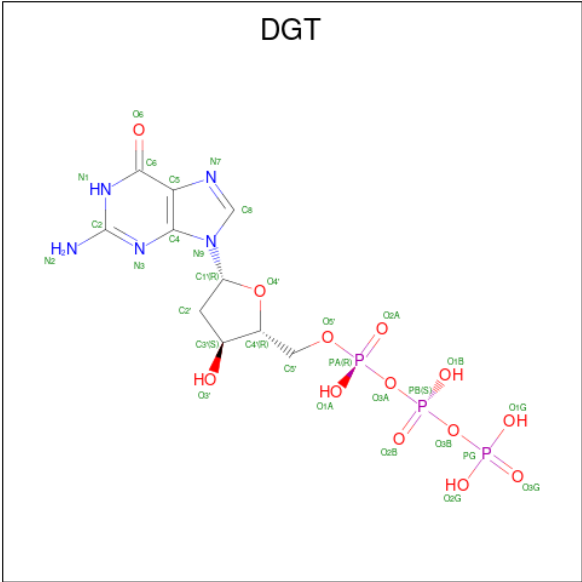
| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 54  | W     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 34    | 23 | 2 | 7 | 1 | 1 |         |
| 54  | n     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 32    | 21 | 2 | 7 | 1 | 1 |         |

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 55  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 55  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |
| 55  | L     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 46    | 27 | 17 | 2 |         |
| 55  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 90    | 71 | 17 | 2 |         |
| 55  | Y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 94    | 75 | 17 | 2 |         |
| 55  | Y     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 55  | d     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 67    | 48 | 17 | 2 |         |
| 55  | h     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 70    | 51 | 17 | 2 |         |
| 55  | m     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 72    | 53 | 17 | 2 |         |

- Molecule 56 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

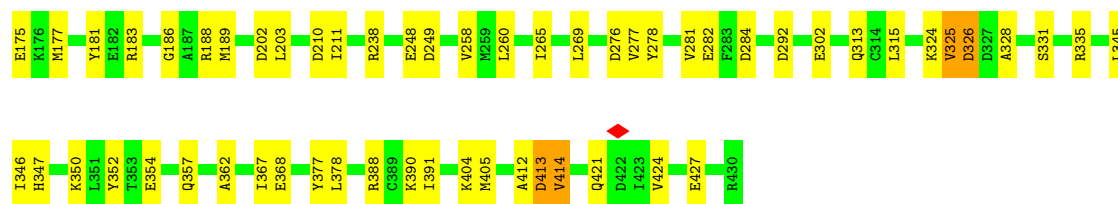


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 56  | O     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

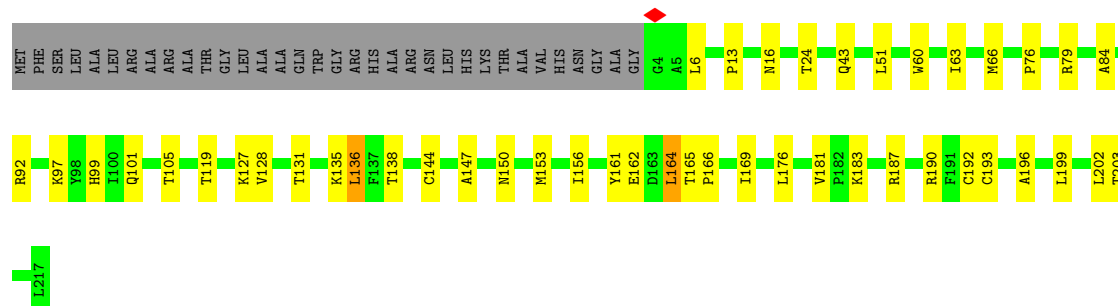
- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 57  | O     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

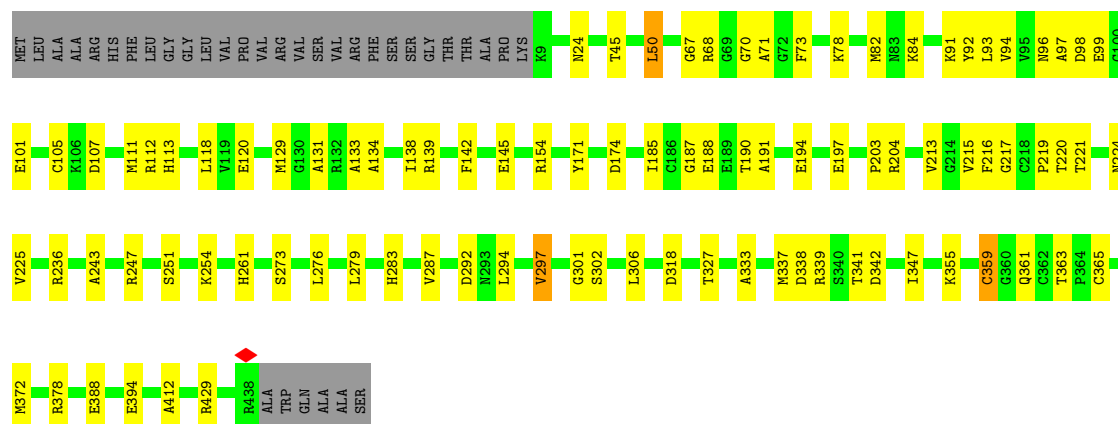




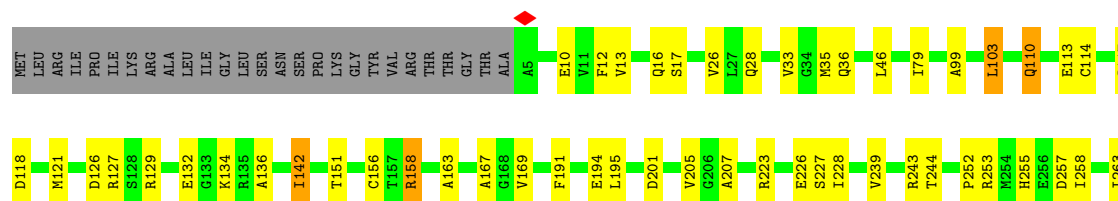
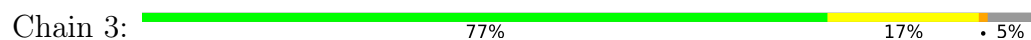
• Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

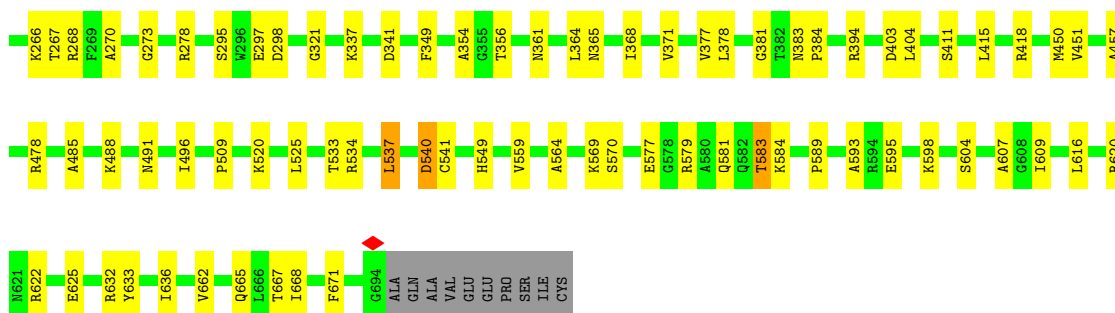


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

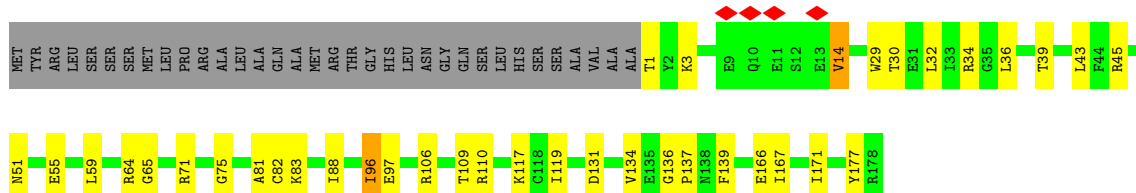


• Molecule 6: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

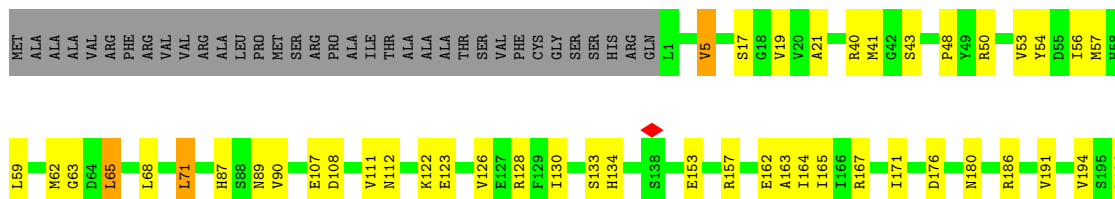




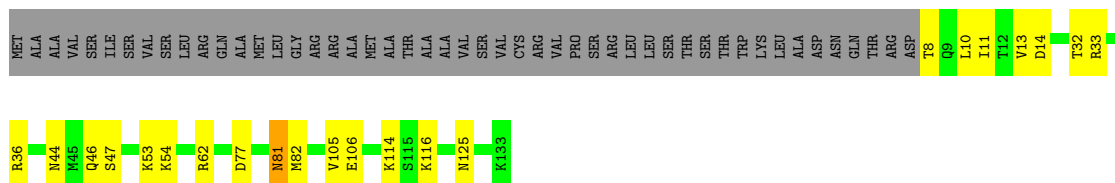
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

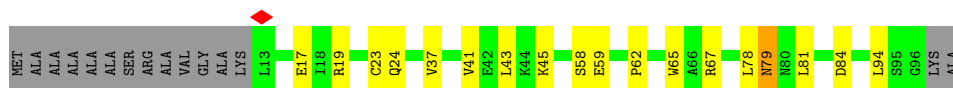


- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



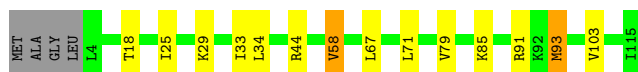
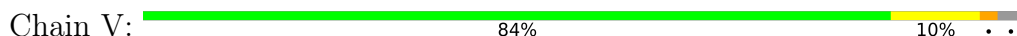
- Molecule 12: Acyl carrier protein, mitochondrial



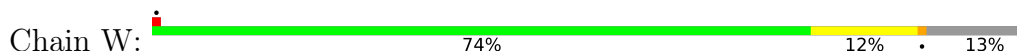
- Molecule 12: Acyl carrier protein, mitochondrial



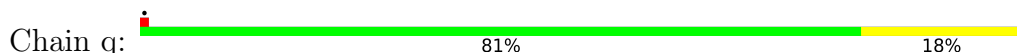
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

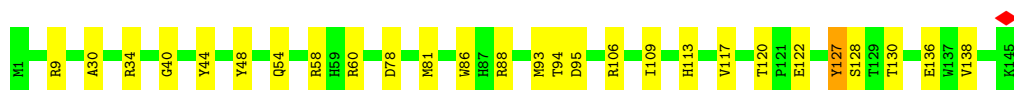


- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

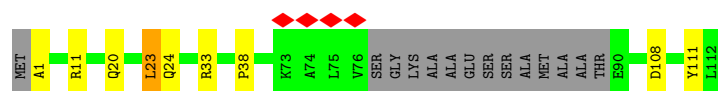
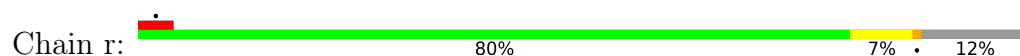


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

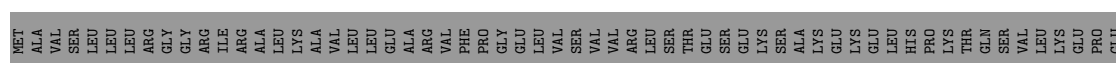




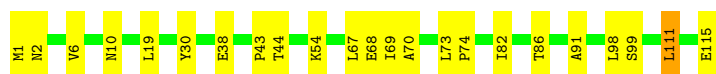
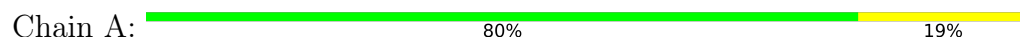
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



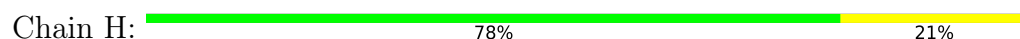
- Molecule 17: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



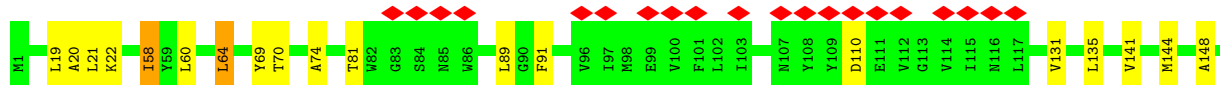
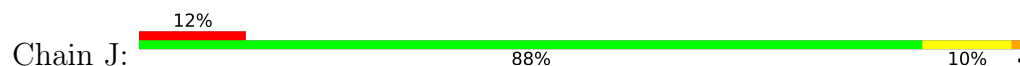
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



- Molecule 19: NADH-ubiquinone oxidoreductase chain 1



- Molecule 20: NADH-ubiquinone oxidoreductase chain 6







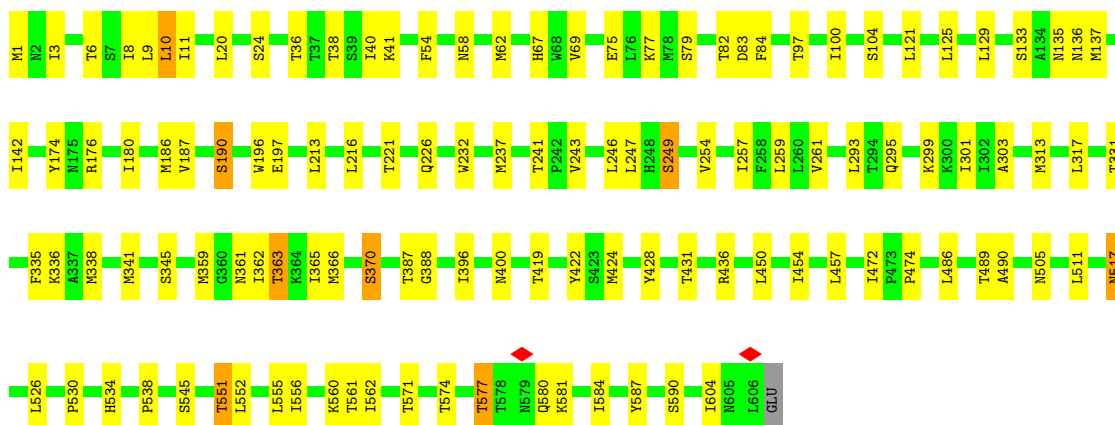
- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 89% 10%



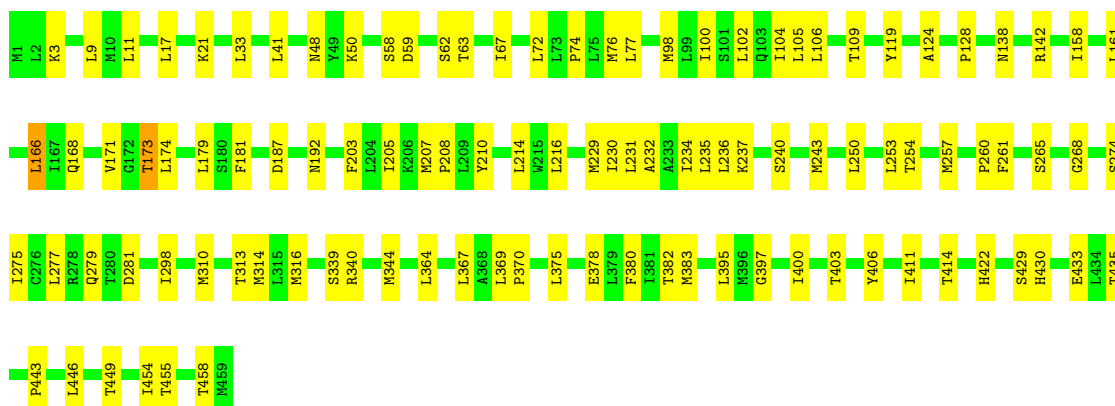
- Molecule 22: NADH-ubiquinone oxidoreductase chain 5

Chain L: 80% 18%



- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

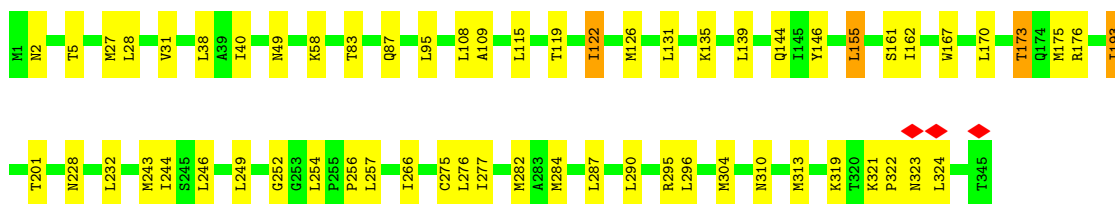
Chain M: 77% 23%



- Molecule 24: NADH-ubiquinone oxidoreductase chain 2

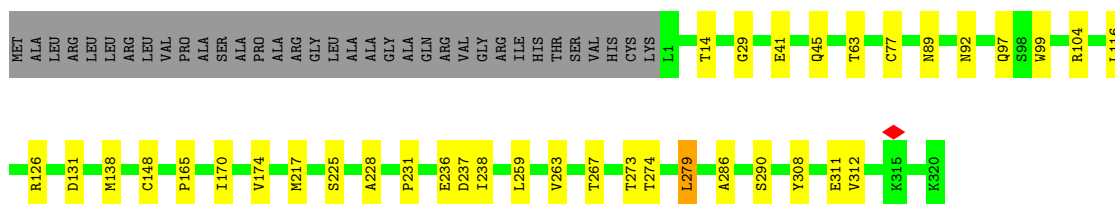
Chain N: 82% 17%





- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 80% 10% 10%



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X: 80% 18% ..



- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain Y: 77% 21% ..



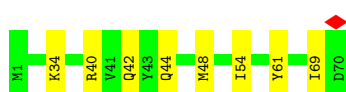
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z: 81% 17% .

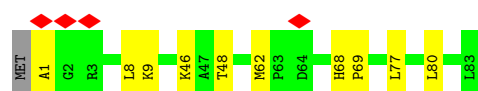
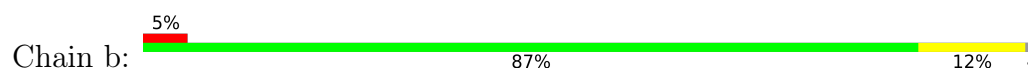


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

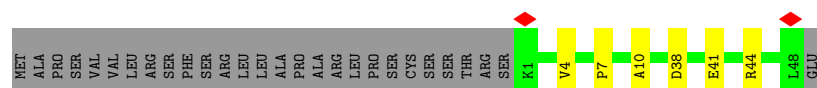
Chain a: 89% 11%



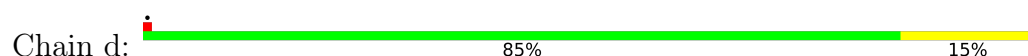
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



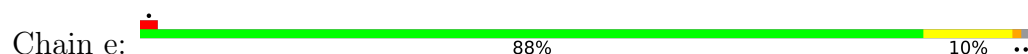
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



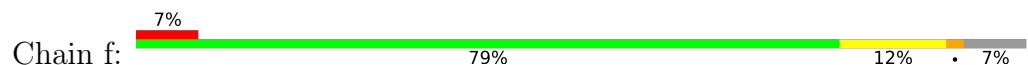
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 subunit C2



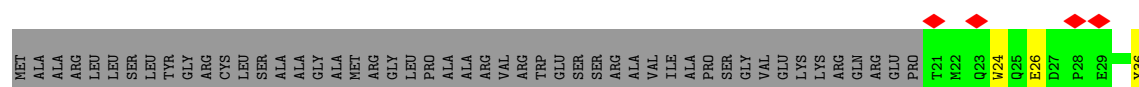
- Molecule 33: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



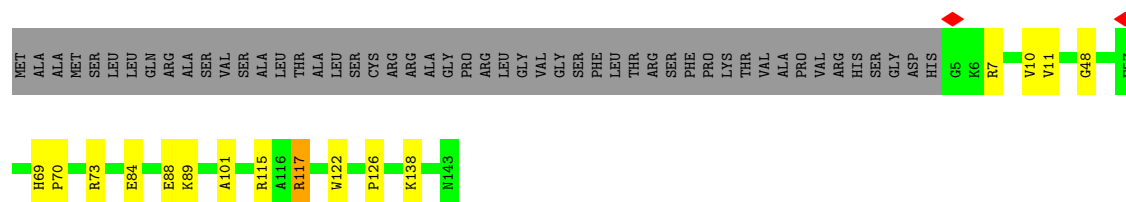
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



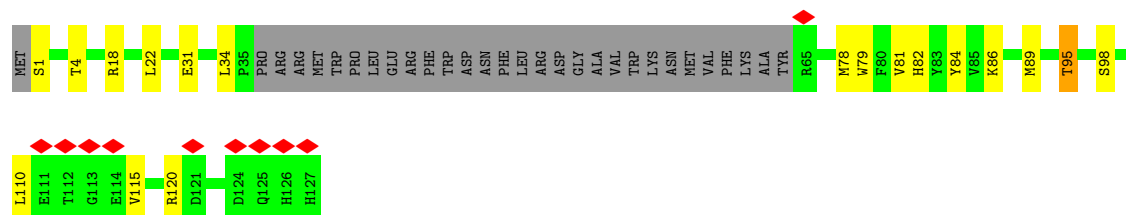
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



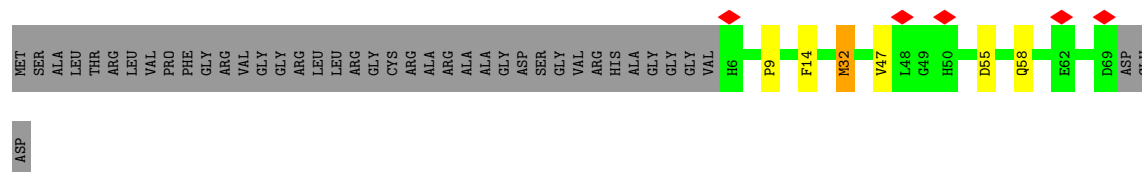
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



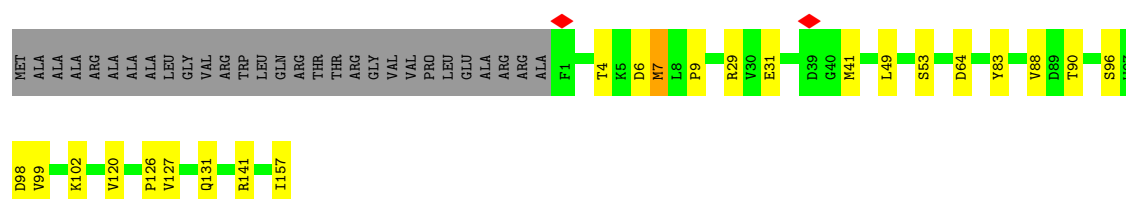
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



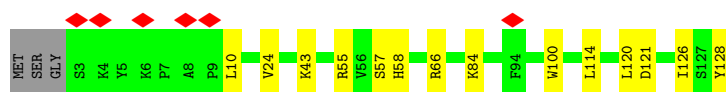
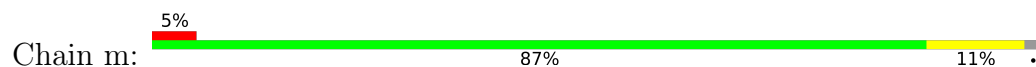
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



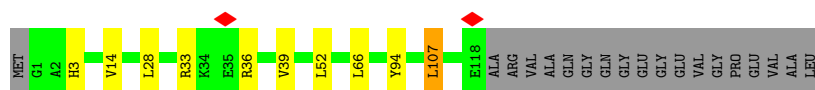
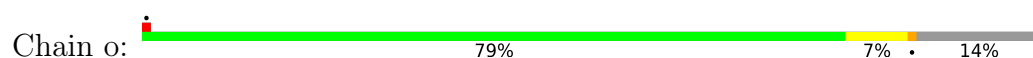
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



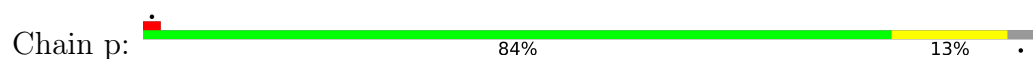
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 95155                                   | 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 ( $e^-/\text{\AA}^2$ ) | 80                                      | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 2600                                    | Depositor |
| Magnification                        | 81000                                   | Depositor |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 0.149                                   | Depositor |
| Minimum map value                    | -0.018                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.008                                   | Depositor |
| Recommended contour level            | 0.018                                   | Depositor |
| Map size (Å)                         | 226.83998, 214.12, 203.51999            | wwPDB     |
| Map dimensions                       | 214, 202, 192                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, AYA, NDP, FMN, 3PE, FES, ZMP, K, FME, CDL, MG, SAC, UQ, 2MR, ZN, SF4, DGT

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   | 6     | 0.30         | 0/1272        | 0.44        | 0/1722        |
| 2   | C     | 0.25         | 0/1771        | 0.40        | 0/2413        |
| 3   | D     | 0.28         | 0/3540        | 0.44        | 1/4795 (0.0%) |
| 4   | 2     | 0.24         | 0/1700        | 0.45        | 0/2316        |
| 5   | 1     | 0.67         | 2/3396 (0.1%) | 0.54        | 5/4586 (0.1%) |
| 6   | 3     | 0.25         | 0/5392        | 0.42        | 0/7305        |
| 7   | 9     | 0.26         | 0/1461        | 0.39        | 0/1974        |
| 8   | P     | 0.24         | 0/2823        | 0.43        | 0/3828        |
| 9   | Q     | 0.24         | 0/1045        | 0.33        | 0/1411        |
| 10  | 7     | 0.23         | 0/773         | 0.38        | 0/1041        |
| 11  | S     | 0.22         | 0/682         | 0.43        | 0/920         |
| 12  | T     | 0.18         | 0/646         | 0.46        | 0/869         |
| 12  | U     | 0.22         | 0/718         | 0.46        | 0/970         |
| 13  | V     | 0.22         | 0/937         | 0.36        | 0/1270        |
| 14  | W     | 0.22         | 0/993         | 0.39        | 0/1335        |
| 15  | q     | 0.24         | 0/1251        | 0.42        | 0/1702        |
| 16  | r     | 0.21         | 0/806         | 0.35        | 0/1090        |
| 17  | s     | 0.25         | 0/353         | 0.41        | 0/479         |
| 18  | A     | 0.27         | 0/948         | 0.48        | 0/1295        |
| 19  | H     | 0.30         | 0/2607        | 0.48        | 0/3564        |
| 20  | J     | 0.24         | 0/1330        | 0.40        | 0/1810        |
| 21  | K     | 0.26         | 0/738         | 0.42        | 0/1002        |
| 22  | L     | 0.28         | 0/4913        | 0.49        | 0/6686        |
| 23  | M     | 0.29         | 0/3709        | 0.47        | 0/5052        |
| 24  | N     | 0.28         | 0/2755        | 0.47        | 0/3751        |
| 25  | O     | 0.23         | 0/2674        | 0.40        | 0/3626        |
| 26  | X     | 0.21         | 0/1434        | 0.44        | 0/1937        |
| 27  | Y     | 0.19         | 0/1061        | 0.32        | 0/1439        |
| 28  | Z     | 0.22         | 0/1198        | 0.36        | 0/1616        |
| 29  | a     | 0.24         | 0/585         | 0.38        | 0/788         |
| 30  | b     | 0.20         | 0/666         | 0.34        | 0/914         |
| 31  | c     | 0.18         | 0/409         | 0.35        | 0/555         |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 32  | d     | 0.21         | 0/1028         | 0.36        | 0/1387         |
| 33  | e     | 0.21         | 0/900          | 0.37        | 0/1199         |
| 34  | f     | 0.22         | 0/468          | 0.50        | 0/630          |
| 35  | g     | 0.20         | 0/878          | 0.37        | 0/1196         |
| 36  | h     | 0.23         | 0/1201         | 0.43        | 0/1626         |
| 37  | i     | 0.21         | 0/846          | 0.41        | 0/1149         |
| 38  | j     | 0.19         | 0/580          | 0.37        | 0/794          |
| 39  | k     | 0.19         | 0/646          | 0.32        | 0/873          |
| 40  | l     | 0.22         | 0/1379         | 0.39        | 0/1882         |
| 41  | m     | 0.22         | 0/1079         | 0.38        | 0/1463         |
| 42  | n     | 0.21         | 0/1596         | 0.39        | 0/2162         |
| 43  | o     | 0.18         | 0/1039         | 0.33        | 0/1394         |
| 44  | p     | 0.20         | 0/1471         | 0.36        | 0/1988         |
| All | All   | 0.28         | 2/67697 (0.0%) | 0.43        | 6/91804 (0.0%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 5   | 1     | 67  | GLY  | C-N   | -30.24 | 0.94        | 1.33     |
| 5   | 1     | 71  | ALA  | C-N   | 19.09  | 1.60        | 1.33     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 5   | 1     | 71  | ALA  | O-C-N  | 12.27 | 135.13      | 122.12   |
| 5   | 1     | 70  | GLY  | N-CA-C | -8.24 | 104.68      | 114.48   |
| 5   | 1     | 71  | ALA  | N-CA-C | 8.09  | 120.10      | 111.28   |
| 3   | D     | 258 | VAL  | N-CA-C | -7.09 | 106.97      | 113.71   |
| 5   | 1     | 71  | ALA  | CA-C-N | -5.93 | 109.85      | 121.53   |
| 5   | 1     | 71  | ALA  | C-N-CA | -5.93 | 109.85      | 121.53   |

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   | 6     | 1241  | 0        | 1250     | 24      | 0            |
| 2   | C     | 1721  | 0        | 1673     | 22      | 0            |
| 3   | D     | 3464  | 0        | 3416     | 69      | 0            |
| 4   | 2     | 1660  | 0        | 1653     | 25      | 0            |
| 5   | 1     | 3321  | 0        | 3277     | 59      | 0            |
| 6   | 3     | 5305  | 0        | 5330     | 86      | 0            |
| 7   | 9     | 1431  | 0        | 1383     | 37      | 0            |
| 8   | P     | 2748  | 0        | 2768     | 46      | 0            |
| 9   | Q     | 1022  | 0        | 1023     | 19      | 0            |
| 10  | 7     | 758   | 0        | 731      | 17      | 0            |
| 11  | S     | 671   | 0        | 688      | 13      | 0            |
| 12  | T     | 637   | 0        | 640      | 10      | 0            |
| 12  | U     | 706   | 0        | 699      | 13      | 0            |
| 13  | V     | 915   | 0        | 954      | 8       | 0            |
| 14  | W     | 970   | 0        | 991      | 11      | 0            |
| 15  | q     | 1209  | 0        | 1170     | 22      | 0            |
| 16  | r     | 796   | 0        | 831      | 8       | 0            |
| 17  | s     | 344   | 0        | 324      | 5       | 0            |
| 18  | A     | 932   | 0        | 967      | 15      | 0            |
| 19  | H     | 2540  | 0        | 2626     | 50      | 0            |
| 20  | J     | 1308  | 0        | 1319     | 17      | 0            |
| 21  | K     | 737   | 0        | 768      | 12      | 0            |
| 22  | L     | 4800  | 0        | 4985     | 75      | 0            |
| 23  | M     | 3632  | 0        | 3853     | 73      | 0            |
| 24  | N     | 2703  | 0        | 2902     | 39      | 0            |
| 25  | O     | 2607  | 0        | 2566     | 23      | 0            |
| 26  | X     | 1396  | 0        | 1379     | 21      | 0            |
| 27  | Y     | 1037  | 0        | 1025     | 18      | 0            |
| 28  | Z     | 1167  | 0        | 1166     | 20      | 0            |
| 29  | a     | 572   | 0        | 583      | 6       | 0            |
| 30  | b     | 651   | 0        | 653      | 7       | 0            |
| 31  | c     | 398   | 0        | 401      | 4       | 0            |
| 32  | d     | 996   | 0        | 1001     | 14      | 0            |
| 33  | e     | 877   | 0        | 871      | 11      | 0            |
| 34  | f     | 456   | 0        | 452      | 5       | 0            |
| 35  | g     | 850   | 0        | 783      | 11      | 0            |
| 36  | h     | 1166  | 0        | 1166     | 13      | 0            |
| 37  | i     | 828   | 0        | 829      | 10      | 0            |
| 38  | j     | 555   | 0        | 506      | 4       | 0            |
| 39  | k     | 626   | 0        | 620      | 4       | 0            |
| 40  | l     | 1323  | 0        | 1216     | 18      | 0            |
| 41  | m     | 1050  | 0        | 1061     | 11      | 0            |
| 42  | n     | 1541  | 0        | 1473     | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | o     | 1014  | 0        | 1002     | 8       | 0            |
| 44  | p     | 1438  | 0        | 1402     | 19      | 0            |
| 45  | 1     | 8     | 0        | 0        | 1       | 0            |
| 45  | 3     | 16    | 0        | 0        | 0       | 0            |
| 45  | 6     | 8     | 0        | 0        | 1       | 0            |
| 45  | 9     | 16    | 0        | 0        | 1       | 0            |
| 46  | 6     | 32    | 0        | 38       | 0       | 0            |
| 46  | A     | 43    | 0        | 60       | 1       | 0            |
| 46  | D     | 51    | 0        | 82       | 4       | 0            |
| 46  | K     | 41    | 0        | 59       | 5       | 0            |
| 46  | L     | 93    | 0        | 140      | 4       | 0            |
| 46  | M     | 87    | 0        | 128      | 6       | 0            |
| 46  | Y     | 28    | 0        | 30       | 1       | 0            |
| 46  | Z     | 51    | 0        | 82       | 0       | 0            |
| 46  | d     | 31    | 0        | 36       | 1       | 0            |
| 46  | h     | 51    | 0        | 82       | 1       | 0            |
| 46  | i     | 42    | 0        | 61       | 5       | 0            |
| 46  | m     | 30    | 0        | 34       | 1       | 0            |
| 47  | 6     | 43    | 0        | 63       | 1       | 0            |
| 47  | 9     | 54    | 0        | 88       | 3       | 0            |
| 47  | H     | 42    | 0        | 58       | 0       | 0            |
| 47  | M     | 54    | 0        | 88       | 6       | 0            |
| 47  | Z     | 47    | 0        | 71       | 3       | 0            |
| 48  | D     | 63    | 0        | 90       | 3       | 0            |
| 49  | 2     | 4     | 0        | 0        | 1       | 0            |
| 49  | 3     | 4     | 0        | 0        | 0       | 0            |
| 50  | 1     | 31    | 0        | 19       | 2       | 0            |
| 51  | 3     | 1     | 0        | 0        | 0       | 0            |
| 52  | P     | 48    | 0        | 26       | 3       | 0            |
| 53  | 7     | 1     | 0        | 0        | 0       | 0            |
| 54  | W     | 34    | 0        | 40       | 3       | 0            |
| 54  | n     | 32    | 0        | 36       | 2       | 0            |
| 55  | L     | 124   | 0        | 136      | 0       | 0            |
| 55  | N     | 90    | 0        | 133      | 6       | 0            |
| 55  | Y     | 151   | 0        | 199      | 4       | 0            |
| 55  | d     | 67    | 0        | 81       | 4       | 0            |
| 55  | h     | 70    | 0        | 87       | 3       | 0            |
| 55  | m     | 72    | 0        | 91       | 1       | 0            |
| 55  | r     | 57    | 0        | 58       | 2       | 0            |
| 56  | O     | 31    | 0        | 12       | 2       | 0            |
| 57  | O     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 67868 | 0        | 68584    | 833     | 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 6.

All (833) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:101:GLU:OE2   | 5:1:302:SER:N     | 1.90                     | 1.05              |
| 10:7:68:HIS:CD2   | 10:7:87:CYS:SG    | 2.68                     | 0.85              |
| 5:1:101:GLU:OE2   | 5:1:302:SER:HB3   | 1.77                     | 0.85              |
| 6:3:520:LYS:O     | 6:3:541:CYS:C     | 2.30                     | 0.75              |
| 8:P:310:LEU:O     | 8:P:314:SER:HB2   | 1.87                     | 0.74              |
| 6:3:12:PHE:HA     | 6:3:16:GLN:O      | 1.88                     | 0.73              |
| 4:2:119:THR:HG21  | 4:2:166:PRO:HB3   | 1.70                     | 0.72              |
| 5:1:101:GLU:OE2   | 5:1:302:SER:CA    | 2.37                     | 0.72              |
| 5:1:101:GLU:OE2   | 5:1:302:SER:CB    | 2.37                     | 0.72              |
| 5:1:93:LEU:O      | 5:1:134:ALA:HA    | 1.94                     | 0.68              |
| 5:1:112:ARG:HB3   | 5:1:145:GLU:HG3   | 1.76                     | 0.67              |
| 1:6:62:LEU:HB2    | 1:6:100:GLY:HA3   | 1.76                     | 0.67              |
| 8:P:216:ASN:O     | 8:P:220:ASP:HB2   | 1.95                     | 0.67              |
| 15:q:78:ASP:HB3   | 15:q:81:MET:HG3   | 1.77                     | 0.66              |
| 7:9:97:GLU:HB2    | 7:9:110:ARG:HB3   | 1.77                     | 0.66              |
| 15:q:40:GLY:HA3   | 15:q:48:TYR:HB2   | 1.76                     | 0.66              |
| 3:D:61:VAL:HG11   | 3:D:83:LEU:HB2    | 1.78                     | 0.65              |
| 27:Y:107:TYR:HB2  | 55:m:201:CDL:HB62 | 1.79                     | 0.65              |
| 7:9:83:LYS:HA     | 7:9:96:ILE:HD12   | 1.78                     | 0.65              |
| 10:7:68:HIS:HD2   | 10:7:87:CYS:SG    | 2.17                     | 0.65              |
| 1:6:119:GLU:O     | 8:P:54:TYR:OH     | 2.15                     | 0.64              |
| 6:3:403:ASP:OD1   | 17:s:64:ARG:NH2   | 2.29                     | 0.64              |
| 5:1:99:GLU:OE2    | 5:1:105:CYS:CA    | 2.46                     | 0.64              |
| 3:D:4:TRP:O       | 23:M:142:ARG:NH2  | 2.31                     | 0.63              |
| 5:1:99:GLU:OE1    | 5:1:107:ASP:HB2   | 1.98                     | 0.63              |
| 6:3:533:THR:O     | 6:3:537:LEU:HB2   | 1.98                     | 0.63              |
| 15:q:34:ARG:HH21  | 15:q:54:GLN:HG3   | 1.62                     | 0.63              |
| 3:D:328:ALA:HB3   | 6:3:126:ASP:HB2   | 1.80                     | 0.63              |
| 22:L:552:LEU:O    | 22:L:556:ILE:HB   | 1.98                     | 0.63              |
| 7:9:137:PRO:HB3   | 15:q:93:MET:HE1   | 1.80                     | 0.63              |
| 14:W:53:GLN:O     | 14:W:102:ARG:NH1  | 2.31                     | 0.63              |
| 24:N:249:LEU:HD22 | 24:N:254:LEU:HD12 | 1.79                     | 0.63              |
| 3:D:269:LEU:HB2   | 3:D:368:GLU:HB2   | 1.81                     | 0.63              |
| 5:1:142:PHE:HB3   | 5:1:145:GLU:HB2   | 1.81                     | 0.62              |
| 23:M:59:ASP:HB3   | 23:M:62:SER:H     | 1.63                     | 0.62              |
| 4:2:97:LYS:H      | 4:2:136:LEU:HA    | 1.65                     | 0.62              |
| 6:3:604:SER:HB2   | 6:3:609:ILE:HB    | 1.82                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2:190:ARG:HD3   | 4:2:196:ALA:HB2   | 1.82                     | 0.61              |
| 4:2:127:LYS:HG3   | 4:2:128:VAL:HG23  | 1.81                     | 0.61              |
| 25:O:45:GLN:NE2   | 25:O:231:PRO:O    | 2.34                     | 0.61              |
| 5:1:215:VAL:HG22  | 5:1:220:THR:HG21  | 1.82                     | 0.61              |
| 22:L:577:THR:O    | 22:L:580:GLN:NE2  | 2.31                     | 0.61              |
| 6:3:142:ILE:HG13  | 6:3:191:PHE:HB3   | 1.82                     | 0.61              |
| 6:3:255:HIS:CE1   | 6:3:257:ASP:HB2   | 2.36                     | 0.61              |
| 5:1:99:GLU:OE2    | 5:1:105:CYS:HA    | 2.00                     | 0.61              |
| 22:L:221:THR:HG23 | 22:L:226:GLN:HB2  | 1.82                     | 0.60              |
| 36:h:7:ARG:NH2    | 37:i:31:GLU:O     | 2.34                     | 0.60              |
| 1:6:79:MET:HB2    | 1:6:84:VAL:HB     | 1.84                     | 0.60              |
| 47:M:501:PC1:H2   | 24:N:276:LEU:HD22 | 1.84                     | 0.60              |
| 1:6:76:ARG:HD2    | 3:D:175:GLU:HG2   | 1.83                     | 0.60              |
| 3:D:282:GLU:HB2   | 3:D:313:GLN:HE22  | 1.67                     | 0.60              |
| 23:M:105:LEU:O    | 23:M:109:THR:OG1  | 2.18                     | 0.60              |
| 4:2:192:CYS:SG    | 4:2:193:CYS:N     | 2.75                     | 0.60              |
| 19:H:293:PHE:O    | 19:H:297:THR:OG1  | 2.18                     | 0.60              |
| 12:U:88:GLU:HA    | 37:i:22:LEU:HB3   | 1.84                     | 0.60              |
| 6:3:632:ARG:HH12  | 11:S:58:SER:HB2   | 1.66                     | 0.60              |
| 35:g:107:GLU:O    | 44:p:141:ARG:NH1  | 2.35                     | 0.59              |
| 20:J:22:LYS:NZ    | 21:K:18:GLY:O     | 2.34                     | 0.59              |
| 20:J:110:ASP:O    | 33:e:73:ARG:NH1   | 2.34                     | 0.59              |
| 22:L:517:ASN:OD1  | 22:L:517:ASN:N    | 2.36                     | 0.59              |
| 8:P:122:LYS:NZ    | 8:P:162:GLU:OE2   | 2.35                     | 0.59              |
| 32:d:11:LEU:HD23  | 46:d:202:3PE:H11  | 1.84                     | 0.59              |
| 12:T:51:ILE:HD11  | 12:T:70:LEU:HD22  | 1.84                     | 0.59              |
| 15:q:60:ARG:HH22  | 15:q:95:ASP:HA    | 1.68                     | 0.59              |
| 16:r:11:ARG:NH2   | 16:r:20:GLN:OE1   | 2.36                     | 0.59              |
| 8:P:176:ASP:OD1   | 8:P:180:ASN:ND2   | 2.36                     | 0.59              |
| 7:9:55:GLU:OE2    | 15:q:34:ARG:NH1   | 2.35                     | 0.59              |
| 5:1:224:ASN:ND2   | 50:1:501:FMN:O2   | 2.32                     | 0.59              |
| 8:P:153:GLU:HG3   | 8:P:165:ILE:HD13  | 1.84                     | 0.59              |
| 23:M:50:LYS:HB2   | 23:M:58:SER:HB3   | 1.84                     | 0.59              |
| 5:1:120:GLU:OE2   | 5:1:236:ARG:NH2   | 2.35                     | 0.59              |
| 6:3:411:SER:HB2   | 6:3:662:VAL:HG12  | 1.85                     | 0.59              |
| 40:l:4:THR:OG1    | 40:l:7:MET:SD     | 2.61                     | 0.59              |
| 3:D:352:TYR:HD1   | 7:9:88:ILE:HG12   | 1.68                     | 0.59              |
| 11:S:62:PRO:HD2   | 11:S:79:ASN:HB3   | 1.85                     | 0.59              |
| 11:S:84:ASP:OD1   | 11:S:84:ASP:N     | 2.36                     | 0.59              |
| 15:q:9:ARG:NH1    | 55:r:201:CDL:OA4  | 2.36                     | 0.59              |
| 5:1:96:ASN:ND2    | 5:1:187:GLY:O     | 2.29                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:H:146:MET:HG3  | 19:H:188:SER:HB3  | 1.85                     | 0.58              |
| 19:H:85:LEU:HD13  | 19:H:108:THR:HB   | 1.86                     | 0.58              |
| 24:N:252:GLY:HA3  | 24:N:290:LEU:HD13 | 1.86                     | 0.58              |
| 9:Q:36:ARG:NH2    | 9:Q:106:GLU:OE2   | 2.36                     | 0.58              |
| 24:N:175:MET:HE1  | 24:N:296:LEU:HD21 | 1.86                     | 0.58              |
| 15:q:78:ASP:H     | 15:q:81:MET:HE2   | 1.67                     | 0.58              |
| 22:L:361:ASN:HD22 | 39:k:62:PHE:HD1   | 1.51                     | 0.58              |
| 1:6:70:MET:HE1    | 3:D:152:MET:HE1   | 1.84                     | 0.58              |
| 3:D:183:ARG:NH1   | 3:D:210:ASP:OD2   | 2.32                     | 0.58              |
| 3:D:144:ILE:HG23  | 3:D:177:MET:HE2   | 1.86                     | 0.58              |
| 19:H:114:TYR:OH   | 20:J:60:LEU:O     | 2.16                     | 0.58              |
| 19:H:139:THR:O    | 19:H:143:GLU:HB2  | 2.04                     | 0.58              |
| 6:3:239:VAL:HG23  | 6:3:253:ARG:HG3   | 1.85                     | 0.58              |
| 6:3:620:ARG:NH1   | 6:3:633:TYR:OH    | 2.37                     | 0.58              |
| 13:V:29:LYS:NZ    | 25:O:237:ASP:OD1  | 2.33                     | 0.58              |
| 24:N:304:MET:HE2  | 25:O:286:ALA:HB1  | 1.86                     | 0.58              |
| 3:D:405:MET:SD    | 3:D:421:GLN:NE2   | 2.75                     | 0.58              |
| 24:N:2:ASN:HB3    | 24:N:5:THR:HG22   | 1.84                     | 0.58              |
| 3:D:175:GLU:OE2   | 3:D:188:ARG:NH1   | 2.36                     | 0.58              |
| 5:1:92:TYR:HB2    | 5:1:220:THR:HG22  | 1.86                     | 0.58              |
| 8:P:130:ILE:HG12  | 8:P:164:ILE:HD12  | 1.85                     | 0.58              |
| 22:L:176:ARG:HD2  | 23:M:400:ILE:HG22 | 1.86                     | 0.58              |
| 23:M:240:SER:OG   | 23:M:316:MET:SD   | 2.58                     | 0.58              |
| 26:X:18:LYS:HA    | 29:a:54:ILE:HD12  | 1.86                     | 0.58              |
| 22:L:135:ASN:ND2  | 22:L:197:GLU:OE1  | 2.37                     | 0.57              |
| 23:M:11:LEU:HB3   | 23:M:100:ILE:HD13 | 1.86                     | 0.57              |
| 9:Q:32:THR:O      | 9:Q:62:ARG:NH2    | 2.37                     | 0.57              |
| 23:M:98:MET:HE1   | 55:N:401:CDL:H801 | 1.86                     | 0.57              |
| 19:H:245:PRO:HB3  | 19:H:258:ASN:HB3  | 1.86                     | 0.57              |
| 5:1:190:THR:HB    | 5:1:204:ARG:HG2   | 1.86                     | 0.57              |
| 8:P:282:ASP:OD2   | 8:P:286:ARG:NH1   | 2.38                     | 0.57              |
| 5:1:91:LYS:HG2    | 5:1:219:PRO:HG2   | 1.86                     | 0.57              |
| 6:3:478:ARG:HH22  | 6:3:485:ALA:HA    | 1.70                     | 0.57              |
| 37:i:120:ARG:NH1  | 43:o:39:VAL:O     | 2.38                     | 0.57              |
| 46:D:502:3PE:H3E1 | 47:M:501:PC1:H3H1 | 1.85                     | 0.57              |
| 23:M:232:ALA:O    | 23:M:237:LYS:NZ   | 2.38                     | 0.57              |
| 6:3:114:CYS:HB3   | 6:3:117:GLN:HB2   | 1.85                     | 0.57              |
| 24:N:122:ILE:O    | 24:N:176:ARG:NH1  | 2.36                     | 0.57              |
| 19:H:175:LEU:HD21 | 47:Z:402:PC1:H2E2 | 1.87                     | 0.57              |
| 12:U:47:GLN:NE2   | 12:U:70:LEU:O     | 2.37                     | 0.57              |
| 26:X:5:GLU:O      | 26:X:53:ARG:NH1   | 2.38                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:335:ARG:NH2   | 7:9:131:ASP:OD1   | 2.38                     | 0.56              |
| 18:A:6:VAL:O      | 18:A:10:ASN:ND2   | 2.38                     | 0.56              |
| 22:L:6:THR:O      | 22:L:10:LEU:HB2   | 2.05                     | 0.56              |
| 25:O:225:SER:O    | 25:O:228:ALA:C    | 2.48                     | 0.56              |
| 5:1:276:LEU:HD11  | 5:1:297:VAL:HG11  | 1.87                     | 0.56              |
| 4:2:76:PRO:HB2    | 4:2:79:ARG:HG2    | 1.86                     | 0.56              |
| 6:3:564:ALA:O     | 6:3:569:LYS:NZ    | 2.39                     | 0.56              |
| 7:9:45:ARG:HH11   | 16:r:24:GLN:HE22  | 1.53                     | 0.56              |
| 22:L:366:MET:O    | 22:L:370:SER:OG   | 2.21                     | 0.56              |
| 22:L:561:THR:HG23 | 46:L:704:3PE:H271 | 1.86                     | 0.56              |
| 25:O:104:ARG:NH2  | 56:O:401:DGT:N7   | 2.52                     | 0.56              |
| 27:Y:35:GLY:HA2   | 55:Y:401:CDL:H322 | 1.87                     | 0.56              |
| 40:l:29:ARG:NH2   | 40:l:31:GLU:OE2   | 2.39                     | 0.56              |
| 2:C:78:LEU:HB3    | 2:C:130:TYR:HB3   | 1.88                     | 0.56              |
| 6:3:227:SER:OG    | 6:3:228:ILE:N     | 2.39                     | 0.56              |
| 7:9:166:GLU:HG3   | 15:q:88:ARG:HD3   | 1.87                     | 0.56              |
| 22:L:362:ILE:HB   | 22:L:431:THR:HA   | 1.87                     | 0.56              |
| 23:M:208:PRO:HD3  | 23:M:236:LEU:HD22 | 1.87                     | 0.56              |
| 4:2:150:ASN:HB3   | 4:2:162:GLU:HB3   | 1.88                     | 0.56              |
| 22:L:190:SER:OG   | 22:L:196:TRP:NE1  | 2.39                     | 0.56              |
| 38:j:55:ASP:OD2   | 38:j:58:GLN:NE2   | 2.39                     | 0.56              |
| 5:1:372:MET:HE1   | 5:1:412:ALA:HA    | 1.87                     | 0.56              |
| 22:L:359:MET:O    | 22:L:436:ARG:NH2  | 2.39                     | 0.56              |
| 12:U:44:SER:HB3   | 42:n:16:LEU:HD11  | 1.87                     | 0.56              |
| 6:3:255:HIS:HE1   | 6:3:257:ASP:HB2   | 1.69                     | 0.56              |
| 6:3:383:ASN:ND2   | 6:3:665:GLN:O     | 2.38                     | 0.56              |
| 23:M:181:PHE:O    | 44:p:152:ARG:NH1  | 2.38                     | 0.56              |
| 3:D:161:ILE:HG23  | 3:D:238:ARG:HG2   | 1.87                     | 0.56              |
| 25:O:170:ILE:HD11 | 25:O:238:ILE:HD11 | 1.88                     | 0.56              |
| 27:Y:103:ARG:NH1  | 55:Y:403:CDL:OA7  | 2.38                     | 0.55              |
| 29:a:34:LYS:NZ    | 29:a:61:TYR:O     | 2.36                     | 0.55              |
| 5:1:247:ARG:NH1   | 5:1:318:ASP:OD2   | 2.39                     | 0.55              |
| 27:Y:14:GLY:O     | 27:Y:78:GLN:NE2   | 2.39                     | 0.55              |
| 18:A:70:ALA:HB2   | 20:J:58:ILE:HD11  | 1.88                     | 0.55              |
| 31:c:41:GLU:OE1   | 31:c:44:ARG:NH2   | 2.39                     | 0.55              |
| 14:W:98:VAL:O     | 14:W:101:GLN:NE2  | 2.39                     | 0.55              |
| 2:C:204:GLU:OE2   | 2:C:210:ARG:NH1   | 2.39                     | 0.55              |
| 7:9:36:LEU:HD21   | 19:H:273:ILE:HD13 | 1.87                     | 0.55              |
| 34:f:32:GLU:O     | 34:f:35:THR:OG1   | 2.24                     | 0.55              |
| 11:S:17:GLU:OE1   | 11:S:67:ARG:NH1   | 2.39                     | 0.55              |
| 23:M:208:PRO:HG2  | 23:M:216:LEU:HD22 | 1.87                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:301:GLY:HA2   | 5:1:333:ALA:HB3   | 1.89                     | 0.55              |
| 6:3:570:SER:HA    | 6:3:583:THR:O     | 2.06                     | 0.55              |
| 24:N:162:ILE:HD12 | 24:N:282:MET:HG2  | 1.87                     | 0.55              |
| 33:e:68:ARG:HH11  | 33:e:71:THR:HG21  | 1.72                     | 0.55              |
| 6:3:540:ASP:OD1   | 6:3:540:ASP:N     | 2.30                     | 0.55              |
| 8:P:108:ASP:OD1   | 8:P:112:ASN:ND2   | 2.40                     | 0.55              |
| 19:H:75:PRO:HG3   | 19:H:219:PRO:HB3  | 1.89                     | 0.55              |
| 7:9:71:ARG:NH1    | 7:9:75:GLY:O      | 2.38                     | 0.54              |
| 8:P:186:ARG:HD2   | 8:P:251:ARG:HG3   | 1.89                     | 0.54              |
| 19:H:110:SER:HB2  | 20:J:60:LEU:HD13  | 1.89                     | 0.54              |
| 11:S:17:GLU:HB3   | 11:S:67:ARG:HB3   | 1.89                     | 0.54              |
| 26:X:39:ASN:HB3   | 28:Z:72:PRO:HG2   | 1.89                     | 0.54              |
| 5:1:306:LEU:HD21  | 5:1:347:ILE:HD11  | 1.88                     | 0.54              |
| 6:3:341:ASP:OD1   | 11:S:67:ARG:NH2   | 2.40                     | 0.54              |
| 18:A:69:ILE:HD11  | 19:H:148:ILE:HG12 | 1.90                     | 0.54              |
| 19:H:24:GLU:OE2   | 19:H:274:ARG:NH1  | 2.40                     | 0.54              |
| 32:d:100:ASP:OD2  | 36:h:117:ARG:NH2  | 2.39                     | 0.54              |
| 24:N:319:LYS:HG2  | 25:O:267:THR:HG21 | 1.89                     | 0.54              |
| 4:2:13:PRO:O      | 4:2:16:ASN:ND2    | 2.41                     | 0.54              |
| 19:H:134:ARG:NH1  | 19:H:206:GLU:OE1  | 2.40                     | 0.54              |
| 22:L:584:ILE:HD12 | 24:N:58:LYS:HG2   | 1.90                     | 0.54              |
| 25:O:77:CYS:O     | 25:O:92:ASN:ND2   | 2.36                     | 0.54              |
| 33:e:27:LYS:HG3   | 36:h:138:LYS:HA   | 1.90                     | 0.54              |
| 2:C:41:GLN:NE2    | 2:C:49:GLU:OE1    | 2.39                     | 0.54              |
| 3:D:51:PHE:HB2    | 3:D:64:LEU:HB3    | 1.89                     | 0.54              |
| 14:W:70:MET:HE1   | 54:W:201:ZMP:H19  | 1.90                     | 0.54              |
| 27:Y:47:SER:OG    | 27:Y:50:GLU:OE1   | 2.24                     | 0.54              |
| 8:P:41:MET:HE1    | 8:P:219:LYS:HD3   | 1.89                     | 0.54              |
| 20:J:144:MET:HG2  | 20:J:152:MET:HE2  | 1.90                     | 0.54              |
| 22:L:100:ILE:O    | 22:L:104:SER:OG   | 2.26                     | 0.54              |
| 33:e:14:ASP:OD1   | 33:e:14:ASP:N     | 2.40                     | 0.54              |
| 3:D:186:GLY:HA3   | 7:9:64:ARG:HG3    | 1.90                     | 0.54              |
| 4:2:164:LEU:HD22  | 4:2:169:ILE:HD13  | 1.89                     | 0.54              |
| 19:H:199:ASP:N    | 19:H:199:ASP:OD1  | 2.41                     | 0.54              |
| 5:1:292:ASP:O     | 5:1:339:ARG:NH1   | 2.40                     | 0.53              |
| 22:L:574:THR:OG1  | 24:N:167:TRP:O    | 2.22                     | 0.53              |
| 23:M:430:HIS:HB2  | 23:M:433:GLU:HG2  | 1.91                     | 0.53              |
| 5:1:118:LEU:HD13  | 5:1:225:VAL:HG13  | 1.90                     | 0.53              |
| 9:Q:125:ASN:O     | 17:s:64:ARG:NH1   | 2.41                     | 0.53              |
| 18:A:82:ILE:HD11  | 30:b:46:LYS:HD3   | 1.90                     | 0.53              |
| 8:P:48:PRO:HA     | 8:P:71:LEU:O      | 2.09                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:H:225:MET:O    | 19:H:229:THR:OG1  | 2.22                     | 0.53              |
| 22:L:100:ILE:HG21 | 22:L:246:LEU:HB2  | 1.89                     | 0.53              |
| 23:M:187:ASP:OD1  | 23:M:192:ASN:ND2  | 2.38                     | 0.53              |
| 5:1:261:HIS:ND1   | 5:1:338:ASP:OD1   | 2.41                     | 0.53              |
| 6:3:110:GLN:NE2   | 6:3:113:GLU:O     | 2.42                     | 0.53              |
| 22:L:176:ARG:HH22 | 23:M:367:LEU:HD13 | 1.74                     | 0.53              |
| 22:L:581:LYS:NZ   | 27:Y:43:ASN:OD1   | 2.42                     | 0.53              |
| 24:N:83:THR:HG22  | 33:e:19:PHE:HB3   | 1.90                     | 0.53              |
| 15:q:9:ARG:HH12   | 55:r:201:CDL:HA22 | 1.73                     | 0.53              |
| 22:L:20:LEU:O     | 22:L:24:SER:HB2   | 2.08                     | 0.53              |
| 22:L:526:LEU:HD12 | 22:L:530:PRO:HG2  | 1.91                     | 0.53              |
| 7:9:29:TRP:HB3    | 7:9:32:LEU:HD12   | 1.91                     | 0.53              |
| 23:M:48:ASN:ND2   | 44:p:89:MET:SD    | 2.82                     | 0.53              |
| 37:i:84:TYR:HB2   | 46:i:201:3PE:H272 | 1.90                     | 0.53              |
| 40:l:41:MET:SD    | 40:l:41:MET:N     | 2.81                     | 0.53              |
| 3:D:347:HIS:ND1   | 6:3:121:MET:SD    | 2.81                     | 0.53              |
| 32:d:108:THR:HA   | 44:p:77:LYS:HA    | 1.90                     | 0.53              |
| 6:3:584:LYS:HE2   | 9:Q:36:ARG:HD2    | 1.91                     | 0.53              |
| 25:O:311:GLU:HG2  | 25:O:312:VAL:HG13 | 1.90                     | 0.53              |
| 32:d:42:GLY:O     | 32:d:46:ASN:ND2   | 2.42                     | 0.53              |
| 5:1:99:GLU:HG2    | 5:1:99:GLU:O      | 2.07                     | 0.53              |
| 6:3:118:ASP:OD2   | 9:Q:46:GLN:NE2    | 2.41                     | 0.53              |
| 16:r:20:GLN:HA    | 16:r:23:LEU:HD23  | 1.90                     | 0.53              |
| 20:J:135:LEU:HD11 | 29:a:42:GLN:HG3   | 1.91                     | 0.53              |
| 22:L:83:ASP:OD1   | 22:L:84:PHE:N     | 2.41                     | 0.53              |
| 23:M:370:PRO:HA   | 23:M:375:LEU:HD22 | 1.90                     | 0.53              |
| 22:L:363:THR:OG1  | 22:L:431:THR:O    | 2.25                     | 0.53              |
| 24:N:87:GLN:NE2   | 36:h:126:PRO:O    | 2.42                     | 0.53              |
| 24:N:131:LEU:HA   | 24:N:135:LYS:HE2  | 1.90                     | 0.53              |
| 6:3:278:ARG:N     | 15:q:136:GLU:O    | 2.42                     | 0.52              |
| 22:L:8:ILE:HA     | 22:L:11:ILE:HD12  | 1.91                     | 0.52              |
| 22:L:365:ILE:HG13 | 22:L:366:MET:HG3  | 1.91                     | 0.52              |
| 41:m:126:ILE:HD13 | 44:p:102:MET:HE2  | 1.92                     | 0.52              |
| 3:D:164:MET:SD    | 3:D:164:MET:N     | 2.82                     | 0.52              |
| 3:D:424:VAL:HG13  | 3:D:427:GLU:HG2   | 1.91                     | 0.52              |
| 8:P:53:VAL:HA     | 8:P:56:ILE:HG12   | 1.90                     | 0.52              |
| 27:Y:8:TYR:HB2    | 27:Y:23:ILE:HG21  | 1.90                     | 0.52              |
| 3:D:148:LEU:HD21  | 3:D:177:MET:HB2   | 1.92                     | 0.52              |
| 19:H:86:TRP:CD1   | 19:H:233:LEU:HD12 | 2.44                     | 0.52              |
| 23:M:76:MET:HE1   | 23:M:230:ILE:HD13 | 1.92                     | 0.52              |
| 1:6:151:PRO:HB2   | 8:P:57:MET:HE3    | 1.92                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:24:ASN:ND2    | 5:1:113:HIS:O     | 2.43                     | 0.52              |
| 6:3:258:ILE:HA    | 6:3:368:ILE:HD12  | 1.91                     | 0.52              |
| 6:3:520:LYS:O     | 6:3:541:CYS:HA    | 2.09                     | 0.52              |
| 22:L:560:LYS:HE3  | 46:L:704:3PE:H221 | 1.90                     | 0.52              |
| 23:M:429:SER:O    | 35:g:36:TYR:OH    | 2.28                     | 0.52              |
| 37:i:81:VAL:HG22  | 46:i:201:3PE:H2A1 | 1.90                     | 0.52              |
| 38:j:14:PHE:HB2   | 39:k:61:GLY:HA3   | 1.92                     | 0.52              |
| 3:D:238:ARG:HH21  | 3:D:412:ALA:HB1   | 1.74                     | 0.52              |
| 4:2:144:CYS:O     | 5:1:139:ARG:NH2   | 2.25                     | 0.52              |
| 11:S:78:LEU:HB2   | 11:S:81:LEU:HD22  | 1.92                     | 0.52              |
| 19:H:288:LEU:HD23 | 19:H:289:LEU:HD23 | 1.92                     | 0.52              |
| 8:P:325:ARG:O     | 8:P:325:ARG:NH1   | 2.38                     | 0.52              |
| 9:Q:13:VAL:O      | 14:W:17:THR:N     | 2.43                     | 0.52              |
| 23:M:173:THR:HB   | 36:h:101:ALA:HB2  | 1.92                     | 0.52              |
| 1:6:164:GLU:HG2   | 7:9:139:PHE:HE1   | 1.75                     | 0.52              |
| 3:D:19:MET:HB2    | 24:N:173:THR:HG22 | 1.92                     | 0.52              |
| 11:S:41:VAL:HG12  | 11:S:45:LYS:HE2   | 1.92                     | 0.52              |
| 23:M:313:THR:HA   | 23:M:316:MET:HE3  | 1.91                     | 0.52              |
| 5:1:154:ARG:HA    | 17:s:52:LEU:HD21  | 1.92                     | 0.52              |
| 6:3:354:ALA:O     | 6:3:361:ASN:ND2   | 2.42                     | 0.52              |
| 22:L:186:MET:O    | 22:L:190:SER:OG   | 2.27                     | 0.52              |
| 25:O:165:PRO:HG3  | 25:O:217:MET:HE2  | 1.91                     | 0.52              |
| 3:D:61:VAL:HG13   | 3:D:82:LEU:HB2    | 1.92                     | 0.51              |
| 5:1:93:LEU:HD13   | 5:1:129:MET:HE1   | 1.90                     | 0.51              |
| 37:i:86:LYS:NZ    | 44:p:41:ASP:OD1   | 2.38                     | 0.51              |
| 40:l:131:GLN:OE1  | 43:o:36:ARG:NH1   | 2.41                     | 0.51              |
| 3:D:63:ARG:HB3    | 3:D:79:HIS:HB2    | 1.92                     | 0.51              |
| 4:2:6:LEU:O       | 4:2:92:ARG:NH2    | 2.42                     | 0.51              |
| 10:7:70:LYS:NZ    | 10:7:72:TYR:OH    | 2.44                     | 0.51              |
| 31:c:38:ASP:OD2   | 32:d:77:LYS:NZ    | 2.41                     | 0.51              |
| 6:3:201:ASP:OD2   | 6:3:268:ARG:NH2   | 2.40                     | 0.51              |
| 6:3:228:ILE:HG12  | 6:3:583:THR:HB    | 1.93                     | 0.51              |
| 35:g:24:TRP:CD1   | 35:g:26:GLU:HB2   | 2.45                     | 0.51              |
| 37:i:89:MET:O     | 37:i:95:THR:OG1   | 2.27                     | 0.51              |
| 3:D:116:GLN:NE2   | 3:D:276:ASP:OD2   | 2.40                     | 0.51              |
| 6:3:577:GLU:OE1   | 6:3:579:ARG:NH1   | 2.44                     | 0.51              |
| 19:H:246:LEU:H    | 19:H:258:ASN:HD22 | 1.59                     | 0.51              |
| 22:L:62:MET:HB2   | 44:p:114:GLN:HG2  | 1.92                     | 0.51              |
| 5:1:191:ALA:HB2   | 5:1:203:PRO:HG3   | 1.93                     | 0.51              |
| 8:P:300:LEU:HB3   | 8:P:305:VAL:HB    | 1.93                     | 0.51              |
| 18:A:73:LEU:O     | 19:H:160:TYR:OH   | 2.25                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:L:424:MET:HE3  | 22:L:428:TYR:HB2  | 1.92                     | 0.51              |
| 2:C:151:ILE:HG23  | 2:C:152:LEU:HG    | 1.91                     | 0.51              |
| 1:6:119:GLU:H     | 19:H:59:GLU:HG2   | 1.75                     | 0.51              |
| 40:l:53:SER:HA    | 40:l:83:TYR:HB3   | 1.92                     | 0.51              |
| 8:P:157:ARG:NH1   | 8:P:163:ALA:O     | 2.44                     | 0.51              |
| 10:7:16:GLN:O     | 10:7:16:GLN:NE2   | 2.43                     | 0.51              |
| 23:M:105:LEU:HD21 | 55:d:201:CDL:H673 | 1.93                     | 0.51              |
| 42:n:138:GLN:NE2  | 42:n:155:PRO:O    | 2.39                     | 0.51              |
| 8:P:311:GLU:HG2   | 8:P:336:PRO:HB3   | 1.93                     | 0.51              |
| 23:M:102:LEU:HD13 | 23:M:230:ILE:HG12 | 1.93                     | 0.51              |
| 23:M:275:ILE:O    | 23:M:279:GLN:HB2  | 2.11                     | 0.51              |
| 47:9:203:PC1:H2D1 | 28:Z:39:ILE:HD11  | 1.93                     | 0.51              |
| 19:H:141:SER:HB2  | 19:H:289:LEU:HD12 | 1.92                     | 0.51              |
| 1:6:40:VAL:HG13   | 1:6:183:LEU:HB3   | 1.93                     | 0.50              |
| 25:O:308:TYR:OH   | 32:d:51:ARG:NH1   | 2.44                     | 0.50              |
| 1:6:189:ARG:NH1   | 52:P:501:NDP:O2X  | 2.44                     | 0.50              |
| 4:2:51:LEU:HD21   | 4:2:84:ALA:HB2    | 1.92                     | 0.50              |
| 5:1:394:GLU:OE1   | 6:3:129:ARG:NH1   | 2.45                     | 0.50              |
| 19:H:179:TRP:HE1  | 28:Z:42:LEU:HG    | 1.76                     | 0.50              |
| 21:K:59:ILE:HD12  | 24:N:27:MET:HG3   | 1.93                     | 0.50              |
| 23:M:339:SER:HB3  | 23:M:344:MET:HE1  | 1.93                     | 0.50              |
| 41:m:114:LEU:HB3  | 41:m:120:LEU:HB2  | 1.93                     | 0.50              |
| 23:M:364:LEU:HB3  | 23:M:369:LEU:HD22 | 1.93                     | 0.50              |
| 3:D:324:LYS:HD3   | 3:D:331:SER:HB3   | 1.93                     | 0.50              |
| 7:9:65:GLY:HA3    | 7:9:136:GLY:O     | 2.11                     | 0.50              |
| 15:q:34:ARG:NH2   | 15:q:58:ARG:O     | 2.41                     | 0.50              |
| 23:M:3:LYS:NZ     | 34:f:27:ASP:OD2   | 2.42                     | 0.50              |
| 24:N:144:GLN:HG2  | 33:e:2:PHE:HB2    | 1.94                     | 0.50              |
| 32:d:104:LYS:NZ   | 32:d:105:GLU:O    | 2.44                     | 0.50              |
| 2:C:33:LEU:HD21   | 13:V:93:MET:HE1   | 1.93                     | 0.50              |
| 13:V:71:LEU:HD13  | 13:V:79:VAL:HG11  | 1.92                     | 0.50              |
| 20:J:19:LEU:HD11  | 21:K:31:LEU:HB3   | 1.94                     | 0.50              |
| 22:L:396:ILE:HG21 | 22:L:490:ALA:HB2  | 1.92                     | 0.50              |
| 23:M:449:THR:HG21 | 46:M:502:3PE:H232 | 1.93                     | 0.50              |
| 2:C:194:PHE:O     | 9:Q:81:ASN:ND2    | 2.44                     | 0.50              |
| 3:D:152:MET:O     | 3:D:156:THR:OG1   | 2.27                     | 0.50              |
| 3:D:155:THR:HB    | 3:D:167:PHE:HA    | 1.93                     | 0.50              |
| 10:7:38:ASN:HB3   | 10:7:43:LEU:HD11  | 1.93                     | 0.50              |
| 23:M:207:MET:HE3  | 23:M:298:ILE:HG12 | 1.94                     | 0.50              |
| 1:6:68:GLU:HG3    | 1:6:160:PRO:HB2   | 1.94                     | 0.50              |
| 14:W:73:ALA:HB1   | 54:W:201:ZMP:H17  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:M:435:THR:HG23 | 35:g:64:PHE:HE2   | 1.77                     | 0.50              |
| 3:D:326:ASP:OD1   | 6:3:127:ARG:NH2   | 2.42                     | 0.49              |
| 5:1:97:ALA:HB3    | 5:1:138:ILE:HA    | 1.93                     | 0.49              |
| 6:3:364:LEU:HD12  | 6:3:491:ASN:HB3   | 1.94                     | 0.49              |
| 6:3:378:LEU:HB3   | 6:3:451:VAL:HG12  | 1.94                     | 0.49              |
| 20:J:148:ALA:HB1  | 20:J:151:MET:HG3  | 1.94                     | 0.49              |
| 22:L:571:THR:HA   | 22:L:574:THR:HG22 | 1.94                     | 0.49              |
| 23:M:33:LEU:HD13  | 46:h:202:3PE:H2C1 | 1.93                     | 0.49              |
| 12:U:51:ILE:HG21  | 12:U:67:ALA:HB1   | 1.94                     | 0.49              |
| 40:l:4:THR:OG1    | 40:l:6:ASP:OD1    | 2.29                     | 0.49              |
| 5:1:97:ALA:HB1    | 5:1:111:MET:SD    | 2.52                     | 0.49              |
| 22:L:97:THR:HG21  | 22:L:125:LEU:HD22 | 1.93                     | 0.49              |
| 22:L:341:MET:HE3  | 22:L:454:ILE:HG12 | 1.94                     | 0.49              |
| 5:1:96:ASN:O      | 5:1:225:VAL:HG23  | 2.12                     | 0.49              |
| 31:c:41:GLU:HG2   | 32:d:19:ARG:HE    | 1.78                     | 0.49              |
| 19:H:24:GLU:HA    | 19:H:271:LEU:HD13 | 1.94                     | 0.49              |
| 42:n:104:ASP:OD1  | 42:n:121:ARG:NH2  | 2.37                     | 0.49              |
| 8:P:63:GLY:HA3    | 8:P:68:LEU:HD13   | 1.93                     | 0.49              |
| 55:N:401:CDL:H861 | 55:d:201:CDL:H651 | 1.95                     | 0.49              |
| 31:c:7:PRO:HG2    | 31:c:10:ALA:HB2   | 1.94                     | 0.49              |
| 55:h:201:CDL:HA21 | 46:i:201:3PE:H122 | 1.93                     | 0.49              |
| 4:2:147:ALA:HB3   | 4:2:153:MET:HE3   | 1.95                     | 0.49              |
| 12:T:22:TYR:HD2   | 12:T:25:ILE:HG12  | 1.77                     | 0.49              |
| 36:h:73:ARG:NH1   | 44:p:60:THR:OG1   | 2.39                     | 0.49              |
| 7:9:59:LEU:O      | 16:r:33:ARG:NH2   | 2.45                     | 0.49              |
| 26:X:74:LYS:NZ    | 29:a:69:ILE:O     | 2.41                     | 0.49              |
| 35:g:88:ARG:NH2   | 44:p:9:TYR:OH     | 2.46                     | 0.49              |
| 3:D:354:GLU:OE2   | 3:D:357:GLN:NE2   | 2.44                     | 0.49              |
| 5:1:287:VAL:HG21  | 5:1:294:LEU:HB2   | 1.95                     | 0.49              |
| 3:D:238:ARG:NH1   | 19:H:279:ARG:O    | 2.46                     | 0.49              |
| 5:1:185:ILE:HG12  | 5:1:359:CYS:HB3   | 1.95                     | 0.49              |
| 22:L:249:SER:HB3  | 22:L:336:LYS:HB3  | 1.95                     | 0.49              |
| 22:L:257:ILE:HD13 | 22:L:313:MET:HB2  | 1.95                     | 0.49              |
| 22:L:363:THR:HG23 | 22:L:431:THR:HB   | 1.93                     | 0.49              |
| 26:X:136:LEU:HD12 | 26:X:137:PRO:HD2  | 1.95                     | 0.49              |
| 8:P:171:ILE:HG13  | 52:P:501:NDP:H42N | 1.94                     | 0.48              |
| 23:M:281:ASP:OD1  | 23:M:340:ARG:NH1  | 2.45                     | 0.48              |
| 44:p:139:GLN:HA   | 44:p:143:LEU:HB2  | 1.94                     | 0.48              |
| 26:X:6:LEU:HD11   | 28:Z:90:LEU:HD13  | 1.95                     | 0.48              |
| 28:Z:58:ARG:NH1   | 30:b:80:LEU:O     | 2.45                     | 0.48              |
| 6:3:595:GLU:OE1   | 6:3:598:LYS:NZ    | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:9:110:ARG:NH2   | 15:q:128:SER:OG   | 2.46                     | 0.48              |
| 8:P:196:LEU:HD13  | 8:P:257:PRO:HG3   | 1.94                     | 0.48              |
| 9:Q:33:ARG:NH2    | 9:Q:77:ASP:OD2    | 2.41                     | 0.48              |
| 14:W:48:THR:HG23  | 14:W:52:MET:HE3   | 1.95                     | 0.48              |
| 22:L:243:VAL:O    | 22:L:247:LEU:HB2  | 2.14                     | 0.48              |
| 5:1:131:ALA:O     | 5:1:171:TYR:OH    | 2.26                     | 0.48              |
| 8:P:134:HIS:CD2   | 52:P:501:NDP:H5N  | 2.49                     | 0.48              |
| 3:D:61:VAL:HG21   | 3:D:83:LEU:HD13   | 1.95                     | 0.48              |
| 3:D:165:THR:HG22  | 19:H:32:GLN:HG3   | 1.95                     | 0.48              |
| 5:1:279:LEU:HD12  | 5:1:283:HIS:HD2   | 1.77                     | 0.48              |
| 5:1:378:ARG:NH2   | 5:1:388:GLU:OE1   | 2.44                     | 0.48              |
| 8:P:21:ALA:HA     | 8:P:90:VAL:O      | 2.13                     | 0.48              |
| 46:i:201:3PE:H2C2 | 46:i:201:3PE:H352 | 1.95                     | 0.48              |
| 41:m:84:LYS:HG3   | 46:m:202:3PE:H11  | 1.96                     | 0.48              |
| 2:C:96:LEU:HB2    | 2:C:105:ILE:HG22  | 1.94                     | 0.48              |
| 2:C:179:GLU:OE1   | 8:P:40:ARG:NH2    | 2.41                     | 0.48              |
| 3:D:413:ASP:OD1   | 3:D:413:ASP:N     | 2.26                     | 0.48              |
| 18:A:6:VAL:HG12   | 18:A:10:ASN:HD21  | 1.78                     | 0.48              |
| 24:N:321:LYS:HD2  | 24:N:322:PRO:HD2  | 1.94                     | 0.48              |
| 25:O:138:MET:HE3  | 56:O:401:DGT:HN2  | 1.78                     | 0.48              |
| 28:Z:104:LYS:HB2  | 28:Z:107:GLU:HB2  | 1.96                     | 0.48              |
| 6:3:26:VAL:HG13   | 6:3:79:ILE:HD13   | 1.96                     | 0.48              |
| 3:D:117:ALA:HA    | 3:D:367:ILE:HG13  | 1.95                     | 0.47              |
| 3:D:128:ILE:HD12  | 3:D:325:VAL:HG11  | 1.96                     | 0.47              |
| 3:D:350:LYS:HG3   | 6:3:121:MET:HG3   | 1.96                     | 0.47              |
| 6:3:243:ARG:HG2   | 6:3:244:THR:HG23  | 1.95                     | 0.47              |
| 18:A:74:PRO:HG3   | 20:J:141:VAL:HG12 | 1.96                     | 0.47              |
| 19:H:113:VAL:HG11 | 19:H:139:THR:HG21 | 1.96                     | 0.47              |
| 23:M:403:THR:HA   | 23:M:406:TYR:CE2  | 2.49                     | 0.47              |
| 3:D:377:TYR:HB3   | 3:D:390:LYS:HB3   | 1.96                     | 0.47              |
| 6:3:384:PRO:HD2   | 6:3:415:LEU:HD21  | 1.96                     | 0.47              |
| 8:P:133:SER:OG    | 8:P:134:HIS:N     | 2.47                     | 0.47              |
| 20:J:69:TYR:HD2   | 21:K:75:LEU:HD22  | 1.80                     | 0.47              |
| 22:L:67:HIS:HD2   | 22:L:77:LYS:HE2   | 1.79                     | 0.47              |
| 24:N:243:MET:HE3  | 32:d:44:MET:HE3   | 1.94                     | 0.47              |
| 42:n:137:LYS:HA   | 42:n:137:LYS:HD3  | 1.73                     | 0.47              |
| 54:n:201:ZMP:H15  | 54:n:201:ZMP:H17  | 1.68                     | 0.47              |
| 1:6:101:THR:OG1   | 1:6:129:CYS:SG    | 2.68                     | 0.47              |
| 7:9:134:VAL:HG21  | 7:9:167:ILE:HG21  | 1.96                     | 0.47              |
| 1:6:164:GLU:HG2   | 7:9:139:PHE:CE1   | 2.49                     | 0.47              |
| 4:2:144:CYS:HB2   | 49:2:301:FES:S2   | 2.54                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:2:150:ASN:OD1   | 4:2:190:ARG:NH2   | 2.47                     | 0.47              |
| 19:H:70:LEU:HD22  | 19:H:118:TRP:HB3  | 1.96                     | 0.47              |
| 22:L:237:MET:HE2  | 22:L:237:MET:HB3  | 1.70                     | 0.47              |
| 24:N:109:ALA:HB3  | 24:N:161:SER:HA   | 1.96                     | 0.47              |
| 26:X:80:PRO:HA    | 26:X:83:GLU:HG2   | 1.95                     | 0.47              |
| 37:i:79:TRP:HD1   | 44:p:40:VAL:HG13  | 1.79                     | 0.47              |
| 4:2:131:THR:HG21  | 4:2:135:LYS:HD3   | 1.97                     | 0.47              |
| 6:3:126:ASP:OD2   | 6:3:127:ARG:NH1   | 2.48                     | 0.47              |
| 18:A:91:ALA:HB1   | 19:H:305:ILE:HD13 | 1.96                     | 0.47              |
| 19:H:141:SER:HA   | 19:H:290:TRP:HE1  | 1.80                     | 0.47              |
| 22:L:295:GLN:HB3  | 22:L:301:ILE:HG12 | 1.97                     | 0.47              |
| 23:M:253:LEU:O    | 23:M:257:MET:HB2  | 2.15                     | 0.47              |
| 1:6:85:VAL:HG21   | 48:D:501:UQ:H352  | 1.97                     | 0.47              |
| 12:T:70:LEU:HD11  | 12:T:76:ILE:HG12  | 1.96                     | 0.47              |
| 19:H:42:PRO:HD2   | 19:H:45:ILE:HG12  | 1.96                     | 0.47              |
| 1:6:101:THR:HA    | 1:6:129:CYS:HB3   | 1.96                     | 0.47              |
| 2:C:167:PRO:HA    | 9:Q:82:MET:HE1    | 1.97                     | 0.47              |
| 3:D:101:PRO:O     | 3:D:105:ARG:NH1   | 2.47                     | 0.47              |
| 10:7:32:GLN:HG2   | 15:q:122:GLU:HA   | 1.97                     | 0.47              |
| 27:Y:68:MET:HE3   | 55:Y:403:CDL:H332 | 1.96                     | 0.47              |
| 41:m:57:SER:OG    | 41:m:58:HIS:N     | 2.48                     | 0.47              |
| 5:1:342:ASP:OD1   | 5:1:429:ARG:NH1   | 2.48                     | 0.47              |
| 6:3:252:PRO:HB3   | 6:3:263:ILE:HG23  | 1.97                     | 0.47              |
| 9:Q:14:ASP:OD1    | 9:Q:14:ASP:N      | 2.48                     | 0.47              |
| 6:3:103:LEU:HD12  | 10:7:69:PRO:HB3   | 1.97                     | 0.46              |
| 15:q:44:TYR:OH    | 15:q:113:HIS:N    | 2.47                     | 0.46              |
| 19:H:26:LYS:HG2   | 19:H:36:GLY:HA3   | 1.97                     | 0.46              |
| 22:L:331:THR:HG23 | 22:L:387:THR:HG22 | 1.96                     | 0.46              |
| 26:X:82:THR:HA    | 26:X:85:TRP:CD1   | 2.49                     | 0.46              |
| 3:D:260:LEU:HB3   | 3:D:265:ILE:HB    | 1.96                     | 0.46              |
| 6:3:36:GLN:NE2    | 9:Q:47:SER:O      | 2.48                     | 0.46              |
| 6:3:377:VAL:HG23  | 6:3:404:LEU:HD11  | 1.98                     | 0.46              |
| 8:P:107:GLU:O     | 8:P:111:VAL:HB    | 2.15                     | 0.46              |
| 24:N:321:LYS:HB3  | 32:d:49:ARG:HD3   | 1.98                     | 0.46              |
| 9:Q:11:ILE:HD13   | 14:W:21:PRO:HB3   | 1.97                     | 0.46              |
| 2:C:77:ASP:HB3    | 2:C:95:ASN:HD22   | 1.79                     | 0.46              |
| 48:D:501:UQ:H451  | 48:D:501:UQ:H471  | 1.61                     | 0.46              |
| 5:1:213:VAL:HG13  | 5:1:217:GLY:HA2   | 1.96                     | 0.46              |
| 10:7:34:GLU:O     | 15:q:127:TYR:OH   | 2.24                     | 0.46              |
| 27:Y:12:PRO:O     | 27:Y:15:THR:OG1   | 2.28                     | 0.46              |
| 24:N:313:MET:HG3  | 25:O:99:TRP:CH2   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:189:MET:HE2   | 3:D:189:MET:HB3   | 1.84                     | 0.46              |
| 6:3:10:GLU:OE2    | 6:3:17:SER:OG     | 2.32                     | 0.46              |
| 6:3:228:ILE:HG21  | 6:3:581:GLN:HB3   | 1.98                     | 0.46              |
| 46:L:704:3PE:H371 | 27:Y:113:GLY:HA2  | 1.98                     | 0.46              |
| 23:M:422:HIS:O    | 41:m:55:ARG:NH1   | 2.47                     | 0.46              |
| 22:L:345:SER:HB3  | 22:L:450:LEU:HD11 | 1.97                     | 0.46              |
| 25:O:29:GLY:O     | 25:O:126:ARG:NH2  | 2.49                     | 0.46              |
| 37:i:82:HIS:ND1   | 44:p:36:TYR:OH    | 2.47                     | 0.46              |
| 40:l:126:PRO:HD3  | 43:o:3:HIS:CE1    | 2.50                     | 0.46              |
| 7:9:83:LYS:HG2    | 7:9:96:ILE:HB     | 1.97                     | 0.46              |
| 8:P:65:LEU:HD13   | 8:P:65:LEU:HA     | 1.85                     | 0.46              |
| 4:2:187:ARG:H     | 4:2:187:ARG:HG2   | 1.62                     | 0.46              |
| 6:3:632:ARG:HH22  | 11:S:59:GLU:H     | 1.63                     | 0.46              |
| 24:N:246:LEU:HD21 | 55:N:401:CDL:H792 | 1.98                     | 0.46              |
| 3:D:155:THR:HG21  | 3:D:170:MET:HB2   | 1.97                     | 0.46              |
| 6:3:520:LYS:O     | 6:3:541:CYS:CA    | 2.63                     | 0.46              |
| 7:9:82:CYS:HA     | 7:9:106:ARG:HH21  | 1.81                     | 0.46              |
| 18:A:99:SER:HB3   | 46:A:201:3PE:H391 | 1.97                     | 0.46              |
| 19:H:149:ILE:HG21 | 19:H:185:TRP:HB2  | 1.98                     | 0.46              |
| 23:M:17:LEU:HD21  | 32:d:54:MET:HE1   | 1.97                     | 0.46              |
| 23:M:106:LEU:HD13 | 23:M:234:ILE:HG21 | 1.98                     | 0.46              |
| 35:g:96:LYS:NZ    | 44:p:7:ASP:OD2    | 2.48                     | 0.46              |
| 6:3:321:GLY:HA2   | 6:3:496:ILE:HG23  | 1.97                     | 0.45              |
| 11:S:79:ASN:N     | 11:S:79:ASN:OD1   | 2.42                     | 0.45              |
| 20:J:21:LEU:HD21  | 20:J:91:PHE:HD2   | 1.81                     | 0.45              |
| 22:L:545:SER:HB2  | 23:M:274:SER:HB3  | 1.98                     | 0.45              |
| 22:L:551:THR:HA   | 22:L:555:LEU:HB2  | 1.97                     | 0.45              |
| 25:O:225:SER:O    | 25:O:228:ALA:O    | 2.34                     | 0.45              |
| 1:6:76:ARG:HD3    | 1:6:77:TYR:CZ     | 2.50                     | 0.45              |
| 46:D:502:3PE:H3C2 | 47:M:501:PC1:H3I3 | 1.97                     | 0.45              |
| 8:P:128:ARG:NH2   | 8:P:220:ASP:O     | 2.49                     | 0.45              |
| 21:K:24:SER:O     | 21:K:24:SER:OG    | 2.34                     | 0.45              |
| 12:U:44:SER:OG    | 54:n:201:ZMP:O7   | 2.27                     | 0.45              |
| 32:d:29:PRO:HG3   | 55:d:201:CDL:H112 | 1.97                     | 0.45              |
| 3:D:284:ASP:OD1   | 7:9:1:THR:OG1     | 2.31                     | 0.45              |
| 5:1:194:GLU:OE2   | 5:1:204:ARG:NH2   | 2.38                     | 0.45              |
| 12:U:76:ILE:O     | 12:U:80:ILE:HG12  | 2.15                     | 0.45              |
| 35:g:118:LEU:HD11 | 44:p:162:MET:HE2  | 1.97                     | 0.45              |
| 22:L:362:ILE:HD13 | 22:L:365:ILE:HD11 | 1.97                     | 0.45              |
| 25:O:97:GLN:NE2   | 25:O:131:ASP:OD2  | 2.49                     | 0.45              |
| 3:D:73:VAL:HG21   | 3:D:414:VAL:HG21  | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:1:215:VAL:H     | 5:1:220:THR:HG21  | 1.82                     | 0.45              |
| 10:7:32:GLN:HE22  | 10:7:34:GLU:HB3   | 1.81                     | 0.45              |
| 15:q:106:ARG:HB2  | 15:q:109:ILE:HG13 | 1.97                     | 0.45              |
| 23:M:250:LEU:O    | 23:M:254:THR:OG1  | 2.35                     | 0.45              |
| 3:D:3:GLN:OE1     | 23:M:142:ARG:NH1  | 2.49                     | 0.45              |
| 23:M:168:GLN:HB2  | 23:M:174:LEU:HD22 | 1.99                     | 0.45              |
| 12:U:49:GLU:HB3   | 39:k:50:TRP:HE1   | 1.82                     | 0.45              |
| 1:6:102:LEU:HD13  | 1:6:110:LEU:HD13  | 1.99                     | 0.45              |
| 2:C:193:GLU:OE2   | 6:3:223:ARG:NH2   | 2.50                     | 0.45              |
| 6:3:266:LYS:O     | 6:3:270:ALA:CB    | 2.65                     | 0.45              |
| 6:3:668:ILE:HA    | 6:3:671:PHE:HB3   | 1.99                     | 0.45              |
| 10:7:12:THR:OG1   | 10:7:14:THR:O     | 2.34                     | 0.45              |
| 23:M:17:LEU:HD11  | 55:N:401:CDL:H141 | 1.99                     | 0.45              |
| 23:M:58:SER:OG    | 23:M:59:ASP:N     | 2.49                     | 0.45              |
| 23:M:310:MET:HG3  | 23:M:455:THR:HG23 | 1.99                     | 0.45              |
| 27:Y:24:THR:HG21  | 27:Y:69:PHE:HD2   | 1.81                     | 0.45              |
| 44:p:5:ASP:N      | 44:p:5:ASP:OD1    | 2.48                     | 0.45              |
| 3:D:211:ILE:HG22  | 3:D:315:LEU:HD11  | 1.98                     | 0.45              |
| 5:1:355:LYS:HE3   | 5:1:355:LYS:HB3   | 1.80                     | 0.45              |
| 21:K:1:FME:HB2    | 21:K:1:FME:HE3    | 1.66                     | 0.45              |
| 25:O:14:THR:HG21  | 25:O:116:LEU:HD22 | 1.99                     | 0.45              |
| 12:T:44:SER:OG    | 54:W:201:ZMP:O5   | 2.30                     | 0.45              |
| 2:C:77:ASP:HB3    | 2:C:95:ASN:HB2    | 1.99                     | 0.45              |
| 6:3:520:LYS:O     | 6:3:541:CYS:O     | 2.34                     | 0.45              |
| 8:P:133:SER:HB3   | 8:P:167:ARG:HG2   | 1.99                     | 0.45              |
| 9:Q:8:THR:O       | 14:W:25:ARG:NH1   | 2.50                     | 0.45              |
| 15:q:117:VAL:O    | 15:q:120:THR:OG1  | 2.31                     | 0.45              |
| 16:r:108:ASP:OD1  | 16:r:108:ASP:N    | 2.46                     | 0.45              |
| 55:h:201:CDL:HB32 | 44:p:51:ILE:HD13  | 1.98                     | 0.45              |
| 1:6:100:GLY:HA2   | 45:6:201:SF4:S4   | 2.57                     | 0.44              |
| 48:D:501:UQ:H372  | 19:H:224:PHE:CZ   | 2.53                     | 0.44              |
| 6:3:156:CYS:SG    | 6:3:158:ARG:HB2   | 2.57                     | 0.44              |
| 6:3:418:ARG:HE    | 17:s:68:ARG:HD2   | 1.81                     | 0.44              |
| 6:3:622:ARG:NH1   | 6:3:625:GLU:OE2   | 2.41                     | 0.44              |
| 8:P:87:HIS:HB2    | 10:7:26:VAL:HG13  | 1.99                     | 0.44              |
| 13:V:34:LEU:HD22  | 13:V:44:ARG:HA    | 1.99                     | 0.44              |
| 22:L:129:LEU:O    | 22:L:133:SER:OG   | 2.32                     | 0.44              |
| 23:M:187:ASP:OD1  | 23:M:187:ASP:N    | 2.42                     | 0.44              |
| 28:Z:34:MET:HE1   | 47:Z:402:PC1:H153 | 1.99                     | 0.44              |
| 46:D:502:3PE:H2C2 | 24:N:284:MET:HB3  | 1.98                     | 0.44              |
| 6:3:194:GLU:HG2   | 6:3:195:LEU:HG    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:3:533:THR:OG1   | 6:3:534:ARG:N     | 2.51                     | 0.44              |
| 19:H:162:LEU:HD23 | 19:H:165:LEU:HD12 | 1.98                     | 0.44              |
| 29:a:48:MET:HE2   | 29:a:48:MET:HB3   | 1.85                     | 0.44              |
| 22:L:241:THR:HG23 | 22:L:299:LYS:HE2  | 1.98                     | 0.44              |
| 23:M:310:MET:HE1  | 23:M:380:PHE:CD1  | 2.52                     | 0.44              |
| 4:2:156:ILE:HB    | 4:2:161:TYR:HE2   | 1.83                     | 0.44              |
| 7:9:45:ARG:HA     | 16:r:11:ARG:HH11  | 1.81                     | 0.44              |
| 23:M:443:PRO:HB3  | 46:M:502:3PE:H3C1 | 2.00                     | 0.44              |
| 27:Y:10:GLU:HG3   | 27:Y:11:VAL:HG13  | 1.98                     | 0.44              |
| 47:9:203:PC1:H352 | 19:H:197:PRO:HG2  | 2.00                     | 0.44              |
| 8:P:5:VAL:HG11    | 8:P:89:ASN:HD21   | 1.82                     | 0.44              |
| 8:P:41:MET:HE3    | 8:P:41:MET:HB2    | 1.78                     | 0.44              |
| 35:g:90:GLU:OE2   | 35:g:93:ARG:NH2   | 2.36                     | 0.44              |
| 35:g:98:ARG:HD3   | 35:g:105:ILE:HA   | 2.00                     | 0.44              |
| 2:C:81:VAL:HG22   | 3:D:388:ARG:HG2   | 2.00                     | 0.44              |
| 2:C:137:MET:HB3   | 2:C:162:PHE:HB2   | 1.99                     | 0.44              |
| 6:3:169:VAL:HG21  | 6:3:191:PHE:HE1   | 1.83                     | 0.44              |
| 7:9:81:ALA:O      | 7:9:106:ARG:NH2   | 2.50                     | 0.44              |
| 19:H:316:PRO:HG3  | 28:Z:56:ARG:HB3   | 1.98                     | 0.44              |
| 23:M:74:PRO:HA    | 23:M:77:LEU:HD12  | 1.99                     | 0.44              |
| 26:X:97:ARG:HD2   | 28:Z:59:LEU:HD13  | 2.00                     | 0.44              |
| 28:Z:126:LEU:HG   | 33:e:75:MET:HE1   | 2.00                     | 0.44              |
| 40:l:6:ASP:OD1    | 40:l:6:ASP:N      | 2.51                     | 0.44              |
| 3:D:145:THR:HG23  | 3:D:181:TYR:OH    | 2.17                     | 0.44              |
| 5:1:361:GLN:N     | 45:1:502:SF4:S2   | 2.90                     | 0.44              |
| 8:P:194:VAL:H     | 8:P:288:HIS:CE1   | 2.36                     | 0.44              |
| 12:T:19:LEU:HD13  | 12:T:19:LEU:HA    | 1.88                     | 0.44              |
| 23:M:166:LEU:HD23 | 23:M:166:LEU:HA   | 1.87                     | 0.44              |
| 26:X:168:PHE:HE2  | 55:d:201:CDL:H542 | 1.81                     | 0.44              |
| 3:D:248:GLU:OE2   | 13:V:85:LYS:NZ    | 2.51                     | 0.44              |
| 3:D:278:TYR:HA    | 3:D:281:VAL:HG22  | 2.00                     | 0.44              |
| 6:3:99:ALA:O      | 6:3:134:LYS:NZ    | 2.50                     | 0.44              |
| 6:3:381:GLY:HA3   | 6:3:457:ALA:HB2   | 2.00                     | 0.44              |
| 8:P:164:ILE:H     | 8:P:164:ILE:HG13  | 1.67                     | 0.44              |
| 2:C:129:TRP:CZ2   | 3:D:78:PRO:HG2    | 2.53                     | 0.44              |
| 3:D:146:ARG:NH2   | 3:D:368:GLU:O     | 2.38                     | 0.44              |
| 5:1:68:ARG:HD2    | 5:1:254:LYS:HE2   | 2.00                     | 0.44              |
| 8:P:17:SER:OG     | 8:P:43:SER:OG     | 2.32                     | 0.44              |
| 9:Q:54:LYS:HA     | 9:Q:54:LYS:HD3    | 1.76                     | 0.44              |
| 22:L:261:VAL:HG12 | 22:L:317:LEU:HD21 | 1.99                     | 0.44              |
| 22:L:400:ASN:HB3  | 22:L:486:LEU:HG   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:L:474:PRO:HD2  | 43:o:66:LEU:HD21  | 2.00                     | 0.44              |
| 24:N:146:TYR:OH   | 36:h:115:ARG:NH1  | 2.51                     | 0.44              |
| 25:O:89:ASN:OD1   | 25:O:89:ASN:N     | 2.51                     | 0.44              |
| 22:L:341:MET:HE2  | 22:L:457:LEU:HD12 | 2.00                     | 0.43              |
| 22:L:428:TYR:CZ   | 22:L:505:ASN:HB3  | 2.52                     | 0.43              |
| 22:L:538:PRO:HB2  | 40:l:88:VAL:HG22  | 1.98                     | 0.43              |
| 33:e:27:LYS:HA    | 33:e:27:LYS:HD3   | 1.58                     | 0.43              |
| 40:l:98:ASP:OD1   | 40:l:98:ASP:N     | 2.51                     | 0.43              |
| 5:1:188:GLU:OE1   | 5:1:190:THR:N     | 2.51                     | 0.43              |
| 6:3:28:GLN:NE2    | 9:Q:114:LYS:O     | 2.52                     | 0.43              |
| 6:3:368:ILE:HG22  | 6:3:394:ARG:HG2   | 2.00                     | 0.43              |
| 7:9:117:LYS:HE3   | 7:9:117:LYS:HB2   | 1.77                     | 0.43              |
| 18:A:54:LYS:HD2   | 18:A:115:GLU:HA   | 1.99                     | 0.43              |
| 22:L:36:THR:O     | 22:L:40:ILE:HG12  | 2.19                     | 0.43              |
| 22:L:121:LEU:HD22 | 22:L:246:LEU:HD23 | 2.00                     | 0.43              |
| 12:U:35:HIS:HB3   | 12:U:38:LYS:HB2   | 1.99                     | 0.43              |
| 28:Z:57:ARG:NH2   | 30:b:48:THR:OG1   | 2.49                     | 0.43              |
| 5:1:50:LEU:HD13   | 5:1:50:LEU:HA     | 1.90                     | 0.43              |
| 5:1:82:MET:SD     | 5:1:221:THR:OG1   | 2.65                     | 0.43              |
| 19:H:114:TYR:OH   | 20:J:64:LEU:N     | 2.51                     | 0.43              |
| 24:N:28:LEU:HA    | 24:N:31:VAL:HG22  | 1.99                     | 0.43              |
| 24:N:139:LEU:HD23 | 24:N:139:LEU:HA   | 1.87                     | 0.43              |
| 26:X:88:LEU:HD23  | 26:X:88:LEU:HA    | 1.87                     | 0.43              |
| 40:l:102:LYS:HA   | 40:l:102:LYS:HD3  | 1.71                     | 0.43              |
| 41:m:121:ASP:OD1  | 41:m:121:ASP:N    | 2.52                     | 0.43              |
| 43:o:28:LEU:HD22  | 43:o:107:LEU:HD11 | 2.00                     | 0.43              |
| 6:3:577:GLU:HB3   | 6:3:636:ILE:HD11  | 2.00                     | 0.43              |
| 23:M:41:LEU:HG    | 23:M:63:THR:HG23  | 1.99                     | 0.43              |
| 4:2:183:LYS:O     | 4:2:187:ARG:NH2   | 2.51                     | 0.43              |
| 6:3:337:LYS:HB3   | 6:3:609:ILE:HD12  | 1.99                     | 0.43              |
| 6:3:349:PHE:H     | 6:3:509:PRO:HB2   | 1.83                     | 0.43              |
| 7:9:51:ASN:ND2    | 15:q:30:ALA:O     | 2.46                     | 0.43              |
| 15:q:128:SER:OG   | 15:q:130:THR:OG1  | 2.35                     | 0.43              |
| 22:L:142:ILE:HG12 | 23:M:370:PRO:HB2  | 2.01                     | 0.43              |
| 23:M:9:LEU:HD23   | 23:M:104:ILE:HD13 | 2.00                     | 0.43              |
| 24:N:115:LEU:O    | 24:N:119:THR:OG1  | 2.35                     | 0.43              |
| 36:h:69:HIS:NE2   | 55:h:201:CDL:OA3  | 2.50                     | 0.43              |
| 2:C:175:ARG:NH2   | 2:C:177:ASP:OD2   | 2.52                     | 0.43              |
| 6:3:205:VAL:HG23  | 6:3:207:ALA:H     | 1.83                     | 0.43              |
| 7:9:30:THR:HB     | 47:Z:402:PC1:H12  | 2.01                     | 0.43              |
| 8:P:59:LEU:HA     | 8:P:62:MET:HE2    | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:J:70:THR:HA    | 20:J:74:ALA:HB3   | 2.00                     | 0.43              |
| 26:X:94:GLN:HE21  | 26:X:94:GLN:HB2   | 1.64                     | 0.43              |
| 30:b:68:HIS:CD2   | 30:b:69:PRO:HD2   | 2.53                     | 0.43              |
| 50:1:501:FMN:H9   | 50:1:501:FMN:H1'1 | 1.78                     | 0.43              |
| 6:3:226:GLU:OE1   | 9:Q:36:ARG:NH2    | 2.43                     | 0.43              |
| 7:9:39:THR:HG23   | 19:H:272:TRP:HE1  | 1.83                     | 0.43              |
| 11:S:19:ARG:HB2   | 11:S:65:TRP:HB2   | 2.01                     | 0.43              |
| 12:T:25:ILE:HG21  | 12:T:42:LEU:HD11  | 2.01                     | 0.43              |
| 24:N:256:PRO:HD2  | 55:N:401:CDL:H872 | 1.99                     | 0.43              |
| 55:N:401:CDL:H572 | 55:N:401:CDL:H312 | 2.01                     | 0.43              |
| 28:Z:125:GLY:HA3  | 33:e:75:MET:HE2   | 2.01                     | 0.43              |
| 1:6:147:ASP:N     | 1:6:147:ASP:OD1   | 2.51                     | 0.43              |
| 8:P:191:VAL:HG11  | 8:P:242:VAL:HG11  | 2.01                     | 0.43              |
| 21:K:14:LEU:HD22  | 46:K:201:3PE:H272 | 2.01                     | 0.43              |
| 23:M:260:PRO:HB3  | 46:M:503:3PE:H381 | 2.00                     | 0.43              |
| 23:M:378:GLU:O    | 23:M:382:THR:OG1  | 2.36                     | 0.43              |
| 25:O:116:LEU:HD11 | 25:O:259:LEU:HD23 | 2.01                     | 0.43              |
| 26:X:8:THR:HG22   | 28:Z:87:ARG:HH21  | 1.84                     | 0.43              |
| 36:h:84:GLU:O     | 36:h:88:GLU:HG2   | 2.19                     | 0.43              |
| 42:n:34:ASP:OD1   | 42:n:34:ASP:N     | 2.51                     | 0.43              |
| 21:K:24:SER:HB2   | 21:K:91:GLN:HE22  | 1.83                     | 0.43              |
| 22:L:336:LYS:HD3  | 22:L:336:LYS:HA   | 1.83                     | 0.43              |
| 27:Y:85:ASP:HB3   | 27:Y:88:ASN:ND2   | 2.34                     | 0.43              |
| 38:j:32:MET:HB3   | 38:j:32:MET:HE3   | 1.81                     | 0.43              |
| 41:m:128:TYR:OH   | 44:p:145:LEU:O    | 2.27                     | 0.43              |
| 2:C:36:TYR:CG     | 2:C:56:GLY:HA3    | 2.54                     | 0.43              |
| 3:D:238:ARG:HH12  | 19:H:279:ARG:HB3  | 1.84                     | 0.43              |
| 46:D:502:3PE:H391 | 47:M:501:PC1:H2I1 | 2.01                     | 0.43              |
| 4:2:199:LEU:HB3   | 4:2:203:THR:HG22  | 2.01                     | 0.43              |
| 5:1:197:GLU:OE2   | 5:1:216:PHE:N     | 2.51                     | 0.43              |
| 7:9:43:LEU:HB2    | 19:H:31:MET:HG2   | 2.00                     | 0.43              |
| 19:H:13:ILE:HD13  | 19:H:13:ILE:HA    | 1.86                     | 0.43              |
| 22:L:187:VAL:HG22 | 23:M:383:MET:HG3  | 2.00                     | 0.43              |
| 23:M:171:VAL:HG21 | 23:M:179:LEU:HD21 | 2.00                     | 0.43              |
| 40:l:9:PRO:HD3    | 41:m:66:ARG:HG2   | 2.01                     | 0.43              |
| 5:1:337:MET:HB3   | 5:1:341:THR:HG21  | 2.01                     | 0.42              |
| 8:P:54:TYR:HA     | 8:P:57:MET:HG2    | 2.00                     | 0.42              |
| 8:P:215:VAL:HA    | 8:P:218:THR:HG22  | 2.00                     | 0.42              |
| 20:J:20:ALA:HB1   | 46:K:201:3PE:H261 | 2.01                     | 0.42              |
| 47:M:501:PC1:H321 | 47:M:501:PC1:H352 | 1.90                     | 0.42              |
| 40:l:157:ILE:HB   | 43:o:33:ARG:HH21  | 1.84                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:151:ILE:O     | 3:D:155:THR:OG1   | 2.31                     | 0.42              |
| 5:1:378:ARG:NE    | 6:3:132:GLU:OE2   | 2.49                     | 0.42              |
| 23:M:119:TYR:CZ   | 23:M:161:LEU:HB2  | 2.55                     | 0.42              |
| 24:N:323:ASN:OD1  | 24:N:324:LEU:N    | 2.52                     | 0.42              |
| 25:O:148:CYS:HA   | 25:O:279:LEU:HD21 | 2.01                     | 0.42              |
| 27:Y:105:HIS:HA   | 46:Y:402:3PE:H11  | 2.01                     | 0.42              |
| 37:i:18:ARG:NH1   | 42:n:170:VAL:O    | 2.46                     | 0.42              |
| 2:C:58:ILE:HD13   | 2:C:120:ILE:HG22  | 2.01                     | 0.42              |
| 3:D:249:ASP:OD2   | 3:D:404:LYS:NZ    | 2.51                     | 0.42              |
| 19:H:172:MET:HB3  | 19:H:172:MET:HE3  | 1.76                     | 0.42              |
| 22:L:75:GLU:HB3   | 22:L:77:LYS:HE3   | 2.00                     | 0.42              |
| 22:L:216:LEU:HD22 | 22:L:259:LEU:HD11 | 2.01                     | 0.42              |
| 23:M:67:ILE:HG22  | 46:M:502:3PE:H3D1 | 2.00                     | 0.42              |
| 23:M:344:MET:HE2  | 23:M:344:MET:HB3  | 1.78                     | 0.42              |
| 24:N:310:ASN:HB2  | 25:O:274:THR:HG22 | 2.01                     | 0.42              |
| 26:X:118:ARG:NH2  | 28:Z:62:GLU:OE2   | 2.53                     | 0.42              |
| 27:Y:94:CYS:HA    | 27:Y:114:CYS:HA   | 2.01                     | 0.42              |
| 4:2:43:GLN:HE22   | 17:s:66:SER:HB3   | 1.84                     | 0.42              |
| 47:9:203:PC1:H351 | 19:H:187:ILE:HD12 | 2.02                     | 0.42              |
| 10:7:11:ILE:HG12  | 10:7:17:VAL:HG11  | 2.00                     | 0.42              |
| 22:L:38:THR:HA    | 22:L:41:LYS:HG2   | 2.01                     | 0.42              |
| 22:L:79:SER:OG    | 22:L:136:ASN:ND2  | 2.49                     | 0.42              |
| 23:M:458:THR:O    | 44:p:149:TYR:OH   | 2.31                     | 0.42              |
| 47:M:501:PC1:H251 | 24:N:277:ILE:HA   | 2.01                     | 0.42              |
| 1:6:186:TRP:HB2   | 47:6:203:PC1:H11  | 2.00                     | 0.42              |
| 3:D:345:LEU:HD22  | 6:3:103:LEU:HB2   | 2.00                     | 0.42              |
| 22:L:174:TYR:CD2  | 22:L:232:TRP:HB3  | 2.54                     | 0.42              |
| 3:D:36:VAL:HG22   | 24:N:49:ASN:HB3   | 2.02                     | 0.42              |
| 22:L:419:THR:HA   | 22:L:422:TYR:CZ   | 2.54                     | 0.42              |
| 23:M:203:PHE:HB2  | 23:M:243:MET:HG3  | 2.01                     | 0.42              |
| 24:N:193:ILE:HG12 | 24:N:266:ILE:HG12 | 2.02                     | 0.42              |
| 40:l:141:ARG:HG2  | 43:o:52:LEU:HD23  | 2.01                     | 0.42              |
| 1:6:67:VAL:HA     | 1:6:70:MET:HE2    | 2.01                     | 0.42              |
| 6:3:371:VAL:HG22  | 6:3:450:MET:HE1   | 2.01                     | 0.42              |
| 15:q:40:GLY:HA2   | 15:q:86:TRP:CH2   | 2.54                     | 0.42              |
| 18:A:111:LEU:H    | 18:A:111:LEU:HG   | 1.69                     | 0.42              |
| 26:X:79:GLU:HG2   | 26:X:80:PRO:HD3   | 2.01                     | 0.42              |
| 28:Z:81:ARG:NH2   | 28:Z:124:TYR:OH   | 2.48                     | 0.42              |
| 32:d:95:LYS:HA    | 32:d:95:LYS:HD3   | 1.79                     | 0.42              |
| 33:e:94:PRO:HG2   | 33:e:97:HIS:HB2   | 2.02                     | 0.42              |
| 42:n:31:ILE:H     | 42:n:31:ILE:HG13  | 1.59                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:3:365:ASN:HB3   | 6:3:488:LYS:HG2   | 2.02                     | 0.42              |
| 8:P:90:VAL:HG21   | 8:P:218:THR:OG1   | 2.19                     | 0.42              |
| 8:P:259:PRO:HG2   | 8:P:262:VAL:HG12  | 2.02                     | 0.42              |
| 19:H:169:GLN:NE2  | 19:H:240:ILE:O    | 2.43                     | 0.42              |
| 19:H:269:THR:O    | 19:H:273:ILE:HG12 | 2.20                     | 0.42              |
| 32:d:2:MET:HG2    | 36:h:122:TRP:CD1  | 2.55                     | 0.42              |
| 40:l:96:SER:HB2   | 40:l:99:VAL:HG22  | 2.01                     | 0.42              |
| 5:1:243:ALA:HA    | 5:1:251:SER:HB2   | 2.02                     | 0.42              |
| 8:P:309:PRO:HG2   | 8:P:312:LEU:HB2   | 2.02                     | 0.42              |
| 11:S:43:LEU:HD11  | 11:S:94:LEU:HD11  | 2.02                     | 0.42              |
| 19:H:61:MET:HB3   | 19:H:61:MET:HE3   | 1.62                     | 0.42              |
| 21:K:21:MET:HB3   | 46:K:201:3PE:H222 | 2.00                     | 0.42              |
| 22:L:180:ILE:HD12 | 23:M:397:GLY:HA2  | 2.00                     | 0.42              |
| 44:p:32:LEU:HD23  | 44:p:32:LEU:HA    | 1.91                     | 0.42              |
| 1:6:92:GLN:NE2    | 19:H:215:TYR:O    | 2.53                     | 0.42              |
| 1:6:189:ARG:HG3   | 8:P:50:ARG:HH12   | 1.85                     | 0.42              |
| 6:3:46:LEU:O      | 9:Q:116:LYS:NZ    | 2.40                     | 0.42              |
| 21:K:21:MET:HE3   | 46:K:201:3PE:H352 | 2.02                     | 0.42              |
| 12:U:40:LEU:HD23  | 12:U:40:LEU:HA    | 1.93                     | 0.42              |
| 28:Z:104:LYS:HB3  | 28:Z:104:LYS:HE2  | 1.91                     | 0.42              |
| 3:D:11:ALA:O      | 24:N:228:ASN:ND2  | 2.48                     | 0.41              |
| 3:D:347:HIS:NE2   | 6:3:126:ASP:HA    | 2.34                     | 0.41              |
| 10:7:1:GLY:N      | 10:7:42:ASP:OD2   | 2.51                     | 0.41              |
| 19:H:175:LEU:O    | 19:H:179:TRP:HB3  | 2.20                     | 0.41              |
| 3:D:106:LEU:HD13  | 3:D:391:ILE:HG21  | 2.01                     | 0.41              |
| 3:D:292:ASP:OD1   | 3:D:292:ASP:N     | 2.47                     | 0.41              |
| 5:1:98:ASP:O      | 5:1:139:ARG:HB2   | 2.20                     | 0.41              |
| 7:9:177:TYR:CZ    | 16:r:38:PRO:HG3   | 2.56                     | 0.41              |
| 9:Q:53:LYS:HB3    | 9:Q:53:LYS:HE2    | 1.79                     | 0.41              |
| 4:2:63:ILE:HA     | 4:2:66:MET:HE3    | 2.02                     | 0.41              |
| 8:P:244:TYR:HB2   | 8:P:337:ALA:HB2   | 2.02                     | 0.41              |
| 22:L:335:PHE:HZ   | 22:L:388:GLY:N    | 2.19                     | 0.41              |
| 24:N:310:ASN:ND2  | 25:O:273:THR:O    | 2.45                     | 0.41              |
| 26:X:129:LYS:HE3  | 26:X:129:LYS:HB3  | 1.93                     | 0.41              |
| 34:f:31:ASP:OD1   | 36:h:89:LYS:NZ    | 2.42                     | 0.41              |
| 34:f:41:SER:O     | 34:f:45:GLN:HB2   | 2.20                     | 0.41              |
| 2:C:16:ASP:N      | 2:C:16:ASP:OD1    | 2.50                     | 0.41              |
| 6:3:295:SER:OG    | 6:3:298:ASP:OD1   | 2.39                     | 0.41              |
| 9:Q:116:LYS:HA    | 9:Q:116:LYS:HD3   | 1.82                     | 0.41              |
| 20:J:69:TYR:HE2   | 21:K:75:LEU:HB3   | 1.85                     | 0.41              |
| 22:L:604:ILE:HD13 | 22:L:604:ILE:HA   | 1.90                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:M:124:ALA:O    | 23:M:128:PRO:HD3  | 2.20                     | 0.41              |
| 23:M:261:PHE:O    | 23:M:265:SER:OG   | 2.29                     | 0.41              |
| 26:X:93:MET:HB2   | 26:X:95:LEU:HG    | 2.01                     | 0.41              |
| 27:Y:49:LEU:HD13  | 27:Y:49:LEU:HA    | 1.91                     | 0.41              |
| 36:h:48:GLY:HA3   | 36:h:70:PRO:HG3   | 2.02                     | 0.41              |
| 4:2:60:TRP:H      | 4:2:60:TRP:CD1    | 2.38                     | 0.41              |
| 5:1:133:ALA:HA    | 5:1:174:ASP:O     | 2.20                     | 0.41              |
| 12:T:55:GLU:OE1   | 14:W:43:ARG:NH2   | 2.51                     | 0.41              |
| 22:L:587:TYR:O    | 22:L:590:SER:OG   | 2.33                     | 0.41              |
| 12:U:39:ASP:OD1   | 12:U:39:ASP:N     | 2.53                     | 0.41              |
| 40:l:127:VAL:HG11 | 43:o:94:TYR:CZ    | 2.55                     | 0.41              |
| 2:C:49:GLU:OE2    | 2:C:106:ARG:NH1   | 2.53                     | 0.41              |
| 6:3:163:ALA:HA    | 6:3:167:ALA:HB3   | 2.02                     | 0.41              |
| 12:T:51:ILE:HD13  | 12:T:51:ILE:HA    | 1.92                     | 0.41              |
| 22:L:3:ILE:HA     | 22:L:6:THR:HG22   | 2.03                     | 0.41              |
| 12:U:52:MET:HE3   | 12:U:52:MET:HB3   | 1.94                     | 0.41              |
| 1:6:101:THR:HG21  | 3:D:85:2MR:HG3    | 2.03                     | 0.41              |
| 3:D:136:TRP:CD2   | 3:D:277:VAL:HG21  | 2.56                     | 0.41              |
| 5:1:84:LYS:HE2    | 5:1:84:LYS:HB2    | 1.91                     | 0.41              |
| 11:S:23:CYS:SG    | 11:S:24:GLN:N     | 2.92                     | 0.41              |
| 13:V:58:VAL:HG23  | 13:V:67:LEU:HD21  | 2.03                     | 0.41              |
| 23:M:158:ILE:HD13 | 23:M:158:ILE:HA   | 1.91                     | 0.41              |
| 23:M:395:LEU:HD21 | 41:m:100:TRP:CE2  | 2.56                     | 0.41              |
| 29:a:40:ARG:N     | 29:a:44:GLN:OE1   | 2.50                     | 0.41              |
| 30:b:8:LEU:HD23   | 30:b:8:LEU:HA     | 1.95                     | 0.41              |
| 42:n:5:PRO:HA     | 42:n:6:PRO:HD3    | 1.93                     | 0.41              |
| 6:3:589:PRO:HB2   | 6:3:593:ALA:HB3   | 2.02                     | 0.41              |
| 7:9:14:VAL:HB     | 30:b:9:LYS:HE3    | 2.02                     | 0.41              |
| 7:9:88:ILE:HD12   | 7:9:88:ILE:HA     | 1.92                     | 0.41              |
| 10:7:34:GLU:N     | 15:q:127:TYR:OH   | 2.54                     | 0.41              |
| 12:T:12:LYS:HB3   | 12:T:12:LYS:HE3   | 1.78                     | 0.41              |
| 13:V:25:ILE:HD12  | 25:O:236:GLU:HB3  | 2.03                     | 0.41              |
| 18:A:38:GLU:HG2   | 18:A:43:PRO:HA    | 2.03                     | 0.41              |
| 21:K:73:VAL:HG21  | 24:N:38:LEU:HD22  | 2.02                     | 0.41              |
| 23:M:231:LEU:HD23 | 23:M:235:LEU:HD12 | 2.02                     | 0.41              |
| 23:M:446:LEU:HB3  | 46:M:502:3PE:H342 | 2.02                     | 0.41              |
| 26:X:19:VAL:HG12  | 26:X:24:LEU:HG    | 2.02                     | 0.41              |
| 38:j:9:PRO:HB2    | 39:k:19:MET:HE1   | 2.01                     | 0.41              |
| 2:C:32:ILE:HG22   | 2:C:33:LEU:HG     | 2.02                     | 0.41              |
| 2:C:145:HIS:HB3   | 2:C:148:LEU:HB2   | 2.03                     | 0.41              |
| 3:D:151:ILE:HG12  | 3:D:170:MET:HE3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:3:525:LEU:HD23  | 6:3:525:LEU:HA    | 1.91                     | 0.41              |
| 12:T:31:SER:H     | 12:T:34:SER:HB2   | 1.85                     | 0.41              |
| 18:A:2:ASN:O      | 18:A:6:VAL:HG23   | 2.21                     | 0.41              |
| 22:L:534:HIS:HB3  | 46:L:701:3PE:H2   | 2.02                     | 0.41              |
| 46:M:502:3PE:H3D2 | 46:M:502:3PE:H3G1 | 1.86                     | 0.41              |
| 24:N:170:LEU:O    | 24:N:295:ARG:NH2  | 2.42                     | 0.41              |
| 26:X:122:GLY:HA3  | 30:b:77:LEU:HD13  | 2.02                     | 0.41              |
| 27:Y:128:LYS:HD3  | 27:Y:128:LYS:HA   | 1.70                     | 0.41              |
| 35:g:111:PHE:HB2  | 35:g:116:ILE:HD11 | 2.03                     | 0.41              |
| 4:2:99:HIS:CE1    | 4:2:101:GLN:HE21  | 2.38                     | 0.41              |
| 8:P:280:THR:HG23  | 8:P:283:LYS:H     | 1.86                     | 0.41              |
| 22:L:237:MET:SD   | 22:L:303:ALA:HB2  | 2.60                     | 0.41              |
| 23:M:21:LYS:HE2   | 35:g:51:VAL:HG21  | 2.02                     | 0.41              |
| 34:f:15:LEU:HD12  | 34:f:15:LEU:HA    | 1.92                     | 0.41              |
| 3:D:68:LEU:HD13   | 19:H:130:PHE:HZ   | 1.86                     | 0.40              |
| 3:D:362:ALA:HA    | 3:D:378:LEU:O     | 2.20                     | 0.40              |
| 7:9:109:THR:HA    | 10:7:14:THR:HG21  | 2.03                     | 0.40              |
| 7:9:134:VAL:HG11  | 7:9:171:ILE:HD11  | 2.02                     | 0.40              |
| 10:7:44:ILE:HG12  | 10:7:88:GLY:HA3   | 2.02                     | 0.40              |
| 16:r:111:TYR:OH   | 28:Z:22:ARG:NH1   | 2.55                     | 0.40              |
| 22:L:419:THR:HA   | 22:L:422:TYR:CE2  | 2.56                     | 0.40              |
| 12:U:36:PHE:HD1   | 12:U:40:LEU:HD12  | 1.85                     | 0.40              |
| 26:X:76:HIS:CE1   | 26:X:114:LEU:HD21 | 2.56                     | 0.40              |
| 27:Y:112:MET:HE3  | 27:Y:112:MET:HB2  | 1.82                     | 0.40              |
| 3:D:302:GLU:HG2   | 7:9:3:LYS:HD2     | 2.03                     | 0.40              |
| 4:2:176:LEU:HD23  | 4:2:176:LEU:HA    | 1.91                     | 0.40              |
| 5:1:73:PHE:CD2    | 5:1:78:LYS:HB2    | 2.56                     | 0.40              |
| 6:3:616:LEU:O     | 6:3:620:ARG:HG2   | 2.21                     | 0.40              |
| 7:9:71:ARG:NH2    | 10:7:38:ASN:O     | 2.55                     | 0.40              |
| 8:P:320:ARG:HD2   | 18:A:30:TYR:HA    | 2.03                     | 0.40              |
| 23:M:277:LEU:HD23 | 23:M:277:LEU:HA   | 1.89                     | 0.40              |
| 36:h:11:VAL:HG11  | 42:n:100:GLU:HA   | 2.02                     | 0.40              |
| 3:D:346:ILE:HG23  | 6:3:117:GLN:HG2   | 2.03                     | 0.40              |
| 6:3:136:ALA:HA    | 6:3:151:THR:HG23  | 2.03                     | 0.40              |
| 19:H:142:TYR:CZ   | 19:H:192:GLU:HA   | 2.56                     | 0.40              |
| 22:L:213:LEU:HD13 | 22:L:213:LEU:HA   | 1.93                     | 0.40              |
| 12:U:25:ILE:HD13  | 12:U:42:LEU:HD11  | 2.03                     | 0.40              |
| 3:D:202:ASP:OD1   | 3:D:203:LEU:N     | 2.49                     | 0.40              |
| 6:3:273:GLY:O     | 6:3:549:HIS:NE2   | 2.45                     | 0.40              |
| 14:W:98:VAL:HG21  | 18:A:44:THR:HA    | 2.02                     | 0.40              |
| 22:L:9:LEU:HD23   | 46:i:201:3PE:H2B1 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:M:210:TYR:HB2  | 23:M:268:GLY:HA3  | 2.04                     | 0.40              |
| 26:X:9:LEU:HD11   | 28:Z:84:GLN:HG3   | 2.03                     | 0.40              |
| 28:Z:119:LEU:HD11 | 33:e:68:ARG:HG3   | 2.02                     | 0.40              |
| 40:l:90:THR:HG22  | 41:m:10:LEU:HD23  | 2.03                     | 0.40              |
| 5:1:92:TYR:O      | 5:1:220:THR:HA    | 2.21                     | 0.40              |
| 6:3:297:GLU:HG3   | 14:W:125:TYR:CZ   | 2.56                     | 0.40              |
| 6:3:604:SER:O     | 6:3:607:ALA:C     | 2.64                     | 0.40              |
| 7:9:34:ARG:HH21   | 28:Z:27:ARG:HG2   | 1.86                     | 0.40              |
| 7:9:119:ILE:HG12  | 45:9:201:SF4:S3   | 2.61                     | 0.40              |
| 13:V:33:ILE:HD13  | 13:V:91:ARG:HG2   | 2.03                     | 0.40              |
| 20:J:91:PHE:CZ    | 46:K:201:3PE:H331 | 2.56                     | 0.40              |
| 22:L:54:PHE:CD1   | 22:L:58:ASN:HA    | 2.57                     | 0.40              |
| 23:M:314:MET:HA   | 23:M:454:ILE:HG22 | 2.02                     | 0.40              |
| 23:M:411:ILE:HA   | 23:M:411:ILE:HD13 | 1.87                     | 0.40              |
| 24:N:155:LEU:HA   | 24:N:155:LEU:HD13 | 1.88                     | 0.40              |
| 55:Y:401:CDL:H262 | 55:Y:401:CDL:H231 | 1.90                     | 0.40              |
| 40:l:64:ASP:OD1   | 41:m:43:LYS:NZ    | 2.43                     | 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   | 6     | 153/224 (68%) | 146 (95%) | 7 (5%)   | 0        | 100         | 100 |
| 2   | C     | 205/263 (78%) | 193 (94%) | 12 (6%)  | 0        | 100         | 100 |
| 3   | D     | 427/463 (92%) | 398 (93%) | 29 (7%)  | 0        | 100         | 100 |
| 4   | 2     | 212/248 (86%) | 189 (89%) | 23 (11%) | 0        | 100         | 100 |
| 5   | 1     | 428/464 (92%) | 399 (93%) | 29 (7%)  | 0        | 100         | 100 |
| 6   | 3     | 688/727 (95%) | 643 (94%) | 45 (6%)  | 0        | 100         | 100 |
| 7   | 9     | 176/212 (83%) | 173 (98%) | 3 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|----------|-------------|-----|
| 8   | P     | 340/377 (90%)  | 310 (91%)  | 30 (9%)  | 0        | 100         | 100 |
| 9   | Q     | 124/175 (71%)  | 119 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 10  | 7     | 94/116 (81%)   | 88 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 11  | S     | 82/99 (83%)    | 73 (89%)   | 9 (11%)  | 0        | 100         | 100 |
| 12  | T     | 77/156 (49%)   | 73 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 12  | U     | 86/156 (55%)   | 80 (93%)   | 6 (7%)   | 0        | 100         | 100 |
| 13  | V     | 110/116 (95%)  | 107 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 14  | W     | 112/131 (86%)  | 105 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 15  | q     | 143/145 (99%)  | 127 (89%)  | 16 (11%) | 0        | 100         | 100 |
| 16  | r     | 95/113 (84%)   | 91 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 17  | s     | 39/104 (38%)   | 38 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 18  | A     | 113/115 (98%)  | 105 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 19  | H     | 316/318 (99%)  | 299 (95%)  | 17 (5%)  | 0        | 100         | 100 |
| 20  | J     | 170/172 (99%)  | 160 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 21  | K     | 96/98 (98%)    | 93 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 22  | L     | 604/607 (100%) | 558 (92%)  | 46 (8%)  | 0        | 100         | 100 |
| 23  | M     | 457/459 (100%) | 439 (96%)  | 18 (4%)  | 0        | 100         | 100 |
| 24  | N     | 343/345 (99%)  | 330 (96%)  | 13 (4%)  | 0        | 100         | 100 |
| 25  | O     | 318/355 (90%)  | 295 (93%)  | 23 (7%)  | 0        | 100         | 100 |
| 26  | X     | 169/172 (98%)  | 158 (94%)  | 11 (6%)  | 0        | 100         | 100 |
| 27  | Y     | 138/141 (98%)  | 138 (100%) | 0        | 0        | 100         | 100 |
| 28  | Z     | 139/144 (96%)  | 134 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 29  | a     | 68/70 (97%)    | 67 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 30  | b     | 81/84 (96%)    | 77 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 31  | c     | 46/76 (60%)    | 45 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 32  | d     | 118/120 (98%)  | 113 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 33  | e     | 103/106 (97%)  | 91 (88%)   | 12 (12%) | 0        | 100         | 100 |
| 34  | f     | 51/57 (90%)    | 42 (82%)   | 9 (18%)  | 0        | 100         | 100 |
| 35  | g     | 99/151 (66%)   | 96 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 36  | h     | 137/189 (72%)  | 129 (94%)  | 8 (6%)   | 0        | 100         | 100 |
| 37  | i     | 94/128 (73%)   | 83 (88%)   | 11 (12%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 38  | j     | 62/105 (59%)    | 58 (94%)   | 4 (6%)   | 0        | 100         | 100 |
| 39  | k     | 75/104 (72%)    | 72 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 40  | l     | 155/186 (83%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 41  | m     | 124/129 (96%)   | 119 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 42  | n     | 176/179 (98%)   | 167 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 43  | o     | 116/137 (85%)   | 107 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| 44  | p     | 168/176 (96%)   | 161 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| All | All   | 8127/9212 (88%) | 7635 (94%) | 492 (6%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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   | 6     | 131/185 (71%) | 126 (96%) | 5 (4%)   | 29          | 63 |
| 2   | C     | 189/227 (83%) | 186 (98%) | 3 (2%)   | 55          | 79 |
| 3   | D     | 370/394 (94%) | 363 (98%) | 7 (2%)   | 50          | 76 |
| 4   | 2     | 184/206 (89%) | 176 (96%) | 8 (4%)   | 26          | 60 |
| 5   | 1     | 345/370 (93%) | 336 (97%) | 9 (3%)   | 40          | 72 |
| 6   | 3     | 580/610 (95%) | 566 (98%) | 14 (2%)  | 43          | 73 |
| 7   | 9     | 152/178 (85%) | 150 (99%) | 2 (1%)   | 61          | 81 |
| 8   | P     | 299/325 (92%) | 290 (97%) | 9 (3%)   | 36          | 69 |
| 9   | Q     | 113/153 (74%) | 109 (96%) | 4 (4%)   | 32          | 65 |
| 10  | 7     | 81/96 (84%)   | 79 (98%)  | 2 (2%)   | 42          | 72 |
| 11  | S     | 74/80 (92%)   | 72 (97%)  | 2 (3%)   | 39          | 71 |
| 12  | T     | 73/135 (54%)  | 69 (94%)  | 4 (6%)   | 19          | 53 |
| 12  | U     | 81/135 (60%)  | 79 (98%)  | 2 (2%)   | 42          | 72 |
| 13  | V     | 100/102 (98%) | 96 (96%)  | 4 (4%)   | 28          | 62 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 14  | W     | 108/114 (95%)  | 103 (95%)  | 5 (5%)   | 24          | 58  |
| 15  | q     | 131/131 (100%) | 128 (98%)  | 3 (2%)   | 44          | 74  |
| 16  | r     | 88/96 (92%)    | 87 (99%)   | 1 (1%)   | 65          | 83  |
| 17  | s     | 40/95 (42%)    | 39 (98%)   | 1 (2%)   | 42          | 72  |
| 18  | A     | 103/103 (100%) | 97 (94%)   | 6 (6%)   | 18          | 51  |
| 19  | H     | 279/279 (100%) | 272 (98%)  | 7 (2%)   | 42          | 72  |
| 20  | J     | 137/137 (100%) | 131 (96%)  | 6 (4%)   | 25          | 60  |
| 21  | K     | 87/87 (100%)   | 86 (99%)   | 1 (1%)   | 65          | 83  |
| 22  | L     | 548/549 (100%) | 530 (97%)  | 18 (3%)  | 33          | 67  |
| 23  | M     | 414/414 (100%) | 406 (98%)  | 8 (2%)   | 50          | 76  |
| 24  | N     | 307/307 (100%) | 293 (95%)  | 14 (5%)  | 24          | 58  |
| 25  | O     | 284/309 (92%)  | 278 (98%)  | 6 (2%)   | 47          | 75  |
| 26  | X     | 153/154 (99%)  | 146 (95%)  | 7 (5%)   | 24          | 58  |
| 27  | Y     | 105/106 (99%)  | 99 (94%)   | 6 (6%)   | 18          | 52  |
| 28  | Z     | 122/123 (99%)  | 119 (98%)  | 3 (2%)   | 42          | 72  |
| 29  | a     | 60/60 (100%)   | 60 (100%)  | 0        | 100         | 100 |
| 30  | b     | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 80  |
| 31  | c     | 42/67 (63%)    | 41 (98%)   | 1 (2%)   | 43          | 73  |
| 32  | d     | 107/107 (100%) | 105 (98%)  | 2 (2%)   | 50          | 76  |
| 33  | e     | 93/94 (99%)    | 90 (97%)   | 3 (3%)   | 34          | 67  |
| 34  | f     | 49/53 (92%)    | 47 (96%)   | 2 (4%)   | 27          | 61  |
| 35  | g     | 92/129 (71%)   | 90 (98%)   | 2 (2%)   | 45          | 74  |
| 36  | h     | 123/162 (76%)  | 121 (98%)  | 2 (2%)   | 55          | 79  |
| 37  | i     | 92/119 (77%)   | 85 (92%)   | 7 (8%)   | 12          | 41  |
| 38  | j     | 60/87 (69%)    | 58 (97%)   | 2 (3%)   | 33          | 67  |
| 39  | k     | 60/78 (77%)    | 58 (97%)   | 2 (3%)   | 33          | 67  |
| 40  | l     | 142/161 (88%)  | 139 (98%)  | 3 (2%)   | 47          | 75  |
| 41  | m     | 112/114 (98%)  | 111 (99%)  | 1 (1%)   | 70          | 85  |
| 42  | n     | 163/164 (99%)  | 163 (100%) | 0        | 100         | 100 |
| 43  | o     | 109/121 (90%)  | 107 (98%)  | 2 (2%)   | 51          | 77  |
| 44  | p     | 155/158 (98%)  | 153 (99%)  | 2 (1%)   | 61          | 81  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 7209/7947 (91%) | 7010 (97%) | 199 (3%) | 38 70       |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 64  | CYS  |
| 1   | 6     | 85  | VAL  |
| 1   | 6     | 95  | VAL  |
| 1   | 6     | 135 | TYR  |
| 1   | 6     | 154 | ILE  |
| 2   | C     | 17  | VAL  |
| 2   | C     | 45  | LEU  |
| 2   | C     | 169 | THR  |
| 3   | D     | 38  | ILE  |
| 3   | D     | 50  | ASN  |
| 3   | D     | 145 | THR  |
| 3   | D     | 325 | VAL  |
| 3   | D     | 326 | ASP  |
| 3   | D     | 413 | ASP  |
| 3   | D     | 414 | VAL  |
| 4   | 2     | 24  | THR  |
| 4   | 2     | 105 | THR  |
| 4   | 2     | 136 | LEU  |
| 4   | 2     | 138 | THR  |
| 4   | 2     | 164 | LEU  |
| 4   | 2     | 165 | THR  |
| 4   | 2     | 181 | VAL  |
| 4   | 2     | 202 | LEU  |
| 5   | 1     | 45  | THR  |
| 5   | 1     | 50  | LEU  |
| 5   | 1     | 94  | VAL  |
| 5   | 1     | 273 | SER  |
| 5   | 1     | 297 | VAL  |
| 5   | 1     | 327 | THR  |
| 5   | 1     | 359 | CYS  |
| 5   | 1     | 363 | THR  |
| 5   | 1     | 365 | CYS  |
| 6   | 3     | 13  | VAL  |
| 6   | 3     | 33  | VAL  |
| 6   | 3     | 35  | MET  |
| 6   | 3     | 103 | LEU  |
| 6   | 3     | 110 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 3     | 142 | ILE  |
| 6   | 3     | 158 | ARG  |
| 6   | 3     | 267 | THR  |
| 6   | 3     | 356 | THR  |
| 6   | 3     | 537 | LEU  |
| 6   | 3     | 540 | ASP  |
| 6   | 3     | 559 | VAL  |
| 6   | 3     | 583 | THR  |
| 6   | 3     | 667 | THR  |
| 7   | 9     | 14  | VAL  |
| 7   | 9     | 96  | ILE  |
| 8   | P     | 5   | VAL  |
| 8   | P     | 19  | VAL  |
| 8   | P     | 65  | LEU  |
| 8   | P     | 71  | LEU  |
| 8   | P     | 123 | GLU  |
| 8   | P     | 126 | VAL  |
| 8   | P     | 207 | VAL  |
| 8   | P     | 224 | VAL  |
| 8   | P     | 254 | ILE  |
| 9   | Q     | 10  | LEU  |
| 9   | Q     | 44  | ASN  |
| 9   | Q     | 81  | ASN  |
| 9   | Q     | 105 | VAL  |
| 10  | 7     | 16  | GLN  |
| 10  | 7     | 87  | CYS  |
| 11  | S     | 37  | VAL  |
| 11  | S     | 79  | ASN  |
| 12  | T     | 16  | LEU  |
| 12  | T     | 19  | LEU  |
| 12  | T     | 40  | LEU  |
| 12  | T     | 75  | GLU  |
| 13  | V     | 18  | THR  |
| 13  | V     | 58  | VAL  |
| 13  | V     | 93  | MET  |
| 13  | V     | 103 | VAL  |
| 14  | W     | 55  | ASP  |
| 14  | W     | 75  | VAL  |
| 14  | W     | 96  | ILE  |
| 14  | W     | 98  | VAL  |
| 14  | W     | 121 | LEU  |
| 15  | q     | 94  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | q     | 127 | TYR  |
| 15  | q     | 138 | VAL  |
| 16  | r     | 23  | LEU  |
| 17  | s     | 42  | THR  |
| 18  | A     | 19  | LEU  |
| 18  | A     | 67  | LEU  |
| 18  | A     | 68  | GLU  |
| 18  | A     | 86  | THR  |
| 18  | A     | 98  | LEU  |
| 18  | A     | 111 | LEU  |
| 19  | H     | 17  | MET  |
| 19  | H     | 62  | ARG  |
| 19  | H     | 102 | ILE  |
| 19  | H     | 172 | MET  |
| 19  | H     | 254 | LEU  |
| 19  | H     | 297 | THR  |
| 19  | H     | 318 | MET  |
| 20  | J     | 58  | ILE  |
| 20  | J     | 64  | LEU  |
| 20  | J     | 81  | THR  |
| 20  | J     | 89  | LEU  |
| 20  | J     | 131 | VAL  |
| 20  | J     | 151 | MET  |
| 21  | K     | 93  | LEU  |
| 22  | L     | 10  | LEU  |
| 22  | L     | 69  | VAL  |
| 22  | L     | 82  | THR  |
| 22  | L     | 137 | MET  |
| 22  | L     | 190 | SER  |
| 22  | L     | 249 | SER  |
| 22  | L     | 254 | VAL  |
| 22  | L     | 293 | LEU  |
| 22  | L     | 338 | MET  |
| 22  | L     | 363 | THR  |
| 22  | L     | 370 | SER  |
| 22  | L     | 472 | ILE  |
| 22  | L     | 489 | THR  |
| 22  | L     | 511 | LEU  |
| 22  | L     | 517 | ASN  |
| 22  | L     | 551 | THR  |
| 22  | L     | 562 | ILE  |
| 22  | L     | 577 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | M     | 72  | LEU  |
| 23  | M     | 138 | ASN  |
| 23  | M     | 166 | LEU  |
| 23  | M     | 173 | THR  |
| 23  | M     | 205 | ILE  |
| 23  | M     | 214 | LEU  |
| 23  | M     | 229 | MET  |
| 23  | M     | 414 | THR  |
| 24  | N     | 40  | ILE  |
| 24  | N     | 95  | LEU  |
| 24  | N     | 108 | LEU  |
| 24  | N     | 122 | ILE  |
| 24  | N     | 126 | MET  |
| 24  | N     | 155 | LEU  |
| 24  | N     | 173 | THR  |
| 24  | N     | 193 | ILE  |
| 24  | N     | 201 | THR  |
| 24  | N     | 232 | LEU  |
| 24  | N     | 244 | ILE  |
| 24  | N     | 257 | LEU  |
| 24  | N     | 275 | CYS  |
| 24  | N     | 287 | LEU  |
| 25  | O     | 41  | GLU  |
| 25  | O     | 63  | THR  |
| 25  | O     | 174 | VAL  |
| 25  | O     | 263 | VAL  |
| 25  | O     | 279 | LEU  |
| 25  | O     | 290 | SER  |
| 12  | U     | 32  | VAL  |
| 12  | U     | 75  | GLU  |
| 26  | X     | 6   | LEU  |
| 26  | X     | 23  | VAL  |
| 26  | X     | 35  | CYS  |
| 26  | X     | 47  | TRP  |
| 26  | X     | 77  | CYS  |
| 26  | X     | 94  | GLN  |
| 26  | X     | 109 | CYS  |
| 27  | Y     | 42  | LEU  |
| 27  | Y     | 49  | LEU  |
| 27  | Y     | 82  | LYS  |
| 27  | Y     | 87  | LEU  |
| 27  | Y     | 104 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | Y     | 106 | SER  |
| 28  | Z     | 95  | ILE  |
| 28  | Z     | 96  | ILE  |
| 28  | Z     | 100 | VAL  |
| 30  | b     | 62  | MET  |
| 31  | c     | 4   | VAL  |
| 32  | d     | 34  | MET  |
| 32  | d     | 119 | VAL  |
| 33  | e     | 27  | LYS  |
| 33  | e     | 54  | GLU  |
| 33  | e     | 67  | LEU  |
| 34  | f     | 34  | LEU  |
| 34  | f     | 35  | THR  |
| 35  | g     | 103 | LEU  |
| 35  | g     | 105 | ILE  |
| 36  | h     | 10  | VAL  |
| 36  | h     | 117 | ARG  |
| 37  | i     | 4   | THR  |
| 37  | i     | 34  | LEU  |
| 37  | i     | 78  | MET  |
| 37  | i     | 95  | THR  |
| 37  | i     | 98  | SER  |
| 37  | i     | 110 | LEU  |
| 37  | i     | 115 | VAL  |
| 38  | j     | 32  | MET  |
| 38  | j     | 47  | VAL  |
| 39  | k     | 32  | THR  |
| 39  | k     | 73  | LEU  |
| 40  | l     | 7   | MET  |
| 40  | l     | 49  | LEU  |
| 40  | l     | 120 | VAL  |
| 41  | m     | 24  | VAL  |
| 43  | o     | 14  | VAL  |
| 43  | o     | 107 | LEU  |
| 44  | p     | 16  | THR  |
| 44  | p     | 49  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 127 | ASN  |
| 4   | 2     | 101 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | 1     | 200 | GLN  |
| 5   | 1     | 356 | HIS  |
| 5   | 1     | 361 | GLN  |
| 6   | 3     | 7   | ASN  |
| 6   | 3     | 237 | ASN  |
| 6   | 3     | 402 | ASN  |
| 6   | 3     | 581 | GLN  |
| 8   | P     | 93  | ASN  |
| 8   | P     | 136 | ASN  |
| 9   | Q     | 29  | HIS  |
| 10  | 7     | 36  | ASN  |
| 10  | 7     | 50  | ASN  |
| 12  | T     | 74  | GLN  |
| 13  | V     | 40  | HIS  |
| 15  | q     | 72  | ASN  |
| 15  | q     | 112 | ASN  |
| 15  | q     | 113 | HIS  |
| 18  | A     | 10  | ASN  |
| 18  | A     | 28  | ASN  |
| 19  | H     | 93  | HIS  |
| 19  | H     | 258 | ASN  |
| 19  | H     | 292 | ASN  |
| 22  | L     | 58  | ASN  |
| 22  | L     | 209 | ASN  |
| 22  | L     | 361 | ASN  |
| 22  | L     | 444 | ASN  |
| 22  | L     | 572 | ASN  |
| 23  | M     | 169 | ASN  |
| 24  | N     | 197 | ASN  |
| 24  | N     | 274 | ASN  |
| 24  | N     | 342 | GLN  |
| 25  | O     | 30  | ASN  |
| 25  | O     | 57  | GLN  |
| 25  | O     | 141 | GLN  |
| 25  | O     | 200 | GLN  |
| 25  | O     | 271 | ASN  |
| 27  | Y     | 9   | HIS  |
| 27  | Y     | 88  | ASN  |
| 28  | Z     | 75  | GLN  |
| 30  | b     | 51  | ASN  |
| 30  | b     | 82  | ASN  |
| 34  | f     | 13  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | g     | 25  | GLN  |
| 35  | g     | 101 | ASN  |
| 36  | h     | 78  | ASN  |
| 36  | h     | 135 | HIS  |
| 36  | h     | 143 | ASN  |
| 37  | i     | 25  | GLN  |
| 40  | l     | 54  | GLN  |
| 40  | l     | 154 | HIS  |
| 43  | o     | 43  | GLN  |
| 43  | o     | 54  | GLN  |
| 43  | o     | 84  | HIS  |
| 44  | p     | 54  | GLN  |
| 44  | p     | 123 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues 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 |
| 37  | SAC  | i     | 1   | 37   | 7,8,9        | 1.02 | 1 (14%)  | 7,9,11      | 2.36 | 3 (42%)  |
| 30  | AYA  | b     | 1   | 30   | 6,7,8        | 1.25 | 1 (16%)  | 6,8,10      | 1.31 | 1 (16%)  |
| 18  | FME  | A     | 1   | 18   | 8,9,10       | 1.02 | 1 (12%)  | 8,9,11      | 0.89 | 0        |
| 23  | FME  | M     | 1   | 23   | 8,9,10       | 1.02 | 0        | 8,9,11      | 0.71 | 0        |
| 19  | FME  | H     | 1   | 19   | 8,9,10       | 0.99 | 0        | 8,9,11      | 0.91 | 0        |
| 16  | AYA  | r     | 1   | 16   | 6,7,8        | 1.33 | 1 (16%)  | 6,8,10      | 1.20 | 1 (16%)  |
| 21  | FME  | K     | 1   | 21   | 8,9,10       | 0.98 | 0        | 8,9,11      | 1.71 | 2 (25%)  |
| 22  | FME  | L     | 1   | 22   | 8,9,10       | 0.95 | 0        | 8,9,11      | 1.05 | 1 (12%)  |
| 3   | 2MR  | D     | 85  | 3    | 10,12,13     | 2.01 | 1 (10%)  | 5,13,15     | 7.20 | 3 (60%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 24  | FME  | N     | 1   | 24   | 8,9,10       | 0.99 | 0        | 8,9,11      | 0.90 | 0        |
| 20  | FME  | J     | 1   | 20   | 8,9,10       | 0.98 | 0        | 8,9,11      | 0.88 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 37  | SAC  | i     | 1   | 37   | -       | 6/7/8/10   | -     |
| 30  | AYA  | b     | 1   | 30   | -       | 1/5/6/8    | -     |
| 18  | FME  | A     | 1   | 18   | -       | 1/7/9/11   | -     |
| 23  | FME  | M     | 1   | 23   | -       | 2/7/9/11   | -     |
| 19  | FME  | H     | 1   | 19   | -       | 2/7/9/11   | -     |
| 16  | AYA  | r     | 1   | 16   | -       | 1/5/6/8    | -     |
| 21  | FME  | K     | 1   | 21   | -       | 4/7/9/11   | -     |
| 22  | FME  | L     | 1   | 22   | -       | 4/7/9/11   | -     |
| 3   | 2MR  | D     | 85  | 3    | -       | 5/10/13/15 | -     |
| 24  | FME  | N     | 1   | 24   | -       | 3/7/9/11   | -     |
| 20  | FME  | J     | 1   | 20   | -       | 0/7/9/11   | -     |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | D     | 85  | 2MR  | CZ-NE | 5.70  | 1.46        | 1.34     |
| 16  | r     | 1   | AYA  | CA-N  | -2.67 | 1.43        | 1.46     |
| 30  | b     | 1   | AYA  | CA-N  | -2.26 | 1.44        | 1.46     |
| 18  | A     | 1   | FME  | CA-N  | -2.01 | 1.43        | 1.46     |
| 37  | i     | 1   | SAC  | C1A-N | 2.01  | 1.40        | 1.34     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | D     | 85  | 2MR  | NE-CZ-NH2  | 14.60 | 132.86      | 119.48   |
| 3   | D     | 85  | 2MR  | CQ2-NH2-CZ | 4.72  | 133.79      | 123.65   |
| 3   | D     | 85  | 2MR  | CD-NE-CZ   | 4.52  | 131.85      | 123.36   |
| 37  | i     | 1   | SAC  | C2A-C1A-N  | 4.38  | 123.38      | 116.12   |
| 21  | K     | 1   | FME  | C-CA-N     | 3.85  | 116.93      | 109.50   |
| 30  | b     | 1   | AYA  | CB-CA-N    | 2.86  | 112.91      | 109.68   |
| 16  | r     | 1   | AYA  | CB-CA-N    | 2.81  | 112.86      | 109.68   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 37  | i     | 1   | SAC  | OAC-C1A-N | -2.33 | 117.86      | 121.98   |
| 37  | i     | 1   | SAC  | C-CA-N    | 2.32  | 113.98      | 109.50   |
| 21  | K     | 1   | FME  | O-C-CA    | -2.24 | 119.00      | 124.77   |
| 22  | L     | 1   | FME  | C-CA-N    | 2.15  | 113.64      | 109.50   |

There are no chirality outliers.

All (29) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 3   | D     | 85  | 2MR  | O-C-CA-CB    |
| 16  | r     | 1   | AYA  | O-C-CA-CB    |
| 19  | H     | 1   | FME  | N-CA-CB-CG   |
| 21  | K     | 1   | FME  | O1-CN-N-CA   |
| 22  | L     | 1   | FME  | CB-CA-N-CN   |
| 22  | L     | 1   | FME  | C-CA-CB-CG   |
| 23  | M     | 1   | FME  | O-C-CA-CB    |
| 24  | N     | 1   | FME  | C-CA-CB-CG   |
| 24  | N     | 1   | FME  | O-C-CA-CB    |
| 37  | i     | 1   | SAC  | O-C-CA-CB    |
| 37  | i     | 1   | SAC  | N-CA-CB-OG   |
| 37  | i     | 1   | SAC  | C-CA-CB-OG   |
| 3   | D     | 85  | 2MR  | NE-CD-CG-CB  |
| 37  | i     | 1   | SAC  | C2A-C1A-N-CA |
| 37  | i     | 1   | SAC  | OAC-C1A-N-CA |
| 21  | K     | 1   | FME  | CA-CB-CG-SD  |
| 18  | A     | 1   | FME  | N-CA-CB-CG   |
| 22  | L     | 1   | FME  | N-CA-CB-CG   |
| 24  | N     | 1   | FME  | N-CA-CB-CG   |
| 21  | K     | 1   | FME  | CB-CG-SD-CE  |
| 21  | K     | 1   | FME  | N-CA-CB-CG   |
| 3   | D     | 85  | 2MR  | CA-CB-CG-CD  |
| 30  | b     | 1   | AYA  | C-CA-N-CT    |
| 22  | L     | 1   | FME  | CB-CG-SD-CE  |
| 23  | M     | 1   | FME  | N-CA-CB-CG   |
| 3   | D     | 85  | 2MR  | N-CA-CB-CG   |
| 37  | i     | 1   | SAC  | C-CA-N-C1A   |
| 19  | H     | 1   | FME  | C-CA-CB-CG   |
| 3   | D     | 85  | 2MR  | C-CA-CB-CG   |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 21  | K     | 1   | FME  | 1       | 0            |
| 3   | D     | 85  | 2MR  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 50  | FMN  | 1     | 501 | -    | 33,33,33     | 0.39 | 0           | 48,50,50    | 0.43 | 0           |
| 46  | 3PE  | h     | 202 | -    | 50,50,50     | 0.30 | 0           | 53,55,55    | 0.27 | 0           |
| 49  | FES  | 2     | 301 | 4    | 0,4,4        | -    | -           | -           |      |             |
| 45  | SF4  | 9     | 201 | 7    | 0,12,12      | -    | -           | -           |      |             |
| 55  | CDL  | h     | 201 | -    | 69,69,99     | 0.35 | 0           | 75,81,111   | 0.43 | 0           |
| 55  | CDL  | d     | 201 | -    | 66,66,99     | 0.36 | 0           | 72,78,111   | 0.36 | 0           |
| 47  | PC1  | Z     | 402 | -    | 46,46,53     | 0.31 | 0           | 52,54,61    | 0.34 | 0           |
| 46  | 3PE  | 6     | 202 | -    | 31,31,50     | 0.37 | 0           | 34,36,55    | 0.35 | 0           |
| 49  | FES  | 3     | 803 | 6    | 0,4,4        | -    | -           | -           |      |             |
| 46  | 3PE  | d     | 202 | -    | 30,30,50     | 0.38 | 0           | 33,35,55    | 0.37 | 0           |
| 48  | UQ   | D     | 501 | -    | 63,63,63     | 0.26 | 0           | 78,79,79    | 0.54 | 1 (1%)      |
| 45  | SF4  | 3     | 802 | 6    | 0,12,12      | -    | -           | -           |      |             |
| 46  | 3PE  | K     | 201 | -    | 40,40,50     | 0.33 | 0           | 43,45,55    | 0.32 | 0           |
| 47  | PC1  | 6     | 203 | -    | 42,42,53     | 0.34 | 0           | 48,50,61    | 0.49 | 0           |
| 55  | CDL  | N     | 401 | -    | 89,89,99     | 0.31 | 0           | 95,101,111  | 0.41 | 0           |
| 46  | 3PE  | M     | 502 | -    | 50,50,50     | 0.30 | 0           | 53,55,55    | 0.32 | 0           |
| 56  | DGT  | O     | 401 | 57   | 32,33,33     | 0.32 | 0           | 48,52,52    | 0.31 | 0           |
| 45  | SF4  | 3     | 801 | 6    | 0,12,12      | -    | -           | -           |      |             |
| 46  | 3PE  | Y     | 402 | -    | 27,27,50     | 0.40 | 0           | 30,32,55    | 0.38 | 0           |
| 46  | 3PE  | A     | 201 | -    | 42,42,50     | 0.33 | 0           | 45,47,55    | 0.33 | 0           |
| 46  | 3PE  | i     | 201 | -    | 41,41,50     | 0.32 | 0           | 44,46,55    | 0.31 | 0           |
| 45  | SF4  | 1     | 502 | 5    | 0,12,12      | -    | -           | -           |      |             |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | 3PE  | M     | 503 | -    | 35,35,50     | 0.35 | 0        | 38,40,55    | 0.30 | 0        |
| 46  | 3PE  | Z     | 401 | -    | 50,50,50     | 0.31 | 0        | 53,55,55    | 0.48 | 1 (1%)   |
| 46  | 3PE  | m     | 202 | -    | 29,29,50     | 0.39 | 0        | 32,34,55    | 0.33 | 0        |
| 47  | PC1  | 9     | 203 | -    | 53,53,53     | 0.30 | 0        | 59,61,61    | 0.45 | 0        |
| 55  | CDL  | Y     | 403 | -    | 56,56,99     | 0.39 | 0        | 62,68,111   | 0.47 | 1 (1%)   |
| 46  | 3PE  | L     | 701 | -    | 50,50,50     | 0.31 | 0        | 53,55,55    | 0.47 | 0        |
| 55  | CDL  | Y     | 401 | -    | 93,93,99     | 0.30 | 0        | 99,105,111  | 0.29 | 0        |
| 46  | 3PE  | D     | 502 | -    | 50,50,50     | 0.30 | 0        | 53,55,55    | 0.37 | 0        |
| 45  | SF4  | 9     | 202 | 7    | 0,12,12      | -    | -        | -           | -    | -        |
| 47  | PC1  | M     | 501 | -    | 53,53,53     | 0.29 | 0        | 59,61,61    | 0.39 | 0        |
| 54  | ZMP  | n     | 201 | -    | 26,31,36     | 0.72 | 1 (3%)   | 30,38,45    | 0.93 | 1 (3%)   |
| 54  | ZMP  | W     | 201 | -    | 28,33,36     | 0.60 | 0        | 32,40,45    | 1.19 | 3 (9%)   |
| 45  | SF4  | 6     | 201 | 1    | 0,12,12      | -    | -        | -           | -    | -        |
| 46  | 3PE  | L     | 704 | -    | 41,41,50     | 0.32 | 0        | 44,46,55    | 0.37 | 0        |
| 55  | CDL  | L     | 702 | -    | 77,77,99     | 0.34 | 0        | 83,89,111   | 0.33 | 0        |
| 47  | PC1  | H     | 401 | -    | 41,41,53     | 0.33 | 0        | 47,49,61    | 0.34 | 0        |
| 55  | CDL  | L     | 703 | -    | 45,45,99     | 0.43 | 0        | 51,57,111   | 0.34 | 0        |
| 52  | NDP  | P     | 501 | -    | 51,52,52     | 0.39 | 0        | 71,80,80    | 0.46 | 0        |
| 55  | CDL  | m     | 201 | -    | 71,71,99     | 0.35 | 0        | 77,83,111   | 0.44 | 1 (1%)   |
| 55  | CDL  | r     | 201 | -    | 56,56,99     | 0.40 | 0        | 62,68,111   | 0.59 | 1 (1%)   |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 50  | FMN  | 1     | 501 | -    | -       | 5/18/18/18   | 0/3/3/3 |
| 46  | 3PE  | h     | 202 | -    | -       | 8/54/54/54   | -       |
| 55  | CDL  | h     | 201 | -    | -       | 18/80/80/110 | -       |
| 45  | SF4  | 9     | 201 | 7    | -       | -            | 0/6/5/5 |
| 49  | FES  | 2     | 301 | 4    | -       | -            | 0/1/1/1 |
| 55  | CDL  | d     | 201 | -    | -       | 21/77/77/110 | -       |
| 47  | PC1  | Z     | 402 | -    | -       | 9/50/50/57   | -       |
| 46  | 3PE  | 6     | 202 | -    | -       | 6/35/35/54   | -       |
| 49  | FES  | 3     | 803 | 6    | -       | -            | 0/1/1/1 |
| 46  | 3PE  | d     | 202 | -    | -       | 7/34/34/54   | -       |
| 48  | UQ   | D     | 501 | -    | -       | 21/63/87/87  | 0/1/1/1 |
| 45  | SF4  | 3     | 802 | 6    | -       | -            | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 46  | 3PE  | K     | 201 | -    | -       | 7/44/44/54     | -       |
| 47  | PC1  | 6     | 203 | -    | -       | 8/46/46/57     | -       |
| 55  | CDL  | N     | 401 | -    | -       | 19/100/100/110 | -       |
| 46  | 3PE  | M     | 502 | -    | -       | 12/54/54/54    | -       |
| 56  | DGT  | O     | 401 | 57   | -       | 8/22/34/34     | 0/3/3/3 |
| 45  | SF4  | 3     | 801 | 6    | -       | -              | 0/6/5/5 |
| 46  | 3PE  | Y     | 402 | -    | -       | 6/31/31/54     | -       |
| 46  | 3PE  | A     | 201 | -    | -       | 11/46/46/54    | -       |
| 46  | 3PE  | i     | 201 | -    | -       | 4/45/45/54     | -       |
| 45  | SF4  | 1     | 502 | 5    | -       | -              | 0/6/5/5 |
| 46  | 3PE  | M     | 503 | -    | -       | 6/39/39/54     | -       |
| 46  | 3PE  | Z     | 401 | -    | -       | 13/54/54/54    | -       |
| 46  | 3PE  | m     | 202 | -    | -       | 2/33/33/54     | -       |
| 47  | PC1  | 9     | 203 | -    | -       | 12/57/57/57    | -       |
| 55  | CDL  | Y     | 403 | -    | -       | 18/67/67/110   | -       |
| 46  | 3PE  | L     | 701 | -    | -       | 10/54/54/54    | -       |
| 55  | CDL  | Y     | 401 | -    | -       | 16/104/104/110 | -       |
| 46  | 3PE  | D     | 502 | -    | -       | 15/54/54/54    | -       |
| 45  | SF4  | 9     | 202 | 7    | -       | -              | 0/6/5/5 |
| 47  | PC1  | M     | 501 | -    | -       | 11/57/57/57    | -       |
| 54  | ZMP  | n     | 201 | -    | -       | 19/36/38/43    | -       |
| 54  | ZMP  | W     | 201 | -    | -       | 11/38/40/43    | -       |
| 45  | SF4  | 6     | 201 | 1    | -       | -              | 0/6/5/5 |
| 46  | 3PE  | L     | 704 | -    | -       | 5/45/45/54     | -       |
| 55  | CDL  | L     | 702 | -    | -       | 18/88/88/110   | -       |
| 47  | PC1  | H     | 401 | -    | -       | 8/45/45/57     | -       |
| 55  | CDL  | L     | 703 | -    | -       | 9/56/56/110    | -       |
| 52  | NDP  | P     | 501 | -    | -       | 3/34/77/77     | 0/5/5/5 |
| 55  | CDL  | m     | 201 | -    | -       | 17/82/82/110   | -       |
| 55  | CDL  | r     | 201 | -    | -       | 15/67/67/110   | -       |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 54  | n     | 201 | ZMP  | C9-C10 | 2.38 | 1.53        | 1.50     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 54  | W     | 201 | ZMP  | O1-C10-C9   | -3.13 | 120.37      | 123.98   |
| 48  | D     | 501 | UQ   | C7-C6-C1    | -2.62 | 115.47      | 118.52   |
| 54  | n     | 201 | ZMP  | O1-C10-C9   | -2.58 | 121.01      | 123.98   |
| 54  | W     | 201 | ZMP  | C15-C14-C13 | -2.53 | 108.18      | 112.39   |
| 54  | W     | 201 | ZMP  | C9-C10-S1   | 2.29  | 116.14      | 113.40   |
| 55  | r     | 201 | CDL  | CA4-OA6-CA5 | 2.24  | 123.16      | 117.80   |
| 55  | Y     | 403 | CDL  | CA4-OA6-CA5 | 2.08  | 122.77      | 117.80   |
| 55  | m     | 201 | CDL  | CA4-OA6-CA5 | 2.03  | 122.66      | 117.80   |
| 46  | Z     | 401 | 3PE  | C2-O21-C21  | 2.02  | 122.64      | 117.80   |

There are no chirality outliers.

All (378) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 46  | 6     | 202 | 3PE  | C11-O13-P-O11 |
| 46  | 6     | 202 | 3PE  | C11-O13-P-O14 |
| 46  | 6     | 202 | 3PE  | O13-C11-C12-N |
| 46  | D     | 502 | 3PE  | C1-O11-P-O12  |
| 46  | D     | 502 | 3PE  | C1-O11-P-O13  |
| 46  | D     | 502 | 3PE  | C1-O11-P-O14  |
| 46  | D     | 502 | 3PE  | C11-O13-P-O11 |
| 46  | D     | 502 | 3PE  | C11-O13-P-O12 |
| 46  | D     | 502 | 3PE  | C11-O13-P-O14 |
| 46  | D     | 502 | 3PE  | O13-C11-C12-N |
| 46  | A     | 201 | 3PE  | C11-O13-P-O11 |
| 46  | A     | 201 | 3PE  | C11-O13-P-O12 |
| 46  | A     | 201 | 3PE  | C11-O13-P-O14 |
| 46  | A     | 201 | 3PE  | O13-C11-C12-N |
| 46  | K     | 201 | 3PE  | C1-O11-P-O13  |
| 46  | K     | 201 | 3PE  | C11-O13-P-O11 |
| 46  | K     | 201 | 3PE  | O13-C11-C12-N |
| 46  | L     | 701 | 3PE  | C1-O11-P-O13  |
| 46  | L     | 701 | 3PE  | C1-O11-P-O14  |
| 46  | L     | 701 | 3PE  | C11-O13-P-O11 |
| 46  | L     | 701 | 3PE  | C11-O13-P-O12 |
| 46  | L     | 701 | 3PE  | C11-O13-P-O14 |
| 46  | L     | 701 | 3PE  | O13-C11-C12-N |
| 46  | L     | 704 | 3PE  | C1-O11-P-O12  |
| 46  | L     | 704 | 3PE  | C11-O13-P-O12 |
| 46  | L     | 704 | 3PE  | O13-C11-C12-N |
| 46  | M     | 502 | 3PE  | C11-O13-P-O11 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | M     | 502 | 3PE  | C11-O13-P-O12   |
| 46  | M     | 503 | 3PE  | C1-O11-P-O13    |
| 46  | M     | 503 | 3PE  | C1-O11-P-O14    |
| 46  | M     | 503 | 3PE  | O13-C11-C12-N   |
| 46  | Y     | 402 | 3PE  | C1-O11-P-O12    |
| 46  | Y     | 402 | 3PE  | C1-O11-P-O13    |
| 46  | Y     | 402 | 3PE  | O13-C11-C12-N   |
| 46  | Z     | 401 | 3PE  | C11-O13-P-O12   |
| 46  | Z     | 401 | 3PE  | O13-C11-C12-N   |
| 46  | d     | 202 | 3PE  | C11-O13-P-O11   |
| 46  | d     | 202 | 3PE  | C11-O13-P-O12   |
| 46  | d     | 202 | 3PE  | C11-O13-P-O14   |
| 46  | d     | 202 | 3PE  | O13-C11-C12-N   |
| 46  | h     | 202 | 3PE  | C1-O11-P-O14    |
| 46  | h     | 202 | 3PE  | C11-O13-P-O14   |
| 46  | h     | 202 | 3PE  | O13-C11-C12-N   |
| 46  | i     | 201 | 3PE  | O13-C11-C12-N   |
| 47  | 6     | 203 | PC1  | C1-O11-P-O12    |
| 47  | 6     | 203 | PC1  | C1-O11-P-O14    |
| 47  | 6     | 203 | PC1  | C1-O11-P-O13    |
| 47  | 9     | 203 | PC1  | C11-O13-P-O14   |
| 47  | 9     | 203 | PC1  | C1-O11-P-O14    |
| 47  | 9     | 203 | PC1  | C1-O11-P-O13    |
| 47  | 9     | 203 | PC1  | O13-C11-C12-N   |
| 47  | M     | 501 | PC1  | C11-O13-P-O12   |
| 47  | M     | 501 | PC1  | C11-O13-P-O11   |
| 47  | Z     | 402 | PC1  | C11-O13-P-O12   |
| 47  | Z     | 402 | PC1  | C11-O13-P-O11   |
| 48  | D     | 501 | UQ   | C14-C16-C17-C18 |
| 50  | 1     | 501 | FMN  | N10-C1'-C2'-O2' |
| 50  | 1     | 501 | FMN  | N10-C1'-C2'-C3' |
| 54  | W     | 201 | ZMP  | C19-C18-C21-O5  |
| 54  | W     | 201 | ZMP  | C20-C18-C21-O5  |
| 54  | W     | 201 | ZMP  | C17-C18-C21-O5  |
| 54  | W     | 201 | ZMP  | S1-C11-C12-N1   |
| 54  | W     | 201 | ZMP  | C12-C11-S1-C10  |
| 54  | W     | 201 | ZMP  | C7-C8-C9-C10    |
| 54  | n     | 201 | ZMP  | C19-C18-C21-O5  |
| 54  | n     | 201 | ZMP  | C20-C18-C21-O5  |
| 54  | n     | 201 | ZMP  | C17-C18-C21-O5  |
| 54  | n     | 201 | ZMP  | O4-C17-C18-C21  |
| 54  | n     | 201 | ZMP  | C16-C17-C18-C21 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | n     | 201 | ZMP  | O4-C17-C18-C19  |
| 54  | n     | 201 | ZMP  | C16-C17-C18-C20 |
| 54  | n     | 201 | ZMP  | O3-C16-C17-O4   |
| 54  | n     | 201 | ZMP  | C17-C16-N2-C15  |
| 54  | n     | 201 | ZMP  | O1-C10-S1-C11   |
| 54  | n     | 201 | ZMP  | C9-C10-S1-C11   |
| 54  | n     | 201 | ZMP  | C7-C8-C9-C10    |
| 55  | r     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | r     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | r     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | r     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | r     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | r     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | r     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | r     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | r     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | r     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | r     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | L     | 702 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | L     | 702 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | L     | 702 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | L     | 702 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | L     | 702 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | L     | 702 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | L     | 702 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | L     | 702 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | L     | 702 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | L     | 702 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | L     | 703 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | L     | 703 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | L     | 703 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | L     | 703 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | L     | 703 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | N     | 401 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | N     | 401 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | N     | 401 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | N     | 401 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | Y     | 401 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | Y     | 401 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | Y     | 401 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | Y     | 401 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | Y     | 403 | CDL  | CA3-OA5-PA1-OA2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | Y     | 403 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | Y     | 403 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | Y     | 403 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | d     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | d     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | d     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | d     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | d     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | d     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | h     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | h     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | h     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | h     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | h     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | h     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | h     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | m     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | m     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | m     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | m     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | m     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | m     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | O     | 401 | DGT  | PB-O3B-PG-O1G   |
| 56  | O     | 401 | DGT  | C5'-O5'-PA-O1A  |
| 48  | D     | 501 | UQ   | C45-C44-C46-C47 |
| 48  | D     | 501 | UQ   | C43-C44-C46-C47 |
| 54  | n     | 201 | ZMP  | O3-C16-N2-C15   |
| 48  | D     | 501 | UQ   | C9-C11-C12-C13  |
| 48  | D     | 501 | UQ   | C24-C26-C27-C28 |
| 48  | D     | 501 | UQ   | C39-C41-C42-C43 |
| 48  | D     | 501 | UQ   | C49-C51-C52-C53 |
| 48  | D     | 501 | UQ   | C12-C11-C9-C10  |
| 55  | d     | 201 | CDL  | O1-C1-CB2-OB2   |
| 55  | m     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 46  | Z     | 401 | 3PE  | C31-C32-C33-C34 |
| 47  | 6     | 203 | PC1  | C11-C12-N-C14   |
| 46  | M     | 503 | 3PE  | C2-C1-O11-P     |
| 47  | H     | 401 | PC1  | C21-C22-C23-C24 |
| 47  | M     | 501 | PC1  | C28-C29-C2A-C2B |
| 47  | H     | 401 | PC1  | C38-C39-C3A-C3B |
| 55  | N     | 401 | CDL  | C81-C82-C83-C84 |
| 46  | L     | 701 | 3PE  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | Z     | 402 | PC1  | C33-C34-C35-C36 |
| 46  | h     | 202 | 3PE  | C35-C36-C37-C38 |
| 46  | M     | 502 | 3PE  | C23-C24-C25-C26 |
| 47  | 6     | 203 | PC1  | C11-C12-N-C13   |
| 47  | 6     | 203 | PC1  | C11-C12-N-C15   |
| 48  | D     | 501 | UQ   | C12-C11-C9-C8   |
| 46  | A     | 201 | 3PE  | C39-C3A-C3B-C3C |
| 54  | n     | 201 | ZMP  | C6-C7-C8-C9     |
| 47  | 6     | 203 | PC1  | C3C-C3D-C3E-C3F |
| 47  | H     | 401 | PC1  | O21-C2-C3-O31   |
| 46  | M     | 502 | 3PE  | C36-C37-C38-C39 |
| 55  | N     | 401 | CDL  | OB5-CB3-CB4-CB6 |
| 46  | D     | 502 | 3PE  | C31-C32-C33-C34 |
| 47  | M     | 501 | PC1  | C37-C38-C39-C3A |
| 46  | D     | 502 | 3PE  | C1-C2-C3-O31    |
| 55  | N     | 401 | CDL  | CA3-CA4-CA6-OA8 |
| 50  | 1     | 501 | FMN  | C5'-O5'-P-O1P   |
| 55  | Y     | 401 | CDL  | C82-C83-C84-C85 |
| 55  | N     | 401 | CDL  | OA6-CA4-CA6-OA8 |
| 47  | H     | 401 | PC1  | C3A-C3B-C3C-C3D |
| 46  | D     | 502 | 3PE  | C37-C38-C39-C3A |
| 54  | n     | 201 | ZMP  | O4-C17-C18-C20  |
| 55  | Y     | 401 | CDL  | C73-C74-C75-C76 |
| 46  | K     | 201 | 3PE  | C2-C1-O11-P     |
| 47  | 9     | 203 | PC1  | C35-C36-C37-C38 |
| 55  | Y     | 403 | CDL  | OB5-CB3-CB4-CB6 |
| 55  | d     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 55  | m     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 48  | D     | 501 | UQ   | C35-C34-C36-C37 |
| 48  | D     | 501 | UQ   | C33-C34-C36-C37 |
| 47  | H     | 401 | PC1  | C1-C2-C3-O31    |
| 55  | m     | 201 | CDL  | CB3-CB4-CB6-OB8 |
| 47  | 9     | 203 | PC1  | C2C-C2D-C2E-C2F |
| 55  | L     | 702 | CDL  | CA5-C11-C12-C13 |
| 55  | r     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 55  | d     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 55  | Y     | 403 | CDL  | O1-C1-CB2-OB2   |
| 46  | h     | 202 | 3PE  | C2-C1-O11-P     |
| 47  | Z     | 402 | PC1  | C21-C22-C23-C24 |
| 54  | W     | 201 | ZMP  | O1-C10-S1-C11   |
| 46  | D     | 502 | 3PE  | O21-C2-C3-O31   |
| 47  | Z     | 402 | PC1  | C2A-C2B-C2C-C2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | D     | 501 | UQ   | C44-C46-C47-C48 |
| 54  | W     | 201 | ZMP  | C9-C10-S1-C11   |
| 54  | n     | 201 | ZMP  | C13-C14-C15-N2  |
| 55  | r     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | O     | 401 | DGT  | PB-O3B-PG-O2G   |
| 55  | Y     | 403 | CDL  | C31-C32-C33-C34 |
| 55  | N     | 401 | CDL  | OB5-CB3-CB4-OB6 |
| 55  | Y     | 403 | CDL  | OB5-CB3-CB4-OB6 |
| 55  | d     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 46  | D     | 502 | 3PE  | C12-C11-O13-P   |
| 46  | M     | 502 | 3PE  | C12-C11-O13-P   |
| 54  | n     | 201 | ZMP  | C16-C17-C18-C19 |
| 47  | M     | 501 | PC1  | O21-C2-C3-O31   |
| 55  | Y     | 401 | CDL  | OB6-CB4-CB6-OB8 |
| 55  | d     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 55  | m     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 47  | H     | 401 | PC1  | O13-C11-C12-N   |
| 47  | M     | 501 | PC1  | O13-C11-C12-N   |
| 47  | Z     | 402 | PC1  | O13-C11-C12-N   |
| 56  | O     | 401 | DGT  | PB-O3A-PA-O1A   |
| 55  | d     | 201 | CDL  | C55-C56-C57-C58 |
| 46  | M     | 503 | 3PE  | C26-C27-C28-C29 |
| 55  | L     | 702 | CDL  | OB5-CB3-CB4-CB6 |
| 55  | L     | 702 | CDL  | OB5-CB3-CB4-OB6 |
| 55  | h     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 46  | K     | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 55  | Y     | 401 | CDL  | CB3-CB4-CB6-OB8 |
| 47  | 9     | 203 | PC1  | C2D-C2E-C2F-C2G |
| 46  | Z     | 401 | 3PE  | C23-C24-C25-C26 |
| 46  | 6     | 202 | 3PE  | C1-O11-P-O14    |
| 46  | K     | 201 | 3PE  | C11-O13-P-O14   |
| 46  | L     | 701 | 3PE  | C1-O11-P-O12    |
| 46  | M     | 502 | 3PE  | O13-C11-C12-N   |
| 46  | M     | 503 | 3PE  | C1-O11-P-O12    |
| 46  | Y     | 402 | 3PE  | C11-O13-P-O11   |
| 46  | Z     | 401 | 3PE  | C1-O11-P-O14    |
| 46  | Z     | 401 | 3PE  | C11-O13-P-O11   |
| 46  | Z     | 401 | 3PE  | C11-O13-P-O14   |
| 46  | d     | 202 | 3PE  | C1-O11-P-O12    |
| 46  | d     | 202 | 3PE  | C1-O11-P-O13    |
| 46  | d     | 202 | 3PE  | C1-O11-P-O14    |
| 46  | i     | 201 | 3PE  | C1-O11-P-O14    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | i     | 201 | 3PE  | C11-O13-P-O14   |
| 47  | 9     | 203 | PC1  | C1-O11-P-O12    |
| 47  | H     | 401 | PC1  | C1-O11-P-O14    |
| 55  | r     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | L     | 702 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | L     | 702 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | L     | 703 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | L     | 703 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | N     | 401 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | N     | 401 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | N     | 401 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | Y     | 401 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | Y     | 401 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | Y     | 401 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | Y     | 401 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | Y     | 403 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | h     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | m     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | m     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | m     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | O     | 401 | DGT  | C5'-O5'-PA-O3A  |
| 56  | O     | 401 | DGT  | C5'-O5'-PA-O2A  |
| 48  | D     | 501 | UQ   | C15-C14-C16-C17 |
| 46  | M     | 502 | 3PE  | C37-C38-C39-C3A |
| 55  | N     | 401 | CDL  | CB4-CB3-OB5-PB2 |
| 55  | h     | 201 | CDL  | C1-CA2-OA2-PA1  |
| 55  | h     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 46  | h     | 202 | 3PE  | C23-C24-C25-C26 |
| 47  | 9     | 203 | PC1  | C3-C2-O21-C21   |
| 48  | D     | 501 | UQ   | C19-C21-C22-C23 |
| 47  | 9     | 203 | PC1  | O11-C1-C2-C3    |
| 55  | h     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 55  | m     | 201 | CDL  | C12-C11-CA5-OA6 |
| 55  | d     | 201 | CDL  | C63-C64-C65-C66 |
| 46  | Z     | 401 | 3PE  | O31-C31-C32-C33 |
| 55  | d     | 201 | CDL  | C57-C58-C59-C60 |
| 48  | D     | 501 | UQ   | C13-C14-C16-C17 |
| 55  | Y     | 403 | CDL  | OA5-CA3-CA4-OA6 |
| 47  | Z     | 402 | PC1  | O21-C21-C22-C23 |
| 55  | h     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 46  | A     | 201 | 3PE  | C2-C1-O11-P     |
| 46  | L     | 701 | 3PE  | C2-C1-O11-P     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | 9     | 203 | PC1  | C29-C2A-C2B-C2C |
| 48  | D     | 501 | UQ   | C34-C36-C37-C38 |
| 54  | n     | 201 | ZMP  | N2-C16-C17-O4   |
| 55  | m     | 201 | CDL  | C72-C73-C74-C75 |
| 46  | Z     | 401 | 3PE  | C3-C2-O21-C21   |
| 55  | r     | 201 | CDL  | CA3-CA4-OA6-CA5 |
| 55  | L     | 702 | CDL  | C12-C13-C14-C15 |
| 46  | M     | 502 | 3PE  | C3D-C3E-C3F-C3G |
| 47  | M     | 501 | PC1  | C21-C22-C23-C24 |
| 54  | W     | 201 | ZMP  | C6-C7-C8-C9     |
| 55  | d     | 201 | CDL  | C59-C60-C61-C62 |
| 55  | N     | 401 | CDL  | OB6-CB4-CB6-OB8 |
| 55  | Y     | 401 | CDL  | C13-C14-C15-C16 |
| 52  | P     | 501 | NDP  | O4D-C1D-N1N-C6N |
| 55  | Y     | 403 | CDL  | CA2-C1-CB2-OB2  |
| 48  | D     | 501 | UQ   | C50-C49-C51-C52 |
| 46  | D     | 502 | 3PE  | O21-C21-C22-C23 |
| 55  | L     | 702 | CDL  | C12-C11-CA5-OA6 |
| 46  | L     | 704 | 3PE  | O11-C1-C2-O21   |
| 55  | d     | 201 | CDL  | C56-C57-C58-C59 |
| 47  | 9     | 203 | PC1  | C3C-C3D-C3E-C3F |
| 54  | n     | 201 | ZMP  | C5-C6-C7-C8     |
| 46  | L     | 704 | 3PE  | C23-C24-C25-C26 |
| 52  | P     | 501 | NDP  | C2D-C1D-N1N-C6N |
| 50  | 1     | 501 | FMN  | C5'-O5'-P-O2P   |
| 46  | A     | 201 | 3PE  | C35-C36-C37-C38 |
| 46  | L     | 701 | 3PE  | C3-C2-O21-C21   |
| 47  | 6     | 203 | PC1  | C3-C2-O21-C21   |
| 55  | h     | 201 | CDL  | CB6-CB4-OB6-CB5 |
| 47  | M     | 501 | PC1  | C3C-C3D-C3E-C3F |
| 46  | D     | 502 | 3PE  | C3D-C3E-C3F-C3G |
| 50  | 1     | 501 | FMN  | O3'-C3'-C4'-C5' |
| 47  | M     | 501 | PC1  | C39-C3A-C3B-C3C |
| 48  | D     | 501 | UQ   | C40-C39-C41-C42 |
| 46  | h     | 202 | 3PE  | C12-C11-O13-P   |
| 46  | i     | 201 | 3PE  | C2B-C2C-C2D-C2E |
| 55  | d     | 201 | CDL  | C62-C63-C64-C65 |
| 54  | W     | 201 | ZMP  | C3-C4-C5-C6     |
| 55  | N     | 401 | CDL  | CA5-C11-C12-C13 |
| 55  | Y     | 403 | CDL  | C72-C71-CB7-OB8 |
| 55  | h     | 201 | CDL  | C72-C71-CB7-OB8 |
| 46  | A     | 201 | 3PE  | C38-C39-C3A-C3B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | A     | 201 | 3PE  | O21-C2-C3-O31   |
| 46  | Y     | 402 | 3PE  | O31-C31-C32-C33 |
| 46  | Z     | 401 | 3PE  | O11-C1-C2-C3    |
| 46  | Z     | 401 | 3PE  | C2E-C2F-C2G-C2H |
| 55  | Y     | 403 | CDL  | C52-C51-CB5-OB6 |
| 55  | Y     | 403 | CDL  | C32-C31-CA7-OA8 |
| 55  | N     | 401 | CDL  | C52-C51-CB5-OB6 |
| 52  | P     | 501 | NDP  | PN-O3-PA-O2A    |
| 56  | O     | 401 | DGT  | PB-O3A-PA-O2A   |
| 46  | 6     | 202 | 3PE  | O21-C21-C22-C23 |
| 48  | D     | 501 | UQ   | C30-C29-C31-C32 |
| 46  | Z     | 401 | 3PE  | C2A-C2B-C2C-C2D |
| 46  | Z     | 401 | 3PE  | C21-C22-C23-C24 |
| 55  | L     | 703 | CDL  | C12-C11-CA5-OA6 |
| 55  | N     | 401 | CDL  | C80-C81-C82-C83 |
| 46  | M     | 502 | 3PE  | O21-C21-C22-C23 |
| 55  | Y     | 401 | CDL  | C32-C31-CA7-OA8 |
| 55  | h     | 201 | CDL  | C32-C31-CA7-OA8 |
| 46  | M     | 502 | 3PE  | O31-C31-C32-C33 |
| 55  | d     | 201 | CDL  | C72-C71-CB7-OB8 |
| 56  | O     | 401 | DGT  | PB-O3B-PG-O3G   |
| 47  | M     | 501 | PC1  | O11-C1-C2-C3    |
| 47  | Z     | 402 | PC1  | O31-C31-C32-C33 |
| 54  | W     | 201 | ZMP  | C16-C17-C18-C21 |
| 46  | h     | 202 | 3PE  | C36-C37-C38-C39 |
| 55  | d     | 201 | CDL  | C61-C62-C63-C64 |
| 55  | N     | 401 | CDL  | CB6-CB4-OB6-CB5 |
| 55  | Y     | 403 | CDL  | CA6-CA4-OA6-CA5 |
| 55  | m     | 201 | CDL  | CA3-CA4-OA6-CA5 |
| 55  | Y     | 403 | CDL  | C52-C51-CB5-OB7 |
| 55  | Y     | 401 | CDL  | C23-C24-C25-C26 |
| 55  | N     | 401 | CDL  | C52-C51-CB5-OB7 |
| 48  | D     | 501 | UQ   | C6-C7-C8-C9     |
| 55  | L     | 702 | CDL  | C1-CA2-OA2-PA1  |
| 55  | L     | 703 | CDL  | C12-C11-CA5-OA7 |
| 46  | K     | 201 | 3PE  | O21-C21-C22-C23 |
| 47  | H     | 401 | PC1  | C24-C25-C26-C27 |
| 55  | Y     | 403 | CDL  | C32-C31-CA7-OA9 |
| 46  | M     | 502 | 3PE  | O22-C21-C22-C23 |
| 47  | Z     | 402 | PC1  | O32-C31-C32-C33 |
| 46  | A     | 201 | 3PE  | O31-C31-C32-C33 |
| 48  | D     | 501 | UQ   | C48-C49-C51-C52 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | 6     | 202 | 3PE  | O22-C21-C22-C23 |
| 55  | h     | 201 | CDL  | C72-C71-CB7-OB9 |
| 46  | Y     | 402 | 3PE  | O32-C31-C32-C33 |
| 55  | Y     | 403 | CDL  | C72-C71-CB7-OB9 |
| 55  | h     | 201 | CDL  | C32-C31-CA7-OA9 |
| 46  | m     | 202 | 3PE  | O31-C31-C32-C33 |
| 47  | M     | 501 | PC1  | C1-C2-C3-O31    |
| 55  | m     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 55  | d     | 201 | CDL  | C32-C31-CA7-OA8 |
| 55  | d     | 201 | CDL  | C72-C71-CB7-OB9 |
| 46  | D     | 502 | 3PE  | C38-C39-C3A-C3B |
| 46  | A     | 201 | 3PE  | O21-C21-C22-C23 |
| 46  | M     | 502 | 3PE  | O32-C31-C32-C33 |
| 55  | Y     | 401 | CDL  | C32-C31-CA7-OA9 |
| 46  | m     | 202 | 3PE  | O32-C31-C32-C33 |

There are no ring outliers.

33 monomers are involved in 76 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 50  | 1     | 501 | FMN  | 2       | 0            |
| 46  | h     | 202 | 3PE  | 1       | 0            |
| 49  | 2     | 301 | FES  | 1       | 0            |
| 45  | 9     | 201 | SF4  | 1       | 0            |
| 55  | h     | 201 | CDL  | 3       | 0            |
| 55  | d     | 201 | CDL  | 4       | 0            |
| 47  | Z     | 402 | PC1  | 3       | 0            |
| 46  | d     | 202 | 3PE  | 1       | 0            |
| 48  | D     | 501 | UQ   | 3       | 0            |
| 46  | K     | 201 | 3PE  | 5       | 0            |
| 47  | 6     | 203 | PC1  | 1       | 0            |
| 55  | N     | 401 | CDL  | 6       | 0            |
| 46  | M     | 502 | 3PE  | 5       | 0            |
| 56  | O     | 401 | DGT  | 2       | 0            |
| 46  | Y     | 402 | 3PE  | 1       | 0            |
| 46  | A     | 201 | 3PE  | 1       | 0            |
| 46  | i     | 201 | 3PE  | 5       | 0            |
| 45  | 1     | 502 | SF4  | 1       | 0            |
| 46  | M     | 503 | 3PE  | 1       | 0            |
| 46  | m     | 202 | 3PE  | 1       | 0            |
| 47  | 9     | 203 | PC1  | 3       | 0            |
| 55  | Y     | 403 | CDL  | 2       | 0            |

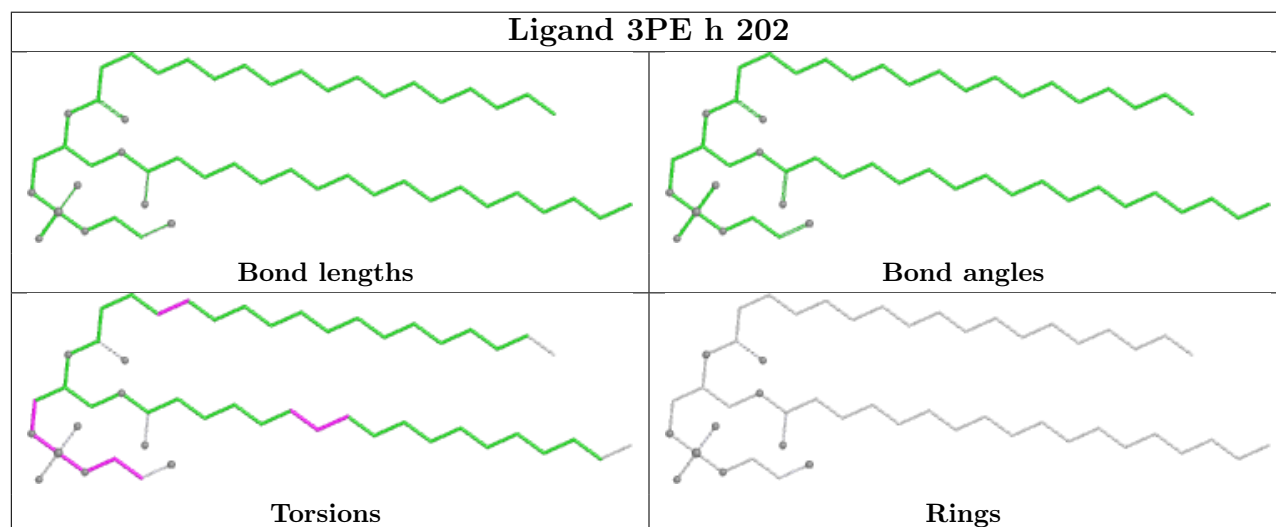
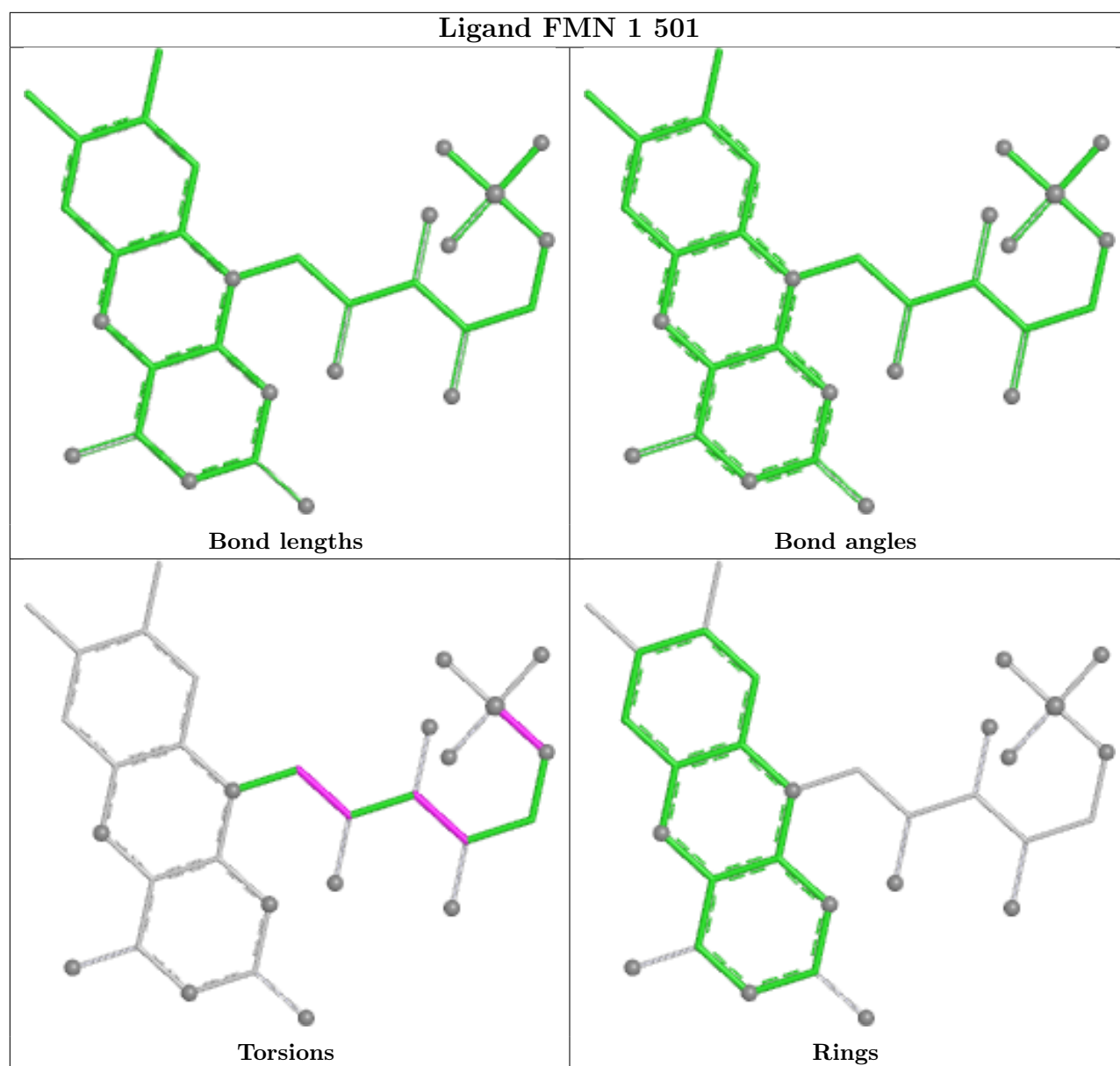
*Continued on next page...*

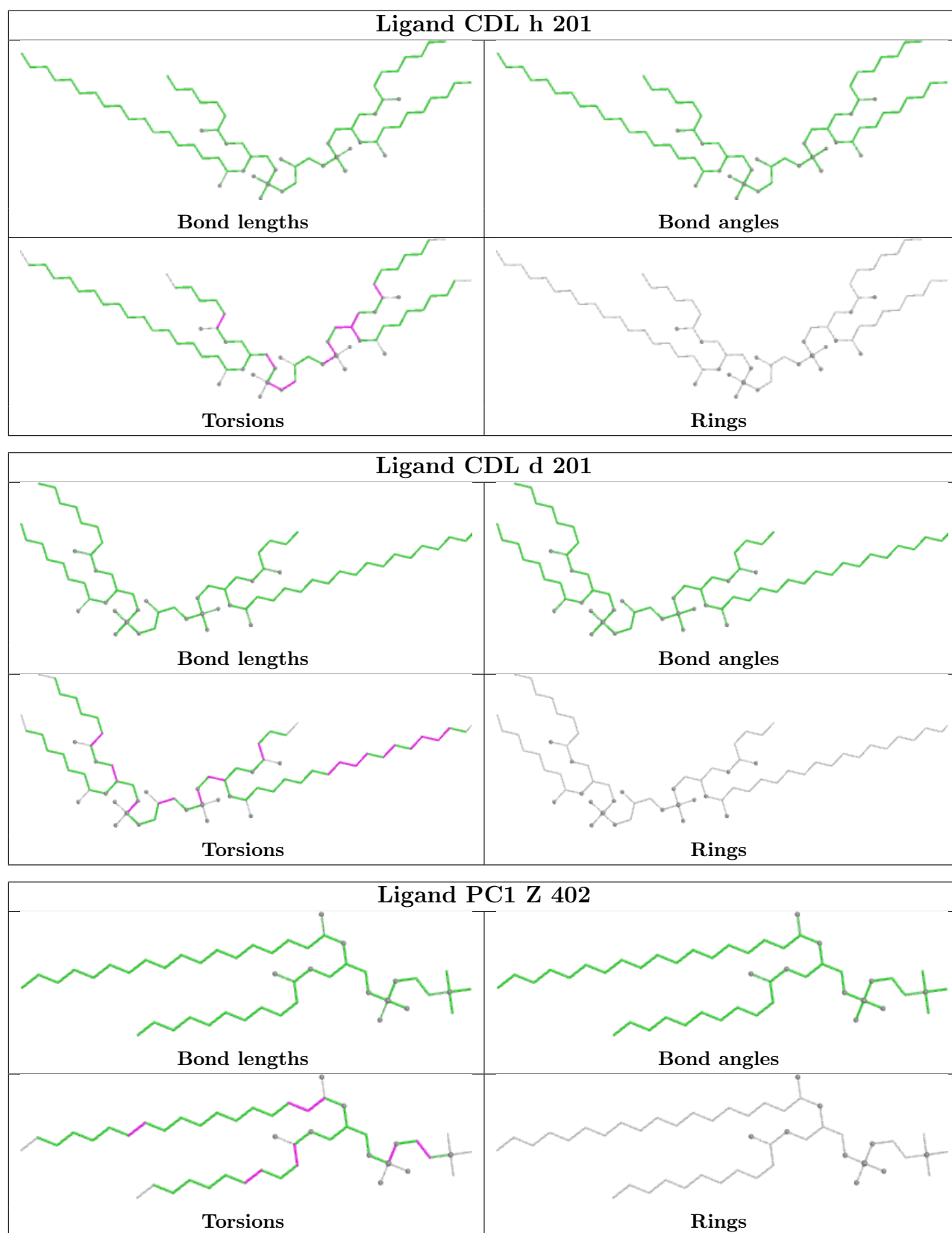


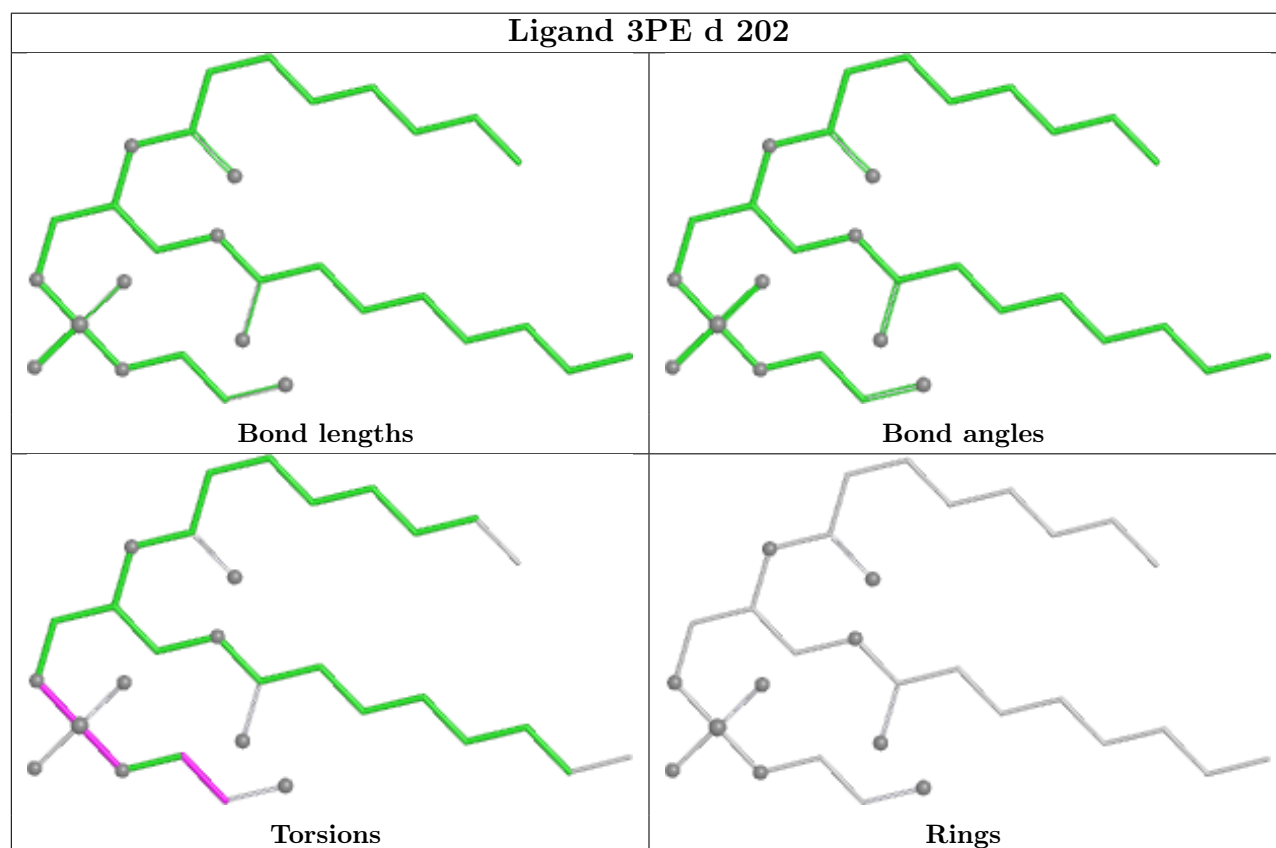
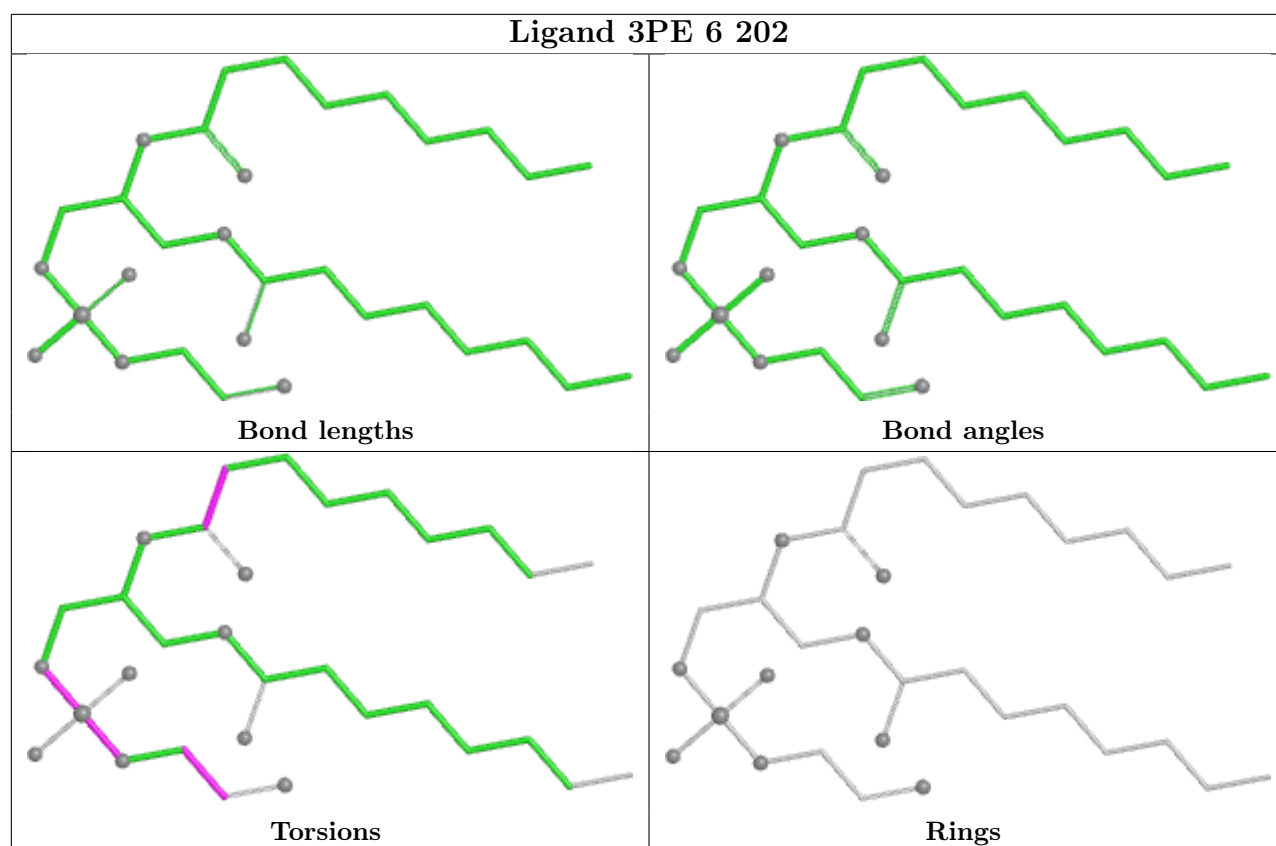
*Continued from previous page...*

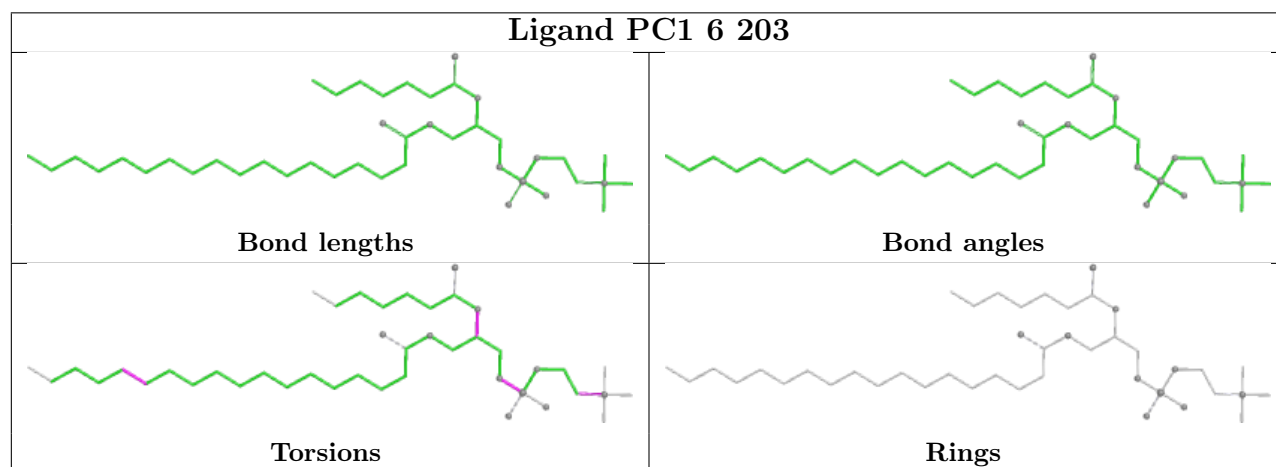
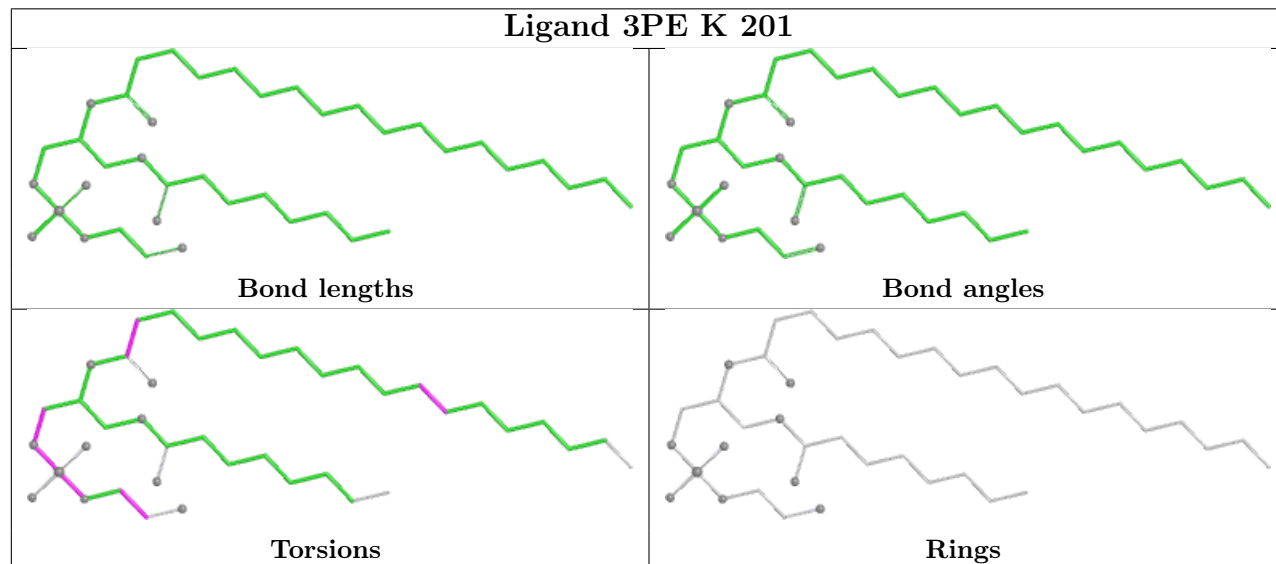
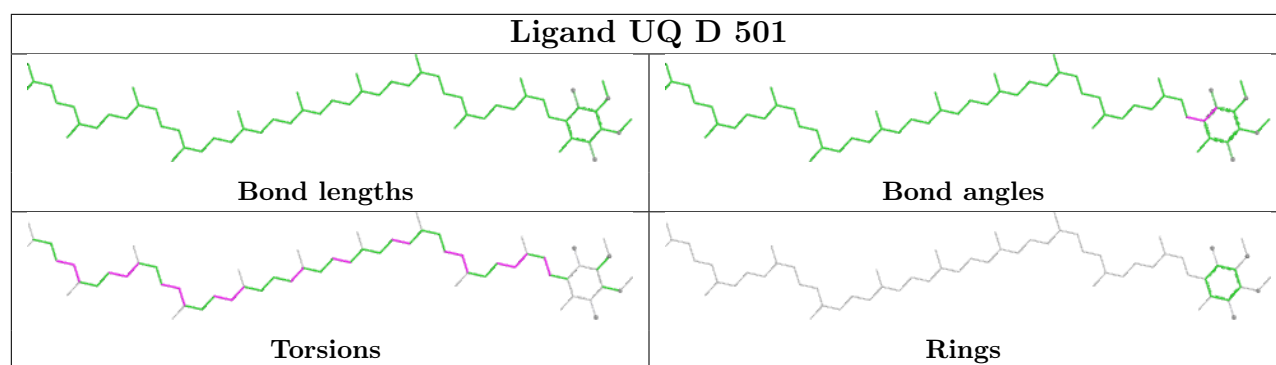
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 46  | L     | 701 | 3PE  | 1       | 0            |
| 55  | Y     | 401 | CDL  | 2       | 0            |
| 46  | D     | 502 | 3PE  | 4       | 0            |
| 47  | M     | 501 | PC1  | 6       | 0            |
| 54  | n     | 201 | ZMP  | 2       | 0            |
| 54  | W     | 201 | ZMP  | 3       | 0            |
| 45  | 6     | 201 | SF4  | 1       | 0            |
| 46  | L     | 704 | 3PE  | 3       | 0            |
| 52  | P     | 501 | NDP  | 3       | 0            |
| 55  | m     | 201 | CDL  | 1       | 0            |
| 55  | r     | 201 | CDL  | 2       | 0            |

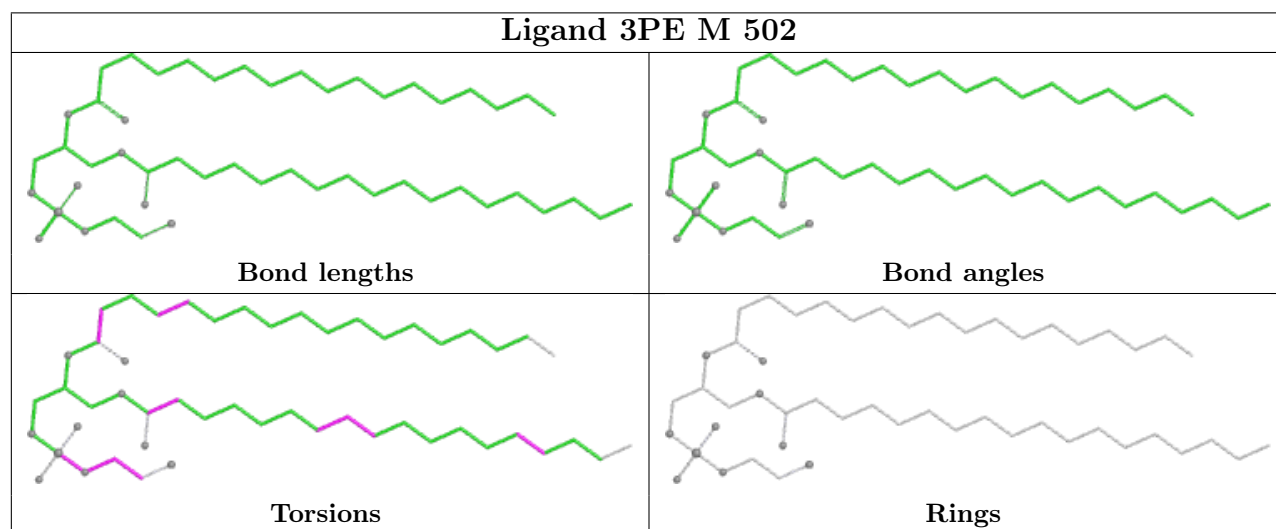
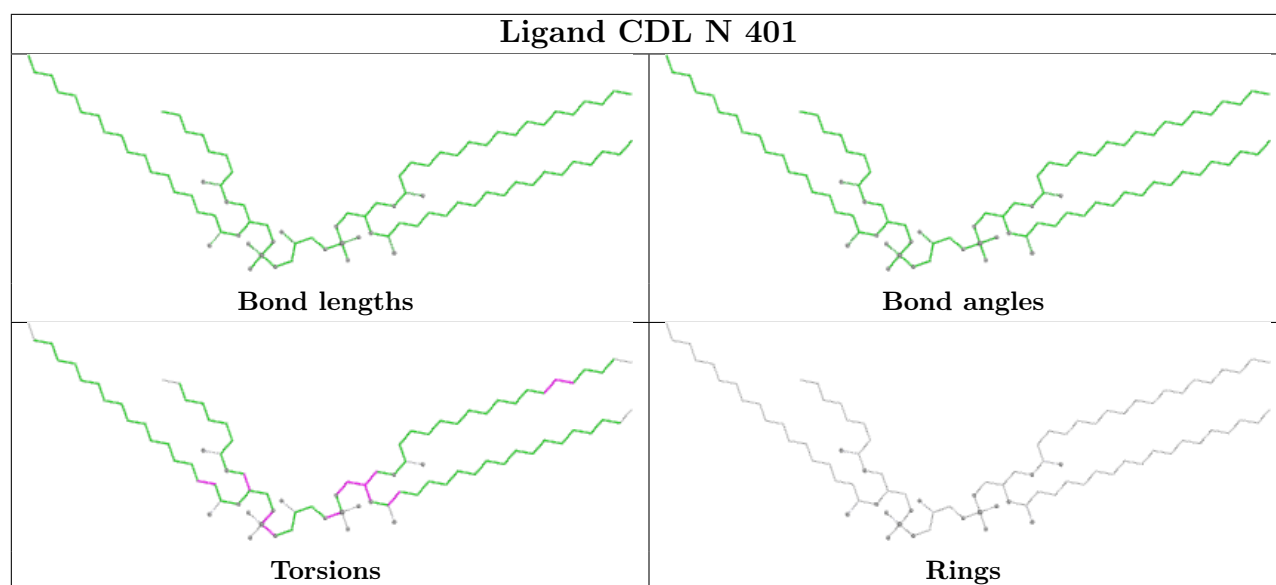
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

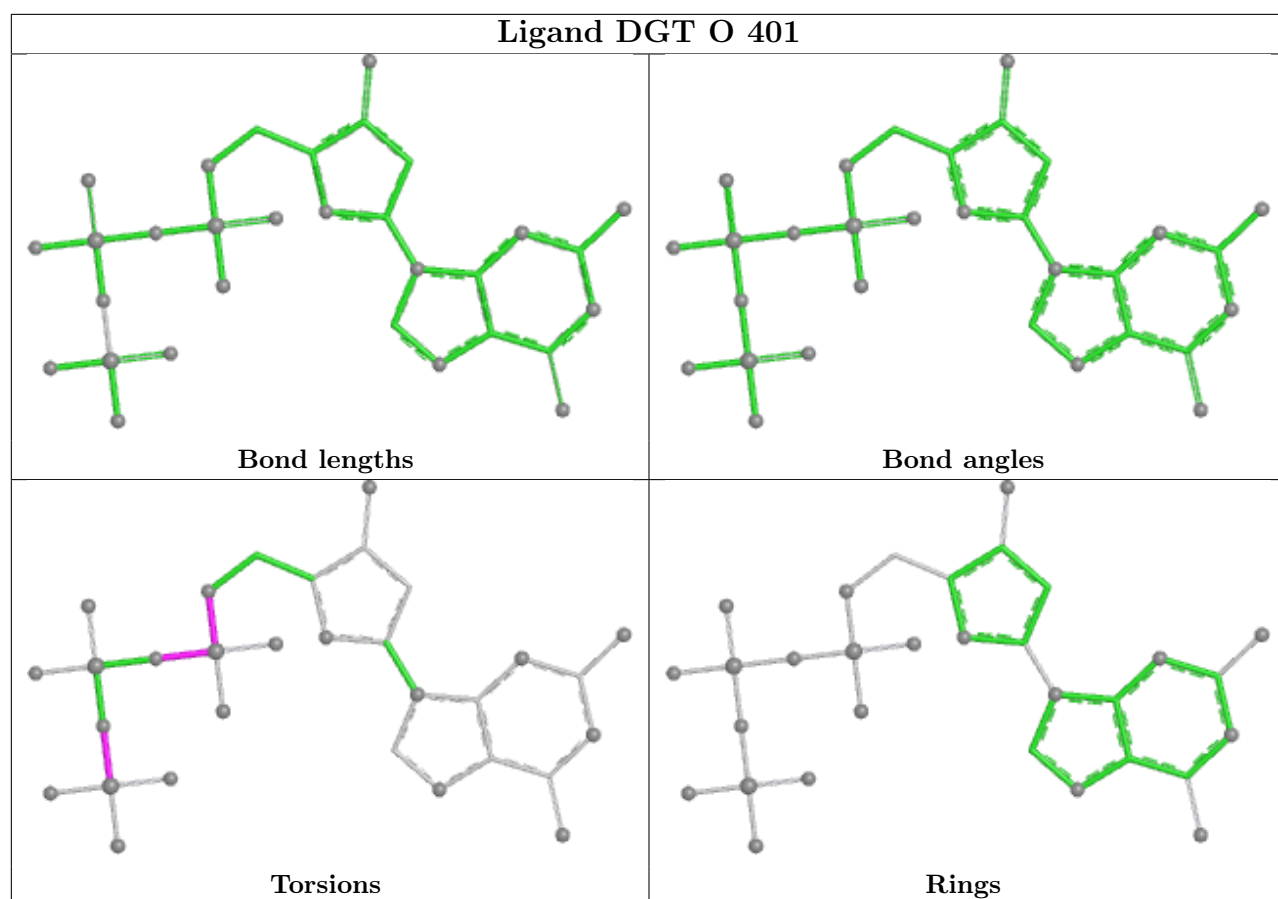


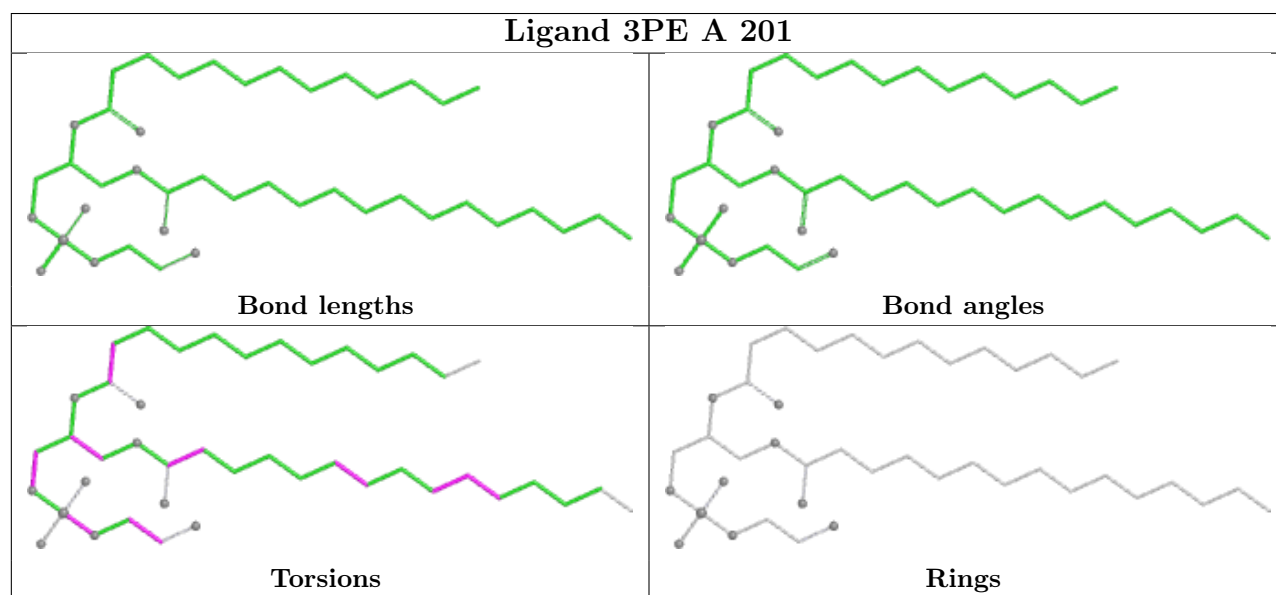
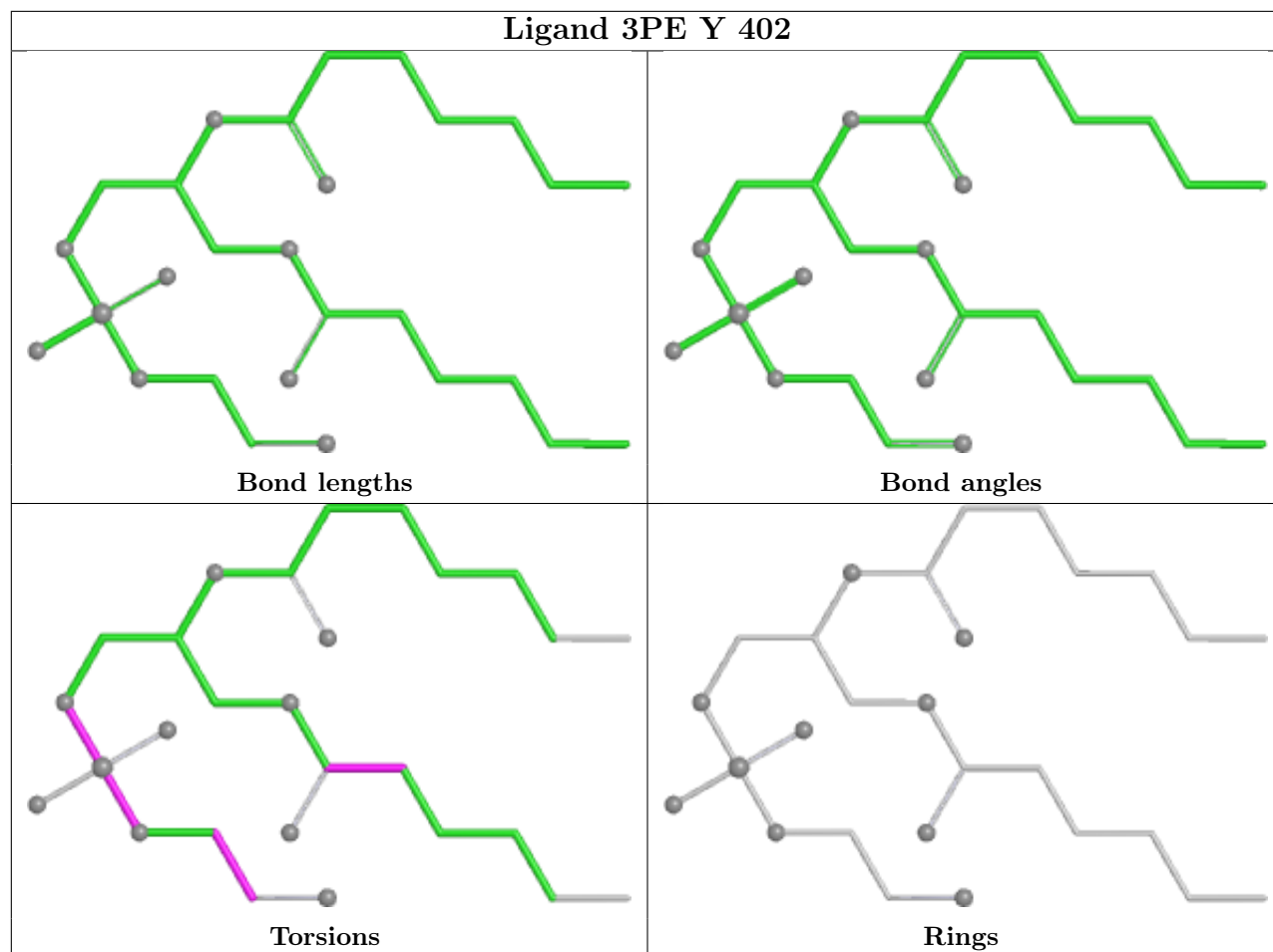




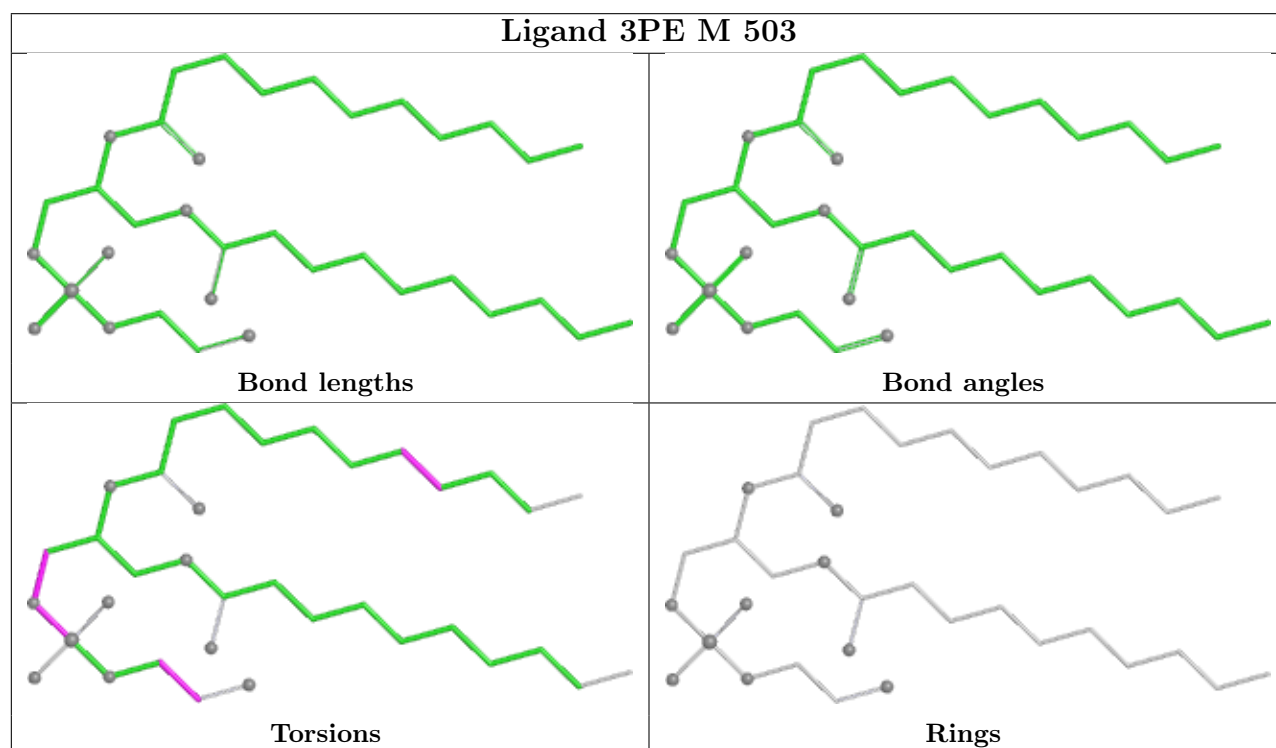
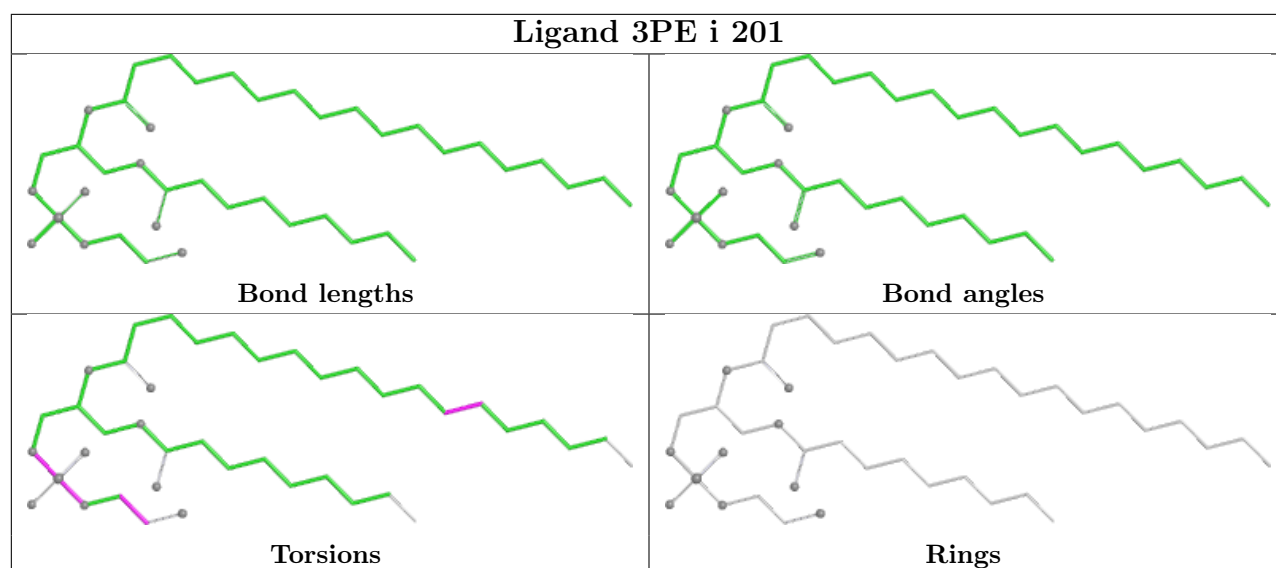


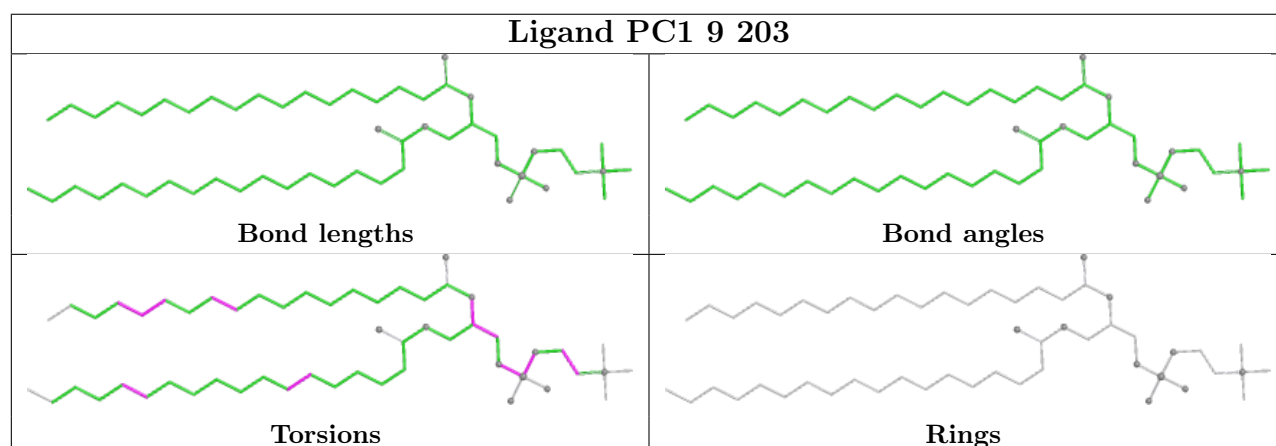
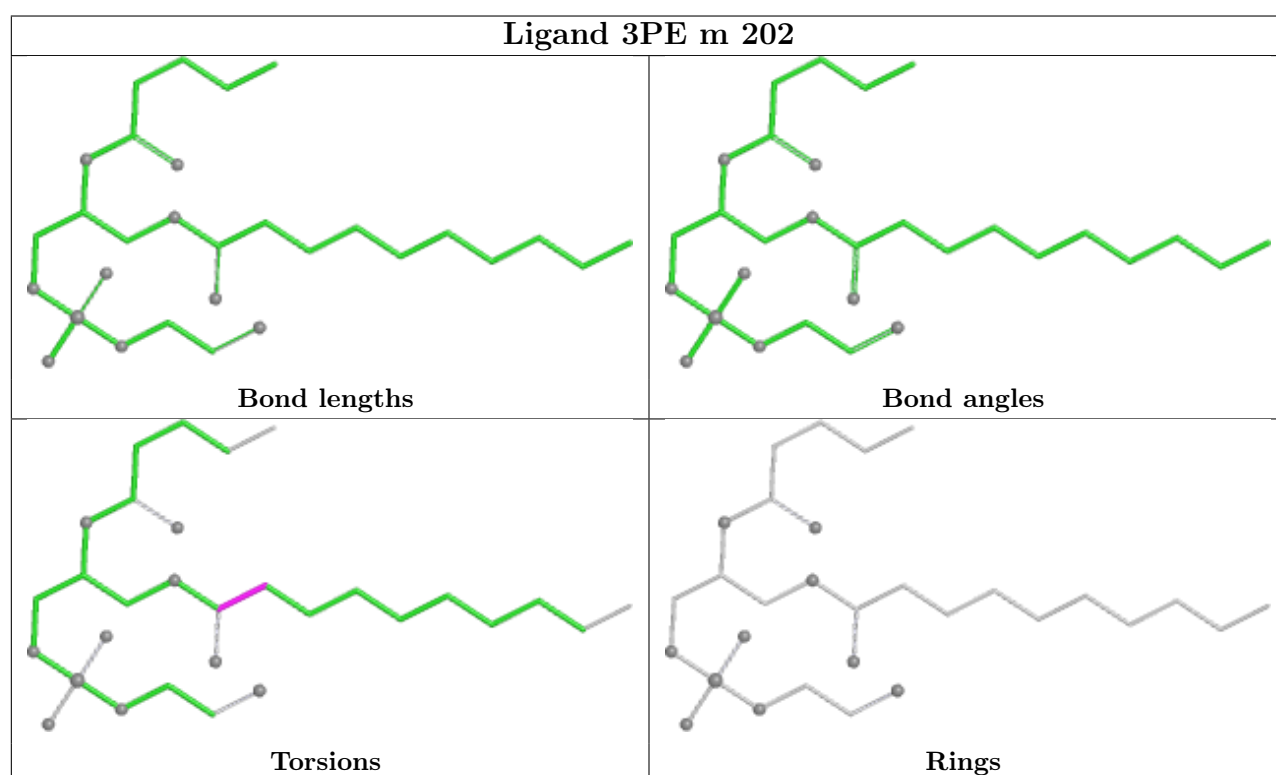
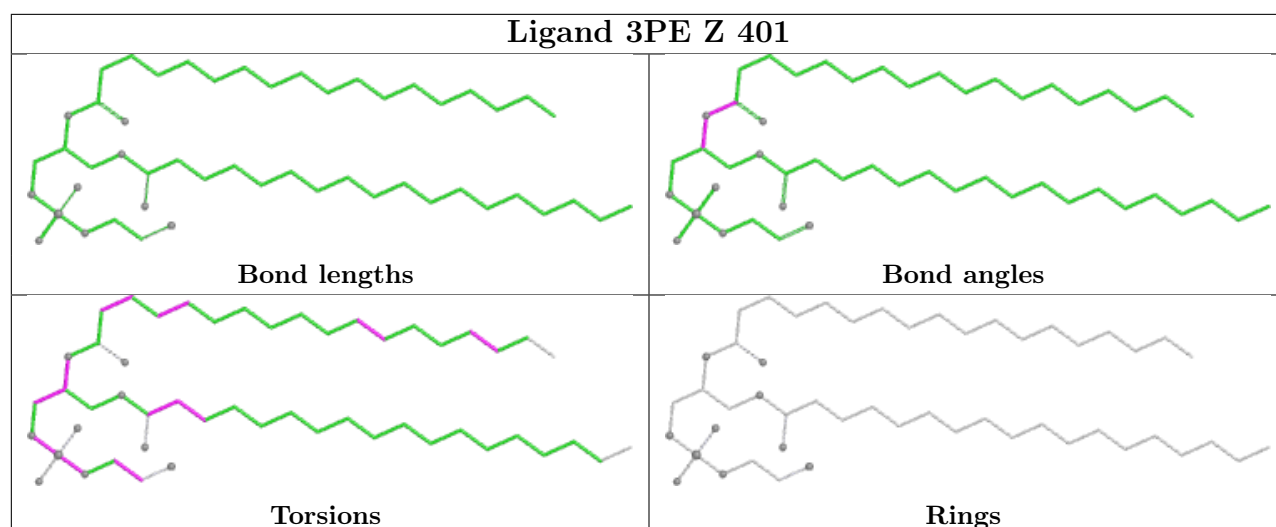


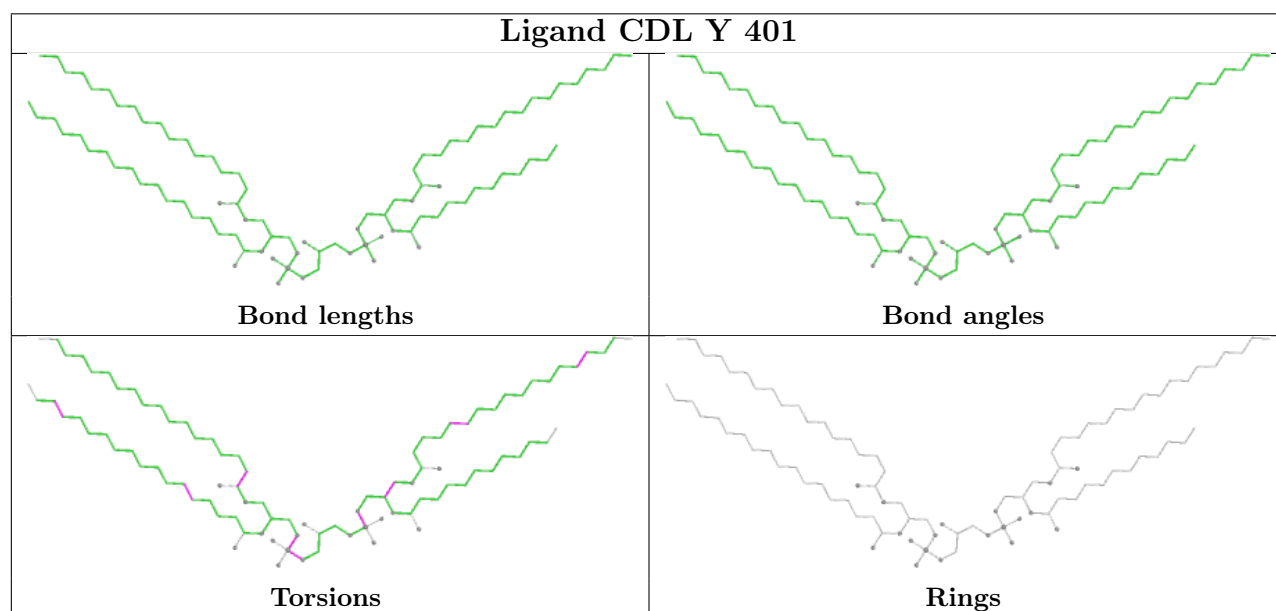
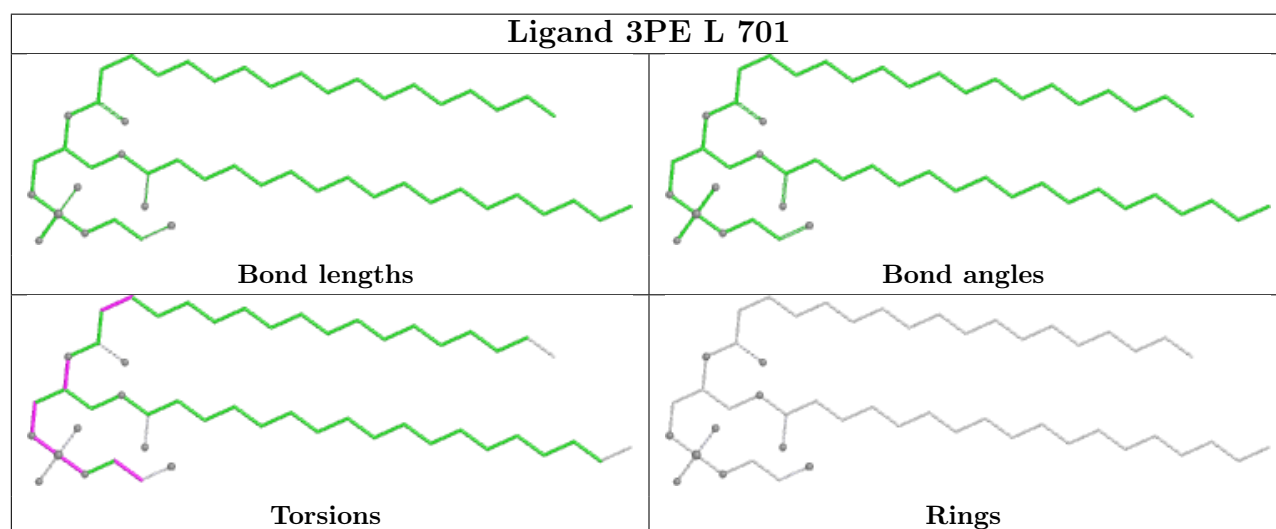
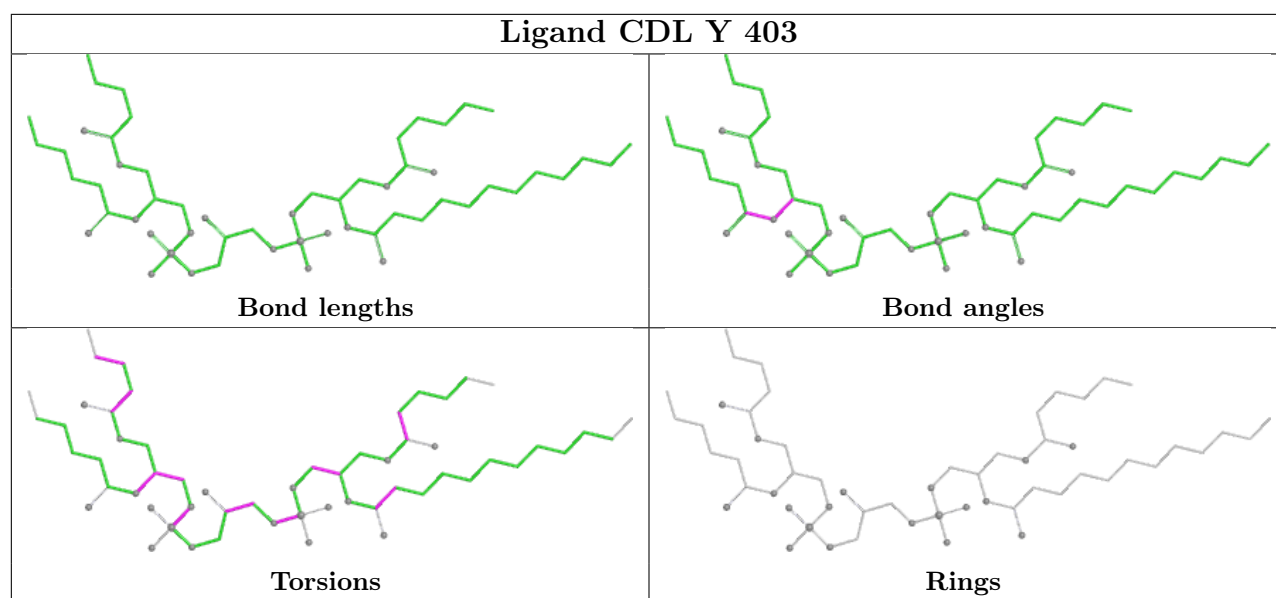


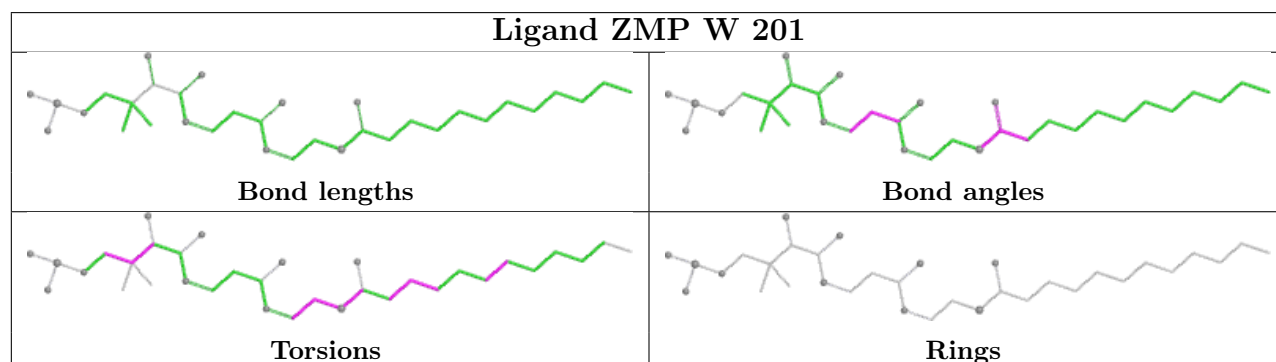
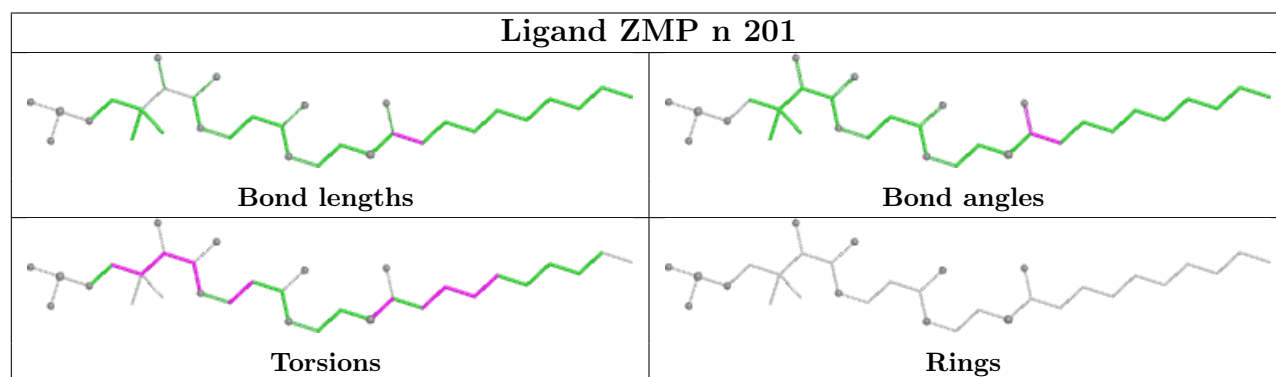
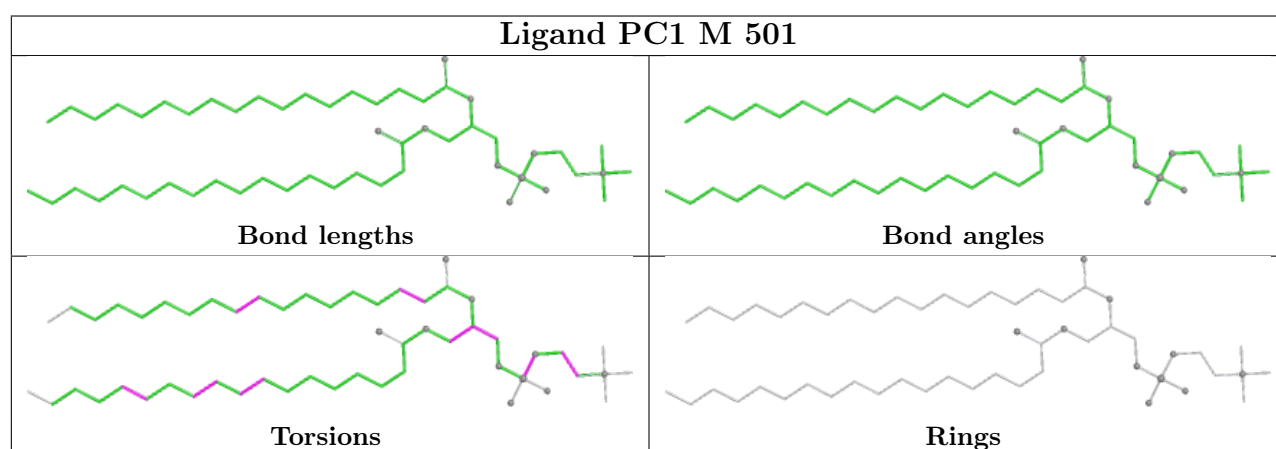
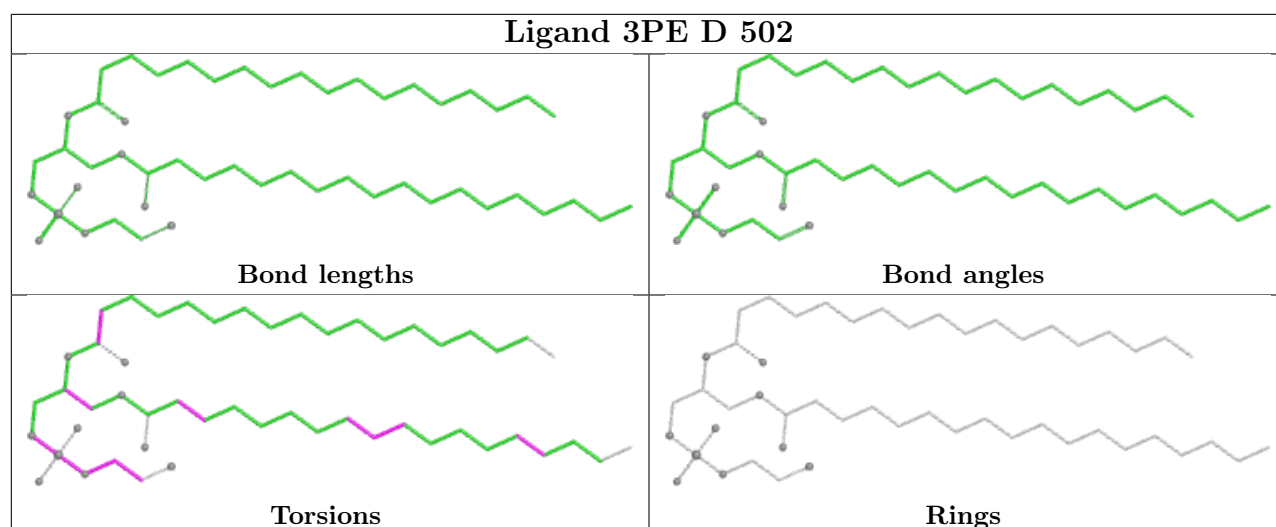


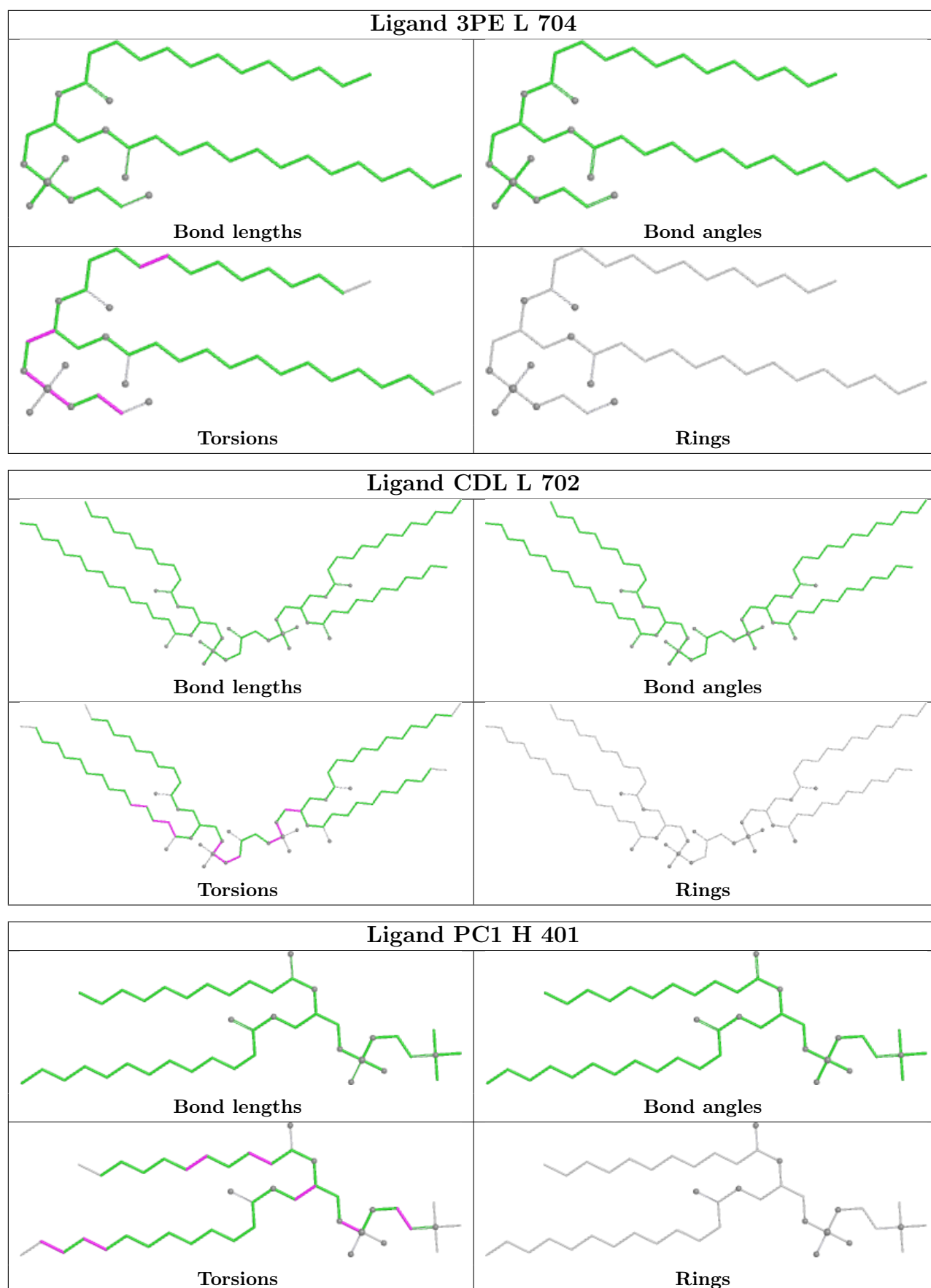


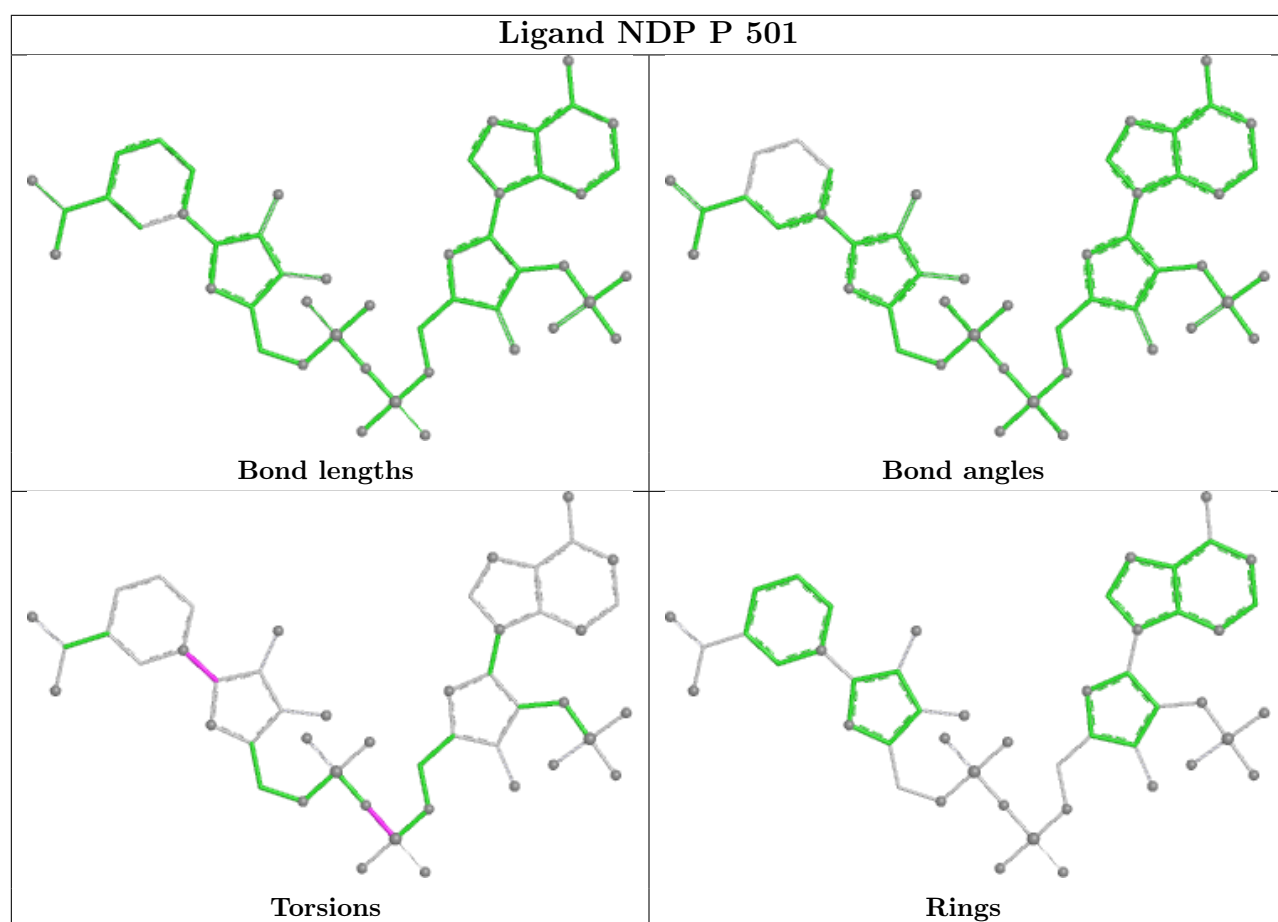
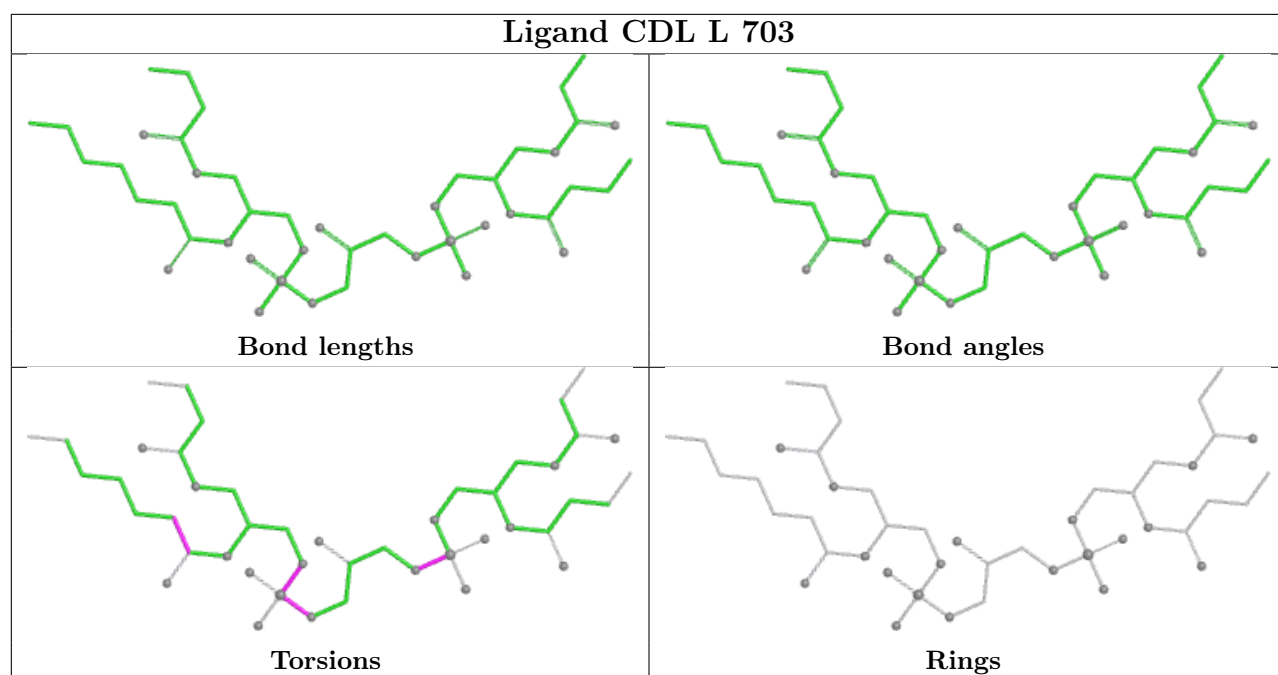


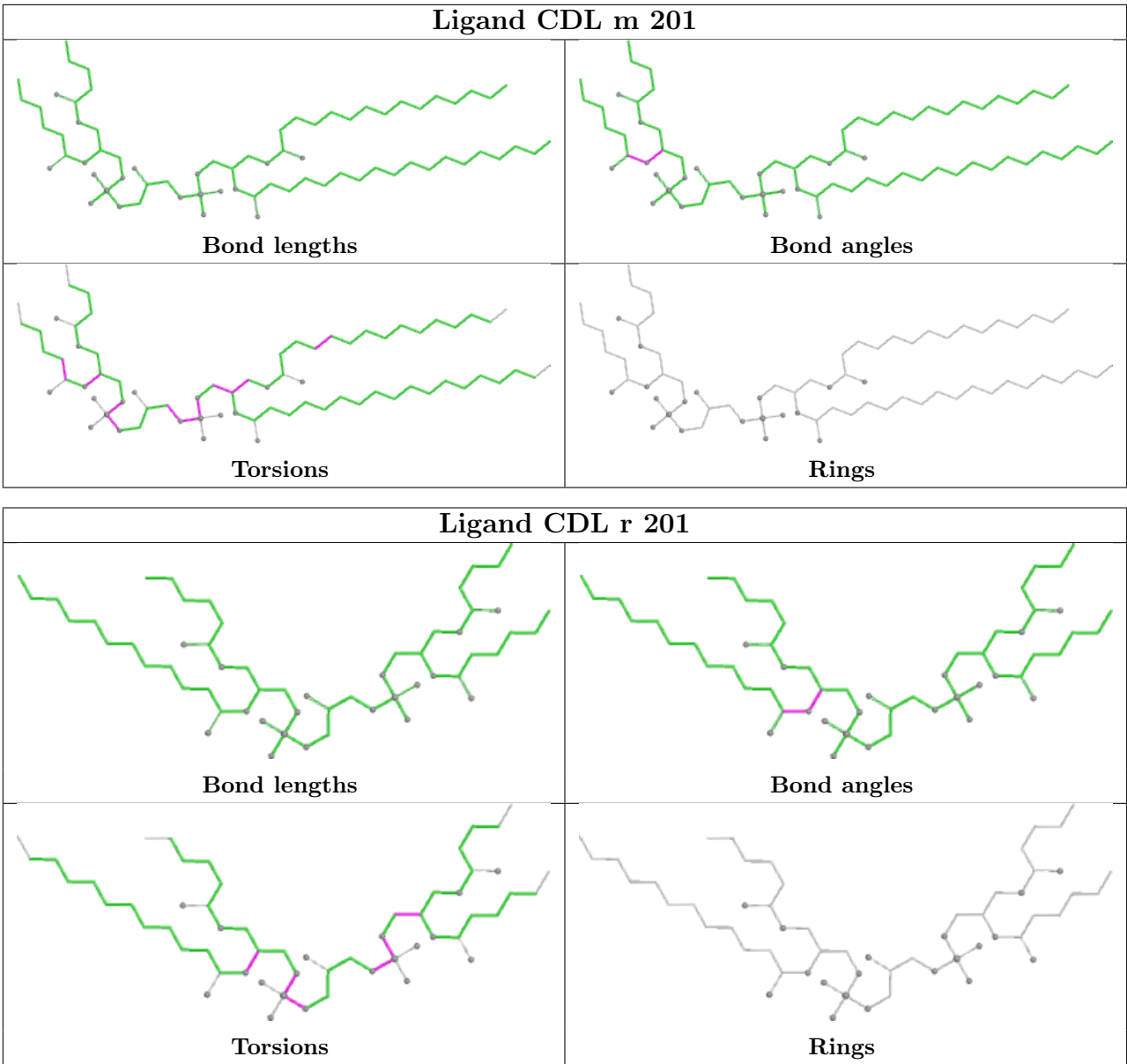












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 5   | 1     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 1     | 67:GLY    | C      | 68:ARG    | N      | 0.94         |



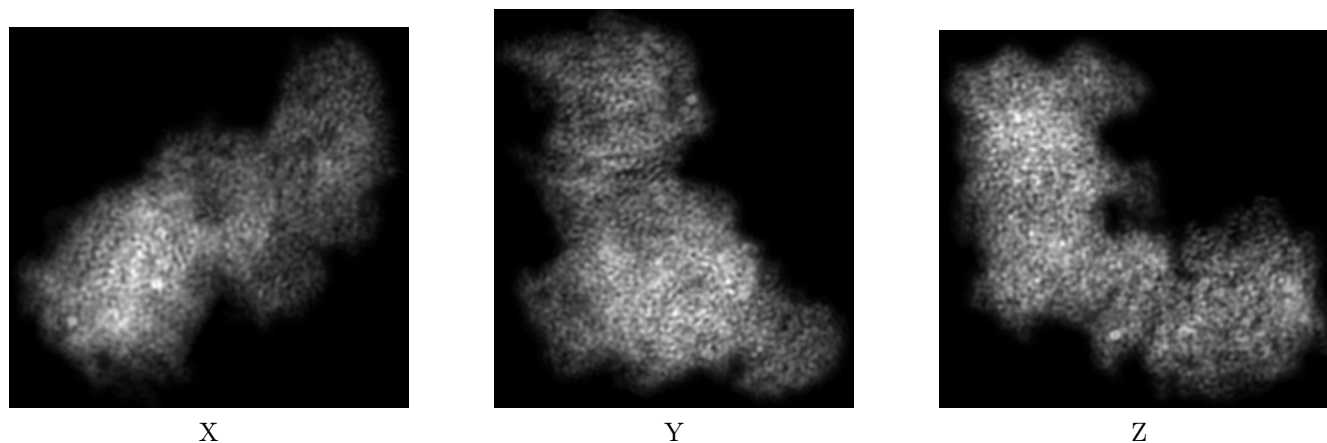
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19145. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

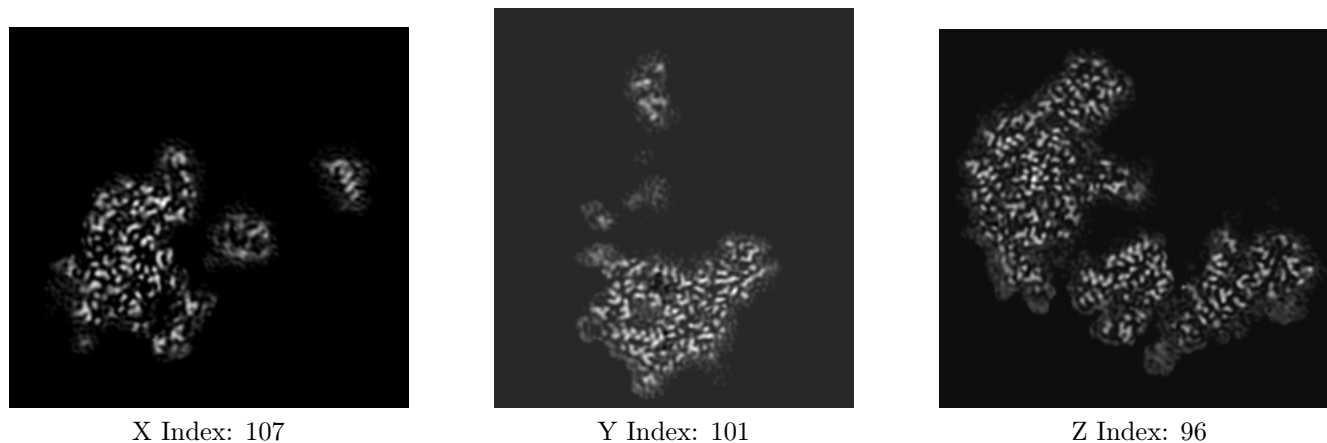
#### 6.1.1 Primary map



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

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

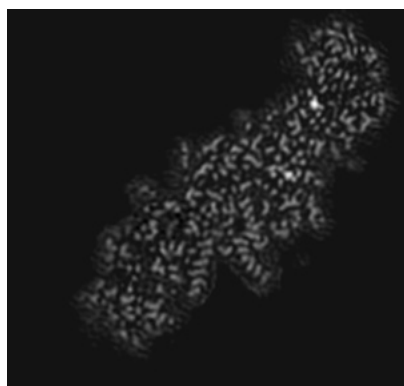
#### 6.2.1 Primary map



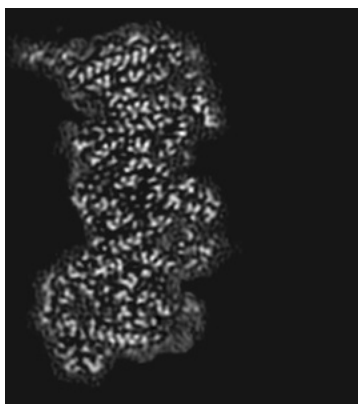
The images above show central slices of the map in three orthogonal directions.

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

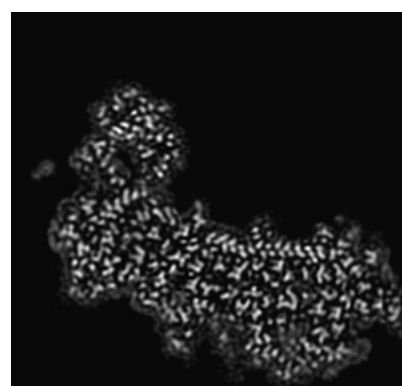
### 6.3.1 Primary map



X Index: 41



Y Index: 63

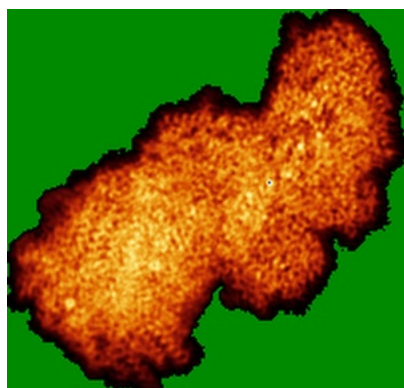


Z Index: 63

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

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

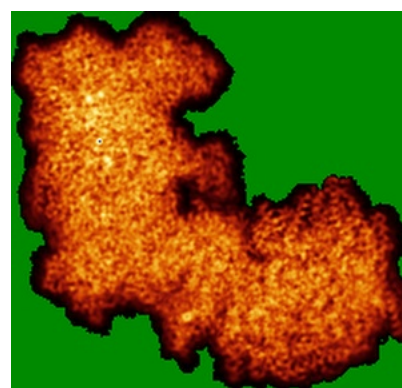
### 6.4.1 Primary map



X



Y

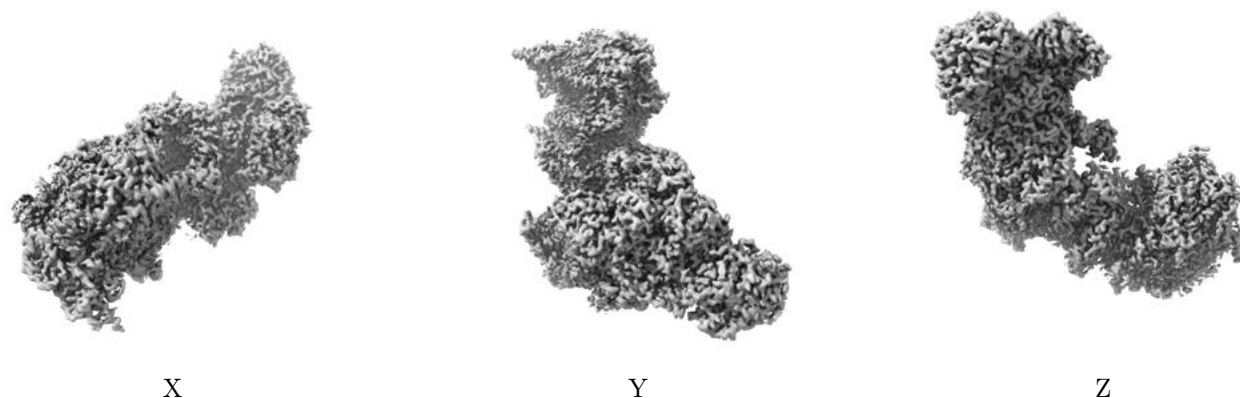


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

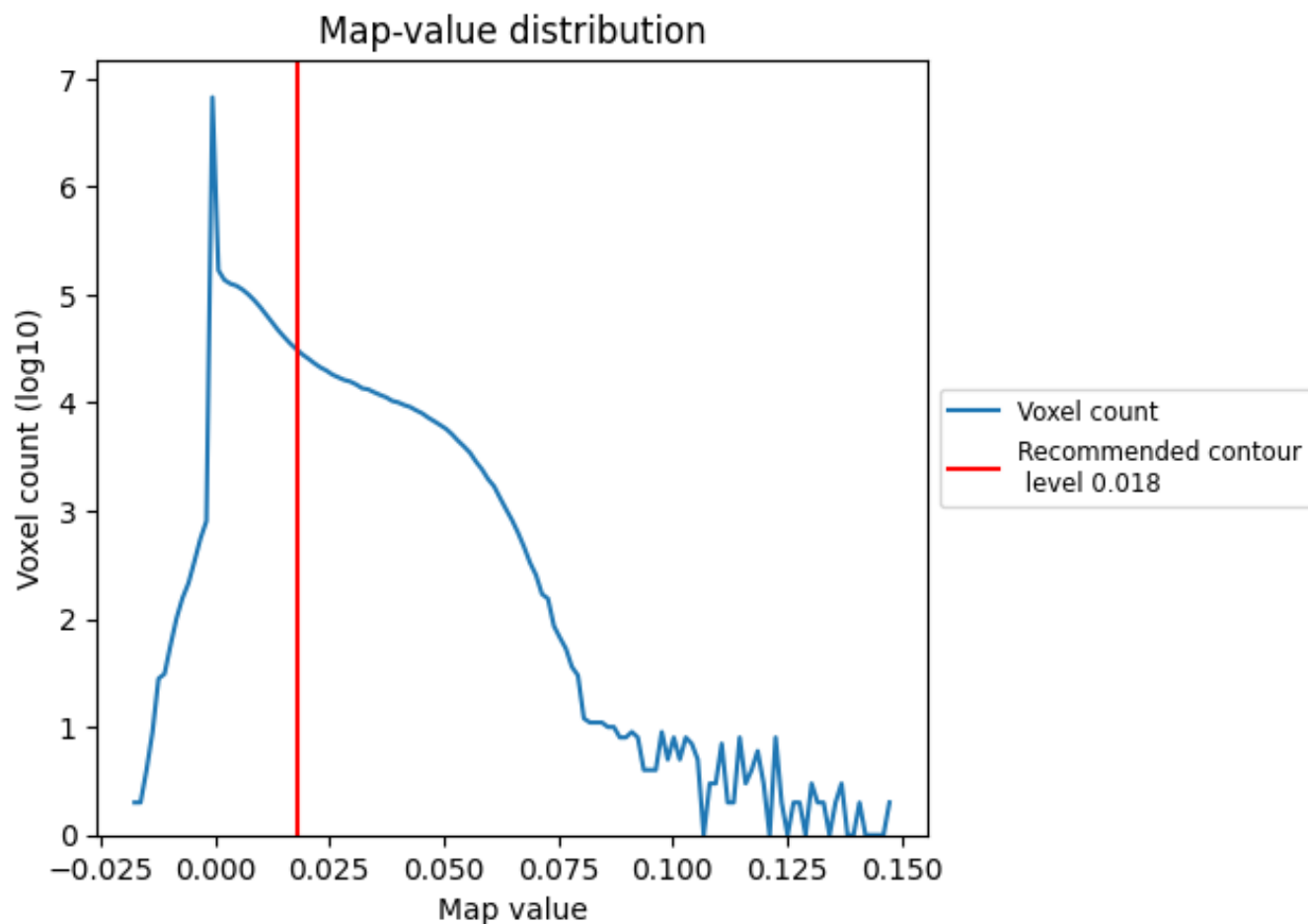
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

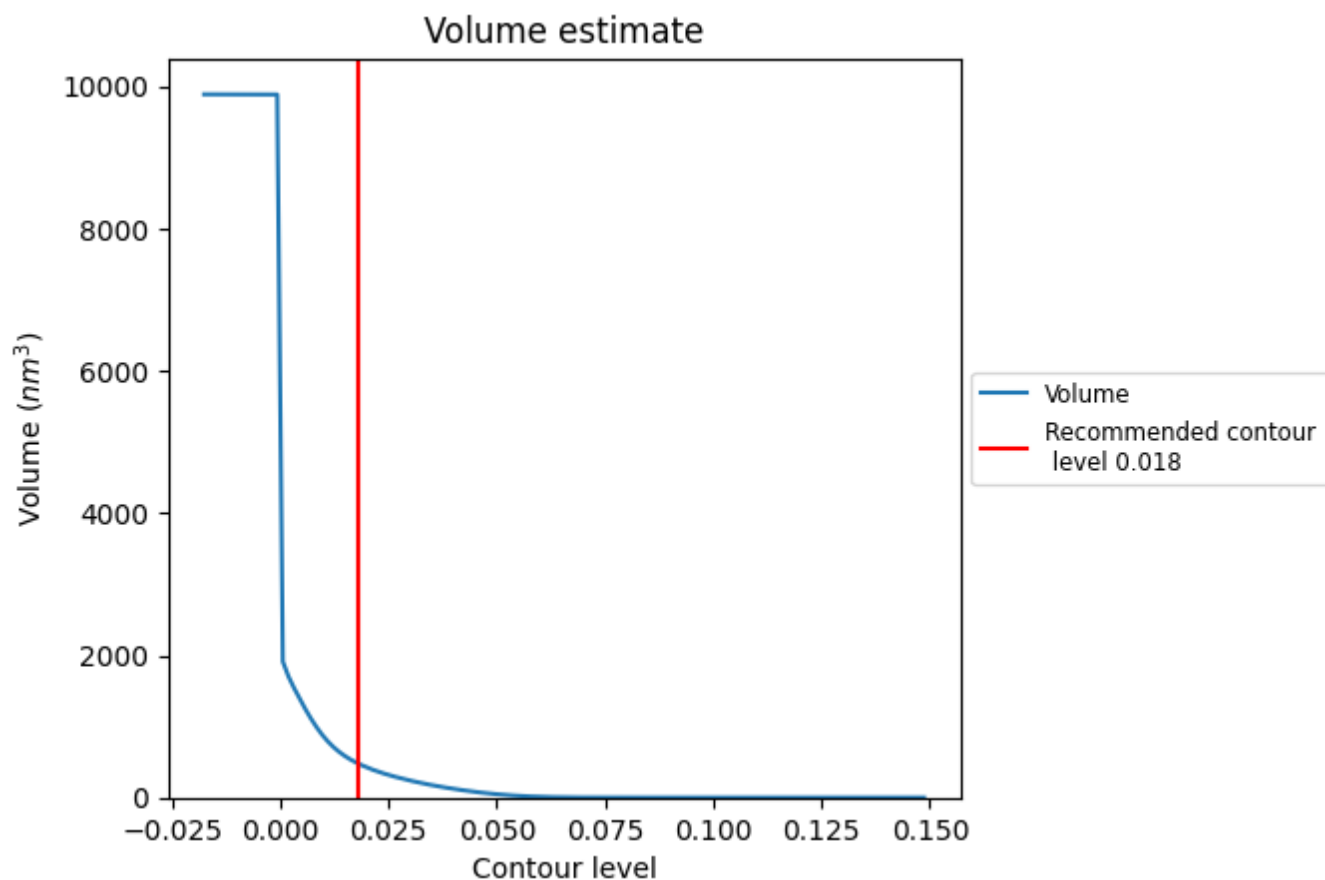
This section contains the results of statistical analysis of the map.

### 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 479 nm<sup>3</sup>; this corresponds to an approximate mass of 433 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.

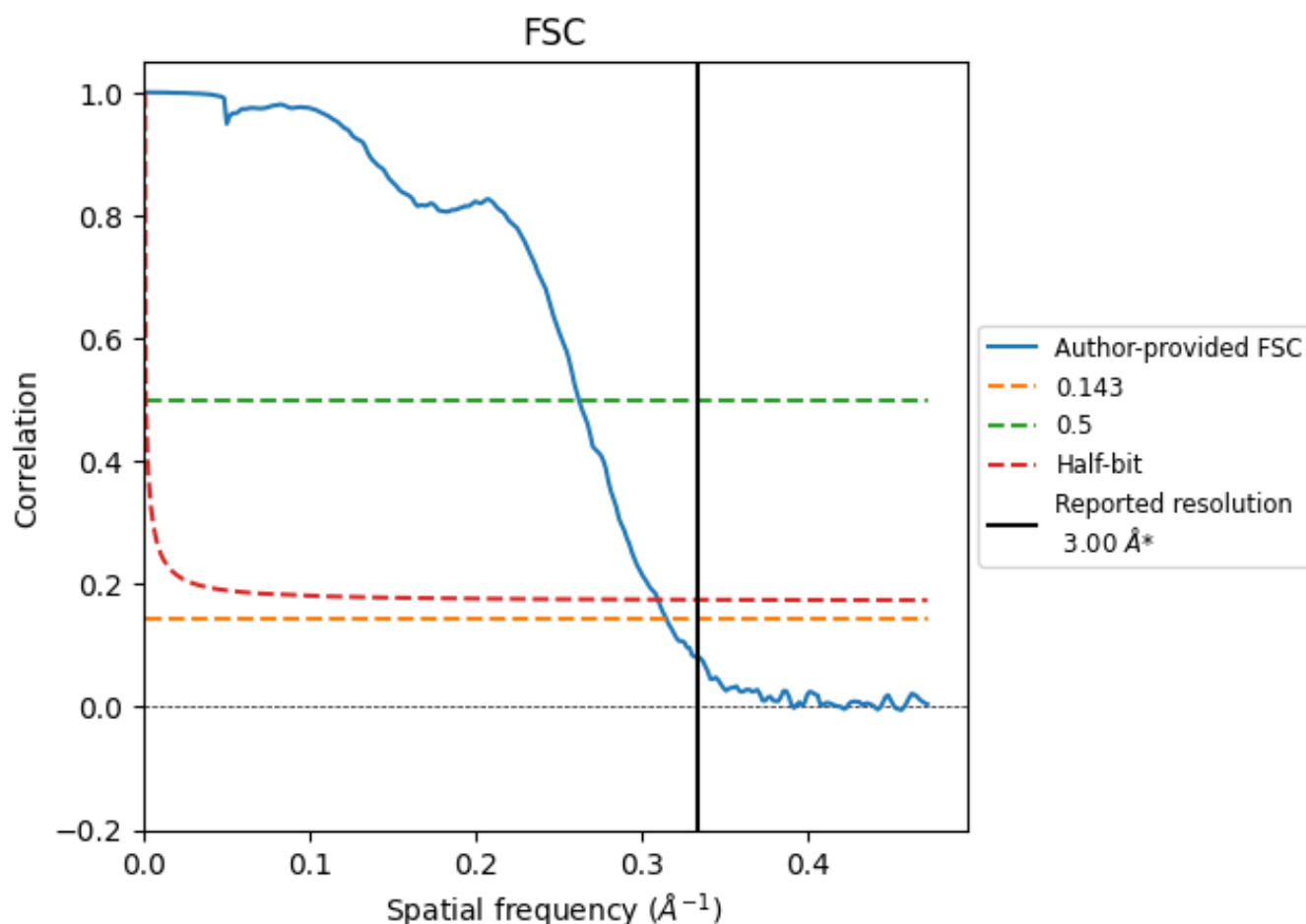
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.333  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

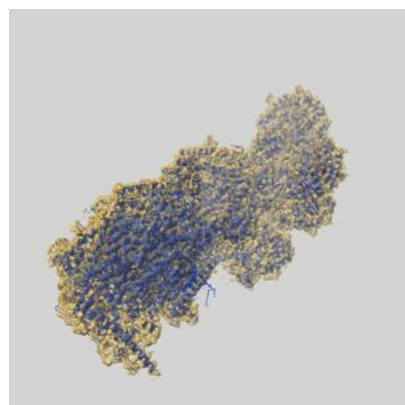
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.00                               | -    | -        |
| Author-provided FSC curve | 3.18                               | 3.82 | 3.23     |
| Unmasked-calculated*      | -                                  | -    | -        |

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

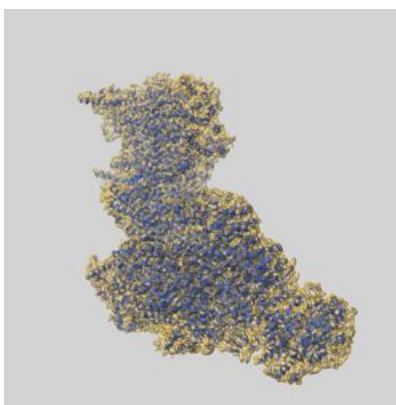
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19145 and PDB model 8RGP. Per-residue inclusion information can be found in section 3 on page 20.

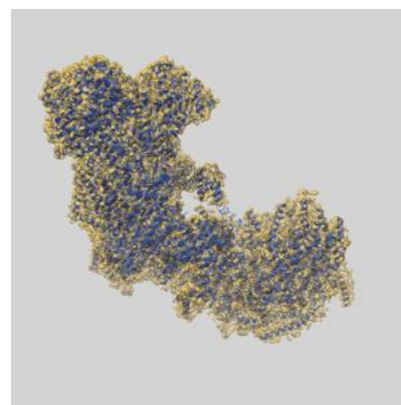
### 9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

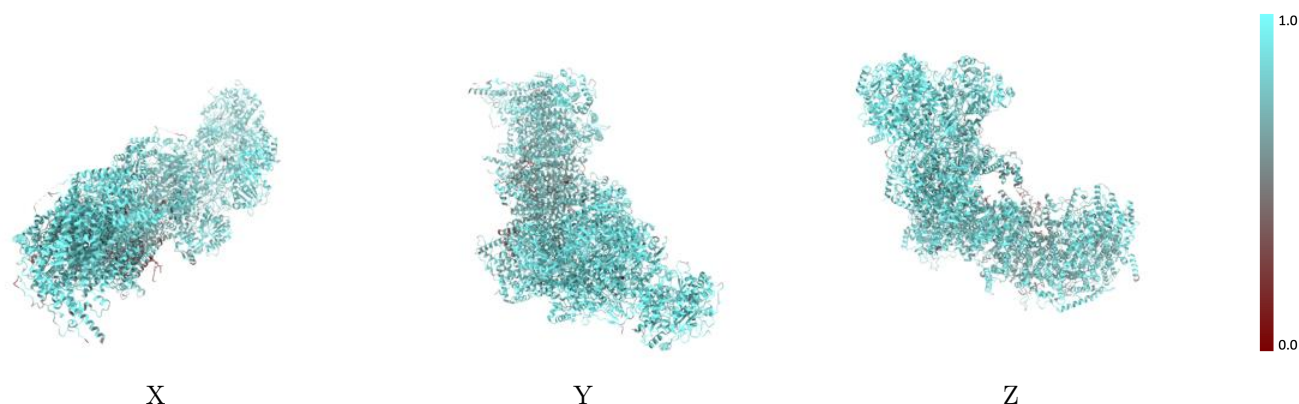


## 9.2 Q-score mapped to coordinate model [i](#)



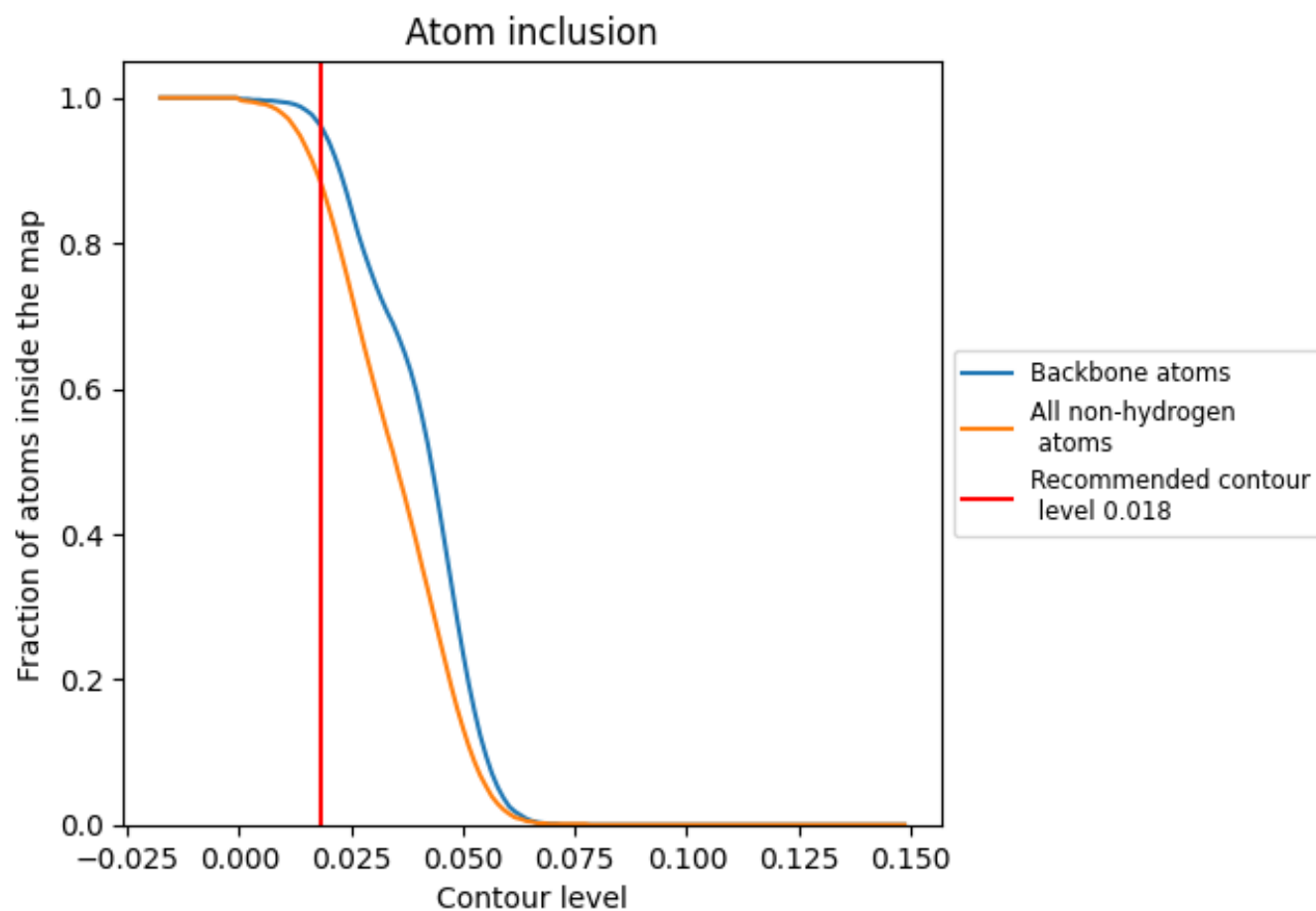
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.018) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8870   |  0.5450   |
| 1     |  0.9190   |  0.5650   |
| 2     |  0.9040   |  0.5490   |
| 3     |  0.9090   |  0.5620   |
| 6     |  0.9440   |  0.5730   |
| 7     |  0.9140   |  0.5630   |
| 9     |  0.9340   |  0.5780   |
| A     |  0.8790   |  0.5470   |
| C     |  0.9390   |  0.5860   |
| D     |  0.8860   |  0.5460   |
| H     |  0.9090   |  0.5490   |
| J     |  0.7760   |  0.4630   |
| K     |  0.8710   |  0.5380   |
| L     |  0.8910   |  0.5450   |
| M     |  0.9020  |  0.5640  |
| N     |  0.9020 |  0.5550 |
| O     |  0.8970 |  0.5430 |
| P     |  0.8910 |  0.5610 |
| Q     |  0.8940 |  0.5730 |
| S     |  0.8880 |  0.5410 |
| T     |  0.7260 |  0.4370 |
| U     |  0.8540 |  0.5220 |
| V     |  0.9020 |  0.5580 |
| W     |  0.8960 |  0.5610 |
| X     |  0.8850 |  0.5310 |
| Y     |  0.7650 |  0.4730 |
| Z     |  0.8700 |  0.5390 |
| a     |  0.9200 |  0.5490 |
| b     |  0.8840 |  0.5260 |
| c     |  0.8420 |  0.5180 |
| d     |  0.8610 |  0.5440 |
| e     |  0.8700 |  0.5280 |
| f     |  0.8130 |  0.4970 |
| g     |  0.8480 |  0.5230 |
| h     |  0.8830 |  0.5480 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.8180 |  0.5000 |
| j     |  0.8520 |  0.4990 |
| k     |  0.8830 |  0.5320 |
| l     |  0.8810 |  0.5450 |
| m     |  0.7870 |  0.5130 |
| n     |  0.9030 |  0.5420 |
| o     |  0.8570 |  0.5160 |
| p     |  0.8830 |  0.5310 |
| q     |  0.9230 |  0.5600 |
| r     |  0.8890 |  0.5540 |
| s     |  0.9370 |  0.5740 |