



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2025 – 10:59 am BST

PDB ID : 9IHQ / pdb\_00009ihq  
EMDB ID : EMD-52877  
Title : Closed state with NUQM and without flavoprotein (classification state 2) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs  
Authors : Grba, D.N.; Hirst, J.  
Deposited on : 2025-02-21  
Resolution : 2.90 Å(reported)  
Based on initial model : 9IHR

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.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

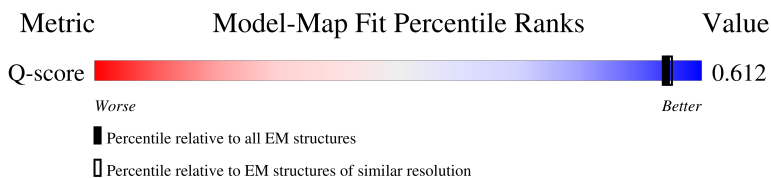
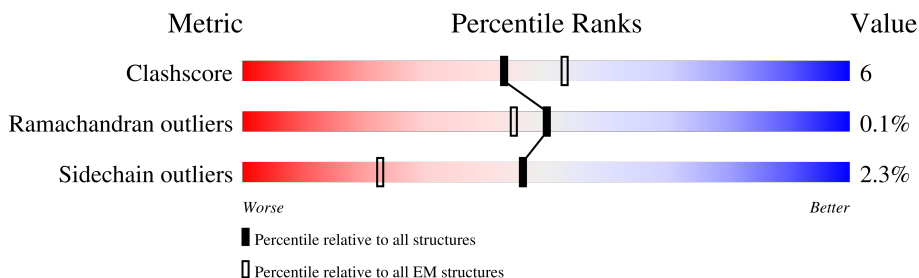
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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.









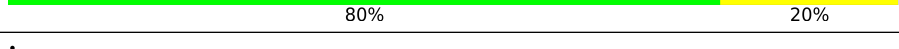
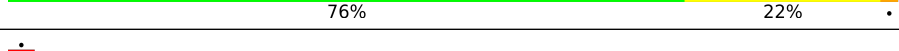
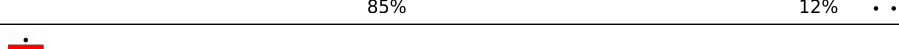
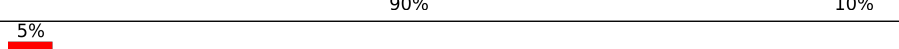

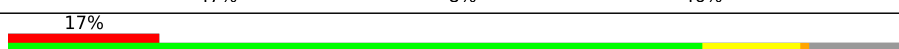


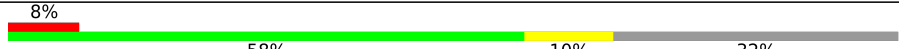


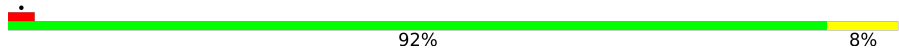


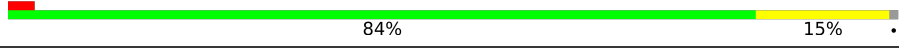
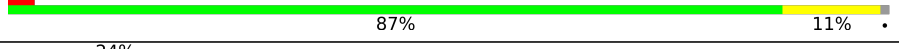



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 210492                      | 15764                       | -                                                        |
| Ramachandran outliers | 207382                      | 16835                       | -                                                        |
| Sidechain outliers    | 206894                      | 16415                       | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

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   | 1     | 190    | <div> <div>14%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>• 11%</div> </div> </div> |
| 2   | A     | 141    | <div> <div>•</div> <div> <div></div> <div>74%</div> <div>24%</div> <div>•</div> </div> </div>       |
| 3   | B     | 204    | <div> <div>•</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>• 14%</div> </div> </div>   |
| 4   | C     | 289    | <div> <div>10%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>17%</div> </div> </div>   |

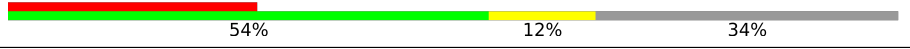



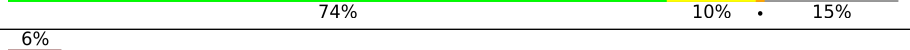
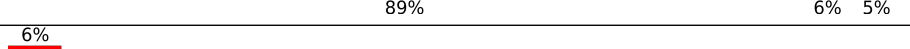
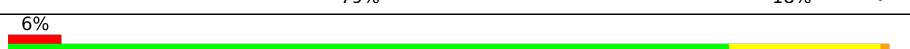
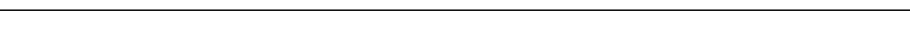
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 5   | D     | 482    |    |
| 6   | G     | 726    |    |
| 7   | H     | 353    |    |
| 8   | I     | 222    |    |
| 9   | J     | 161    |    |
| 10  | K     | 82     |    |
| 11  | L     | 642    |    |
| 12  | M     | 491    |    |
| 13  | N     | 523    |    |
| 14  | O     | 193    |    |
| 15  | P     | 384    |    |
| 16  | Q     | 159    |  |
| 17  | R     | 139    |  |
| 18  | S     | 90     |  |
| 19  | T     | 138    |  |
| 20  | U     | 130    |  |
| 21  | V     | 134    |  |
| 22  | W     | 122    |  |
| 23  | X     | 184    |  |
| 24  | Y     | 216    |  |
| 25  | Z     | 147    |  |
| 26  | a     | 150    |  |
| 27  | b     | 79     |  |
| 28  | c     | 182    |  |
| 29  | d     | 78     |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 30  | e     | 106    |    |
| 31  | f     | 86     |    |
| 32  | g     | 239    |    |
| 33  | h     | 182    |    |
| 34  | i     | 74     |    |
| 35  | j     | 59     |    |
| 36  | k     | 61     |    |
| 37  | l     | 156    |    |
| 38  | m     | 81     |    |
| 39  | n     | 111    |    |
| 40  | o     | 87     |    |
| 41  | p     | 92     |  |
| 42  | q     | 140    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 44  | SF4  | I     | 301 | -         | -        | X       | -                |
| 44  | SF4  | I     | 302 | -         | -        | X       | -                |

## 2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 64071 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 Altered inheritance of mitochondria protein 41, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1     | 169      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1383  | 879 | 231 | 272 | 1 |         |       |

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | A     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1133  | 764 | 166 | 199 | 4 |         |       |

- Molecule 3 is a protein called BA75\_00622T0.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | B     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1407  | 901 | 241 | 249 | 16 |         |       |

- Molecule 4 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | C     | 240      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1970  | 1273 | 331 | 361 | 5 |         |       |

- Molecule 5 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | D     | 451      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3621  | 2310 | 619 | 674 | 18 |         |       |

- Molecule 6 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | G     | 592      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4563  | 2862 | 798 | 882 | 21 |         |       |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | H     | 353      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2809  | 1903 | 414 | 478 | 14 |         |       |

- Molecule 8 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 8   | I     | 192      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1556  | 988 | 259 | 299 | 10 |         |       |

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | J     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1313  | 878 | 180 | 252 | 3 |         |       |

- Molecule 10 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 10  | K     | 80       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 617   | 400 | 93 | 118 | 6 |         |       |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | L     | 642      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5115  | 3454 | 766 | 866 | 29 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | M     | 491      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3868  | 2597 | 593 | 663 | 15 |         |       |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | N     | 506      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4045  | 2723 | 594 | 714 | 14 |         |       |

- Molecule 14 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | O     | 193      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1575  | 1019 | 257 | 294 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| O     | 0       | ACE      | -      | acetylation | UNP E1UWB9 |

- Molecule 15 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | P     | 368      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2922  | 1862 | 510 | 547 | 3 |         |       |

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | Q     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 711   | 451 | 119 | 139 | 2 |         |       |

- Molecule 17 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | R     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 978   | 610 | 179 | 186 | 3 |         |       |

- Molecule 18 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 18  | S     | 90       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 697   | 454 | 117 | 126 |  |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| S     | 0       | ACE      | -      | acetylation | UNP E1UWD3 |

- Molecule 19 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | T     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 745   | 467 | 119 | 158 | 1 |         |       |

- Molecule 20 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | U     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 681   | 427 | 102 | 152 |   |         |       |

- Molecule 21 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | V     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1025  | 658 | 165 | 201 | 1 |         |       |

- Molecule 22 is a protein called BA75\_04796T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | W     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 626 | 177 | 171 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | X     | 184      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1450  | 905 | 253 | 282 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| X     | 0       | ACE      | -      | acetylation | UNP E1UWB8 |

- Molecule 24 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 24  | Y     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1012 | 274 | 289 | 3 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Z     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1176  | 758 | 212 | 202 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| Z     | 0       | ACE      | -      | acetylation | UNP E1UWD8 |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | a     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1215  | 756 | 228 | 225 | 6 |         |       |

- Molecule 27 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | b     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 419 | 111 | 109 | 2 |         |       |

- Molecule 28 is a protein called BA75\_00589T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | c     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1256  | 799 | 221 | 234 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| c     | 0       | ACE      | -      | acetylation | UNP E1UWC1 |

- Molecule 29 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | d     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 616   | 406 | 106 | 103 | 1 |         |       |

- Molecule 30 is a protein called BA75\_05084T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | e     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 531 | 154 | 157 | 6 |         |       |

- Molecule 31 is a protein called NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | f     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 428 | 113 | 101 |   |         |       |

- Molecule 32 is a protein called NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | g     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1280  | 815 | 210 | 252 | 3 |         |       |

- Molecule 33 is a protein called NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | h     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1078  | 699 | 183 | 196 |   |         |       |

- Molecule 34 is a protein called NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | i     | 69       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 552   | 358 | 95 | 97 | 2 |         |       |

- Molecule 35 is a protein called Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | j     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 460   | 319 | 76 | 64 | 1 |         |       |

- Molecule 36 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | k     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 368   | 240 | 71 | 56 | 1 |         |       |

- Molecule 37 is a protein called NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | l     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 706 | 175 | 200 | 1 |         |       |

- Molecule 38 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | m     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 418 | 116 | 108 |   |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | n     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 861   | 550 | 155 | 155 | 1 |         |       |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | o     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 682   | 428 | 126 | 122 | 6 |         |       |

- Molecule 41 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | p     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 740   | 457 | 135 | 144 | 4 |         |       |

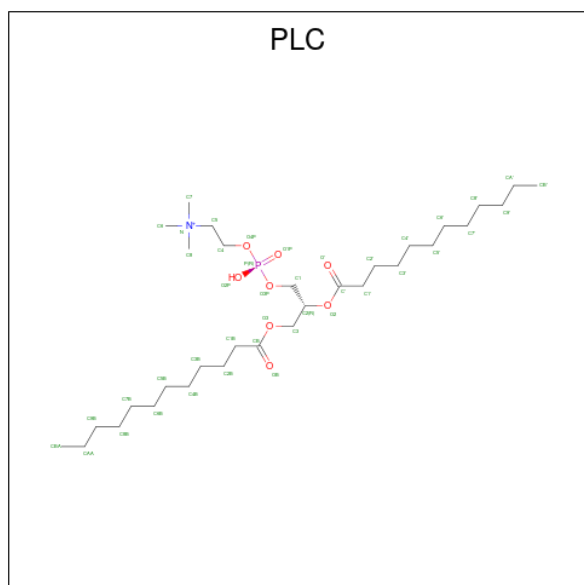
- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | q     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 741 | 201 | 211 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| q     | 0       | ACE      | -      | acetylation | UNP E1UWE0 |

- Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $C_{32}H_{65}NO_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 43  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 43  | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 43  | D     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 24    | 14 | 1 | 8 | 1 |         |

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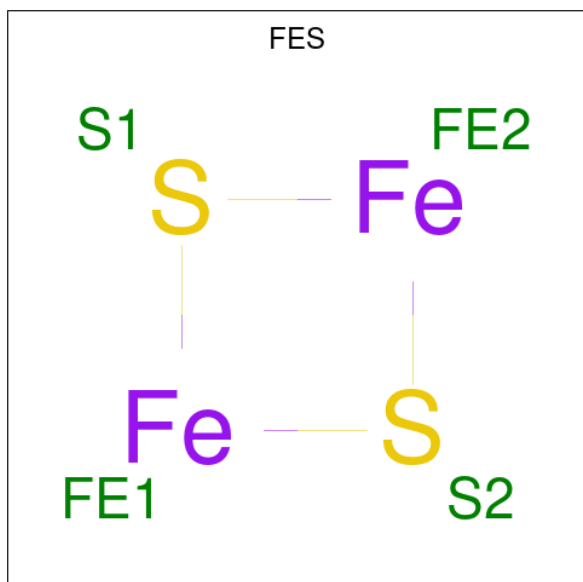
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 43  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 43  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 32    | 22 | 1 | 8 | 1 |         |
| 43  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | P     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 43  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 43  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 43  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 12 | 1 | 8 | 1 |         |
| 43  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 43  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | d     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | g     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |
| 43  | h     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | q     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 43  | q     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |

- Molecule 44 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 44  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 44  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 44  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 44  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 44  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).

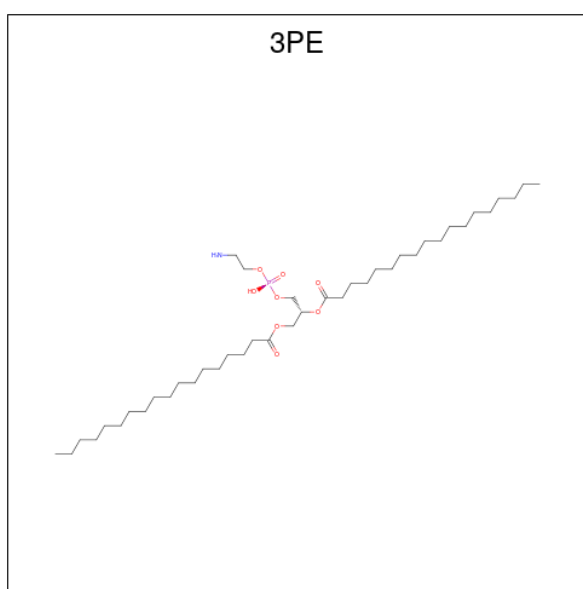


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 46  | G     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 47 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 47  | H     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |

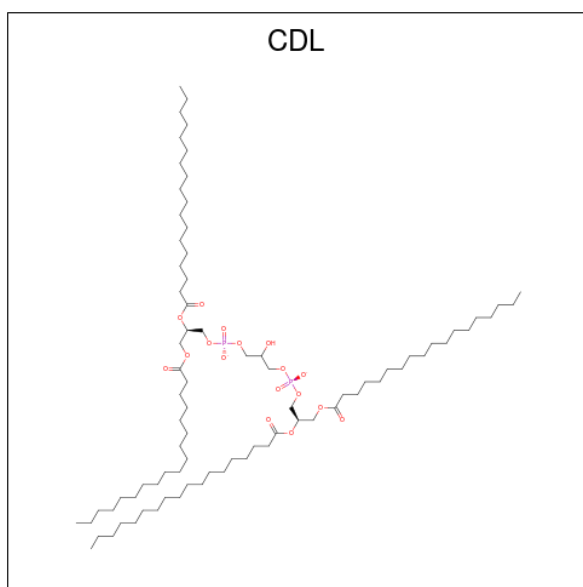
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 47  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 47  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 47  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 47  | O     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 47  | O     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 47  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 26    | 16 | 1 | 8 | 1 |         |
| 47  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 47  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 47  | f     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 47  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 27    | 17 | 1 | 8 | 1 |         |
| 47  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 25    | 15 | 1 | 8 | 1 |         |
| 47  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |

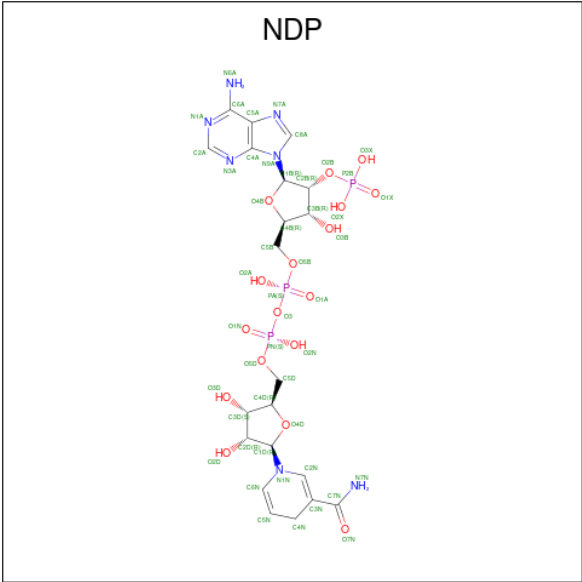
- Molecule 48 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).





| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 48  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 75    | 56 | 17 | 2 |         |
| 48  | P     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 42    | 23 | 17 | 2 |         |
| 48  | Z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 30 | 17 | 2 |         |
| 48  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 59    | 40 | 17 | 2 |         |
| 48  | c     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 60    | 41 | 17 | 2 |         |

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

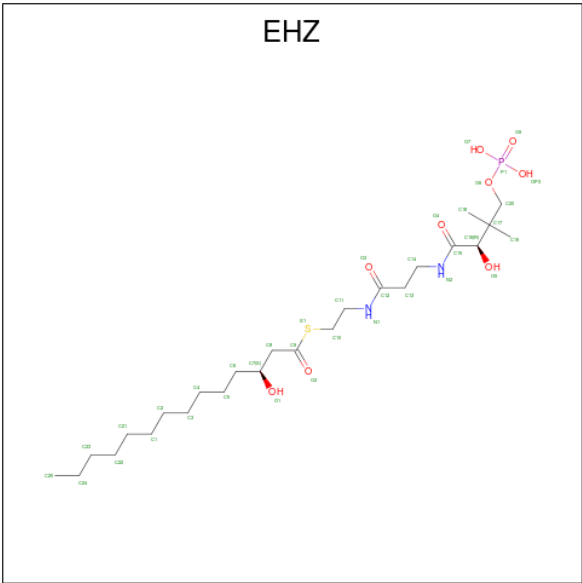


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 49  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 50  | R     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 51 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).

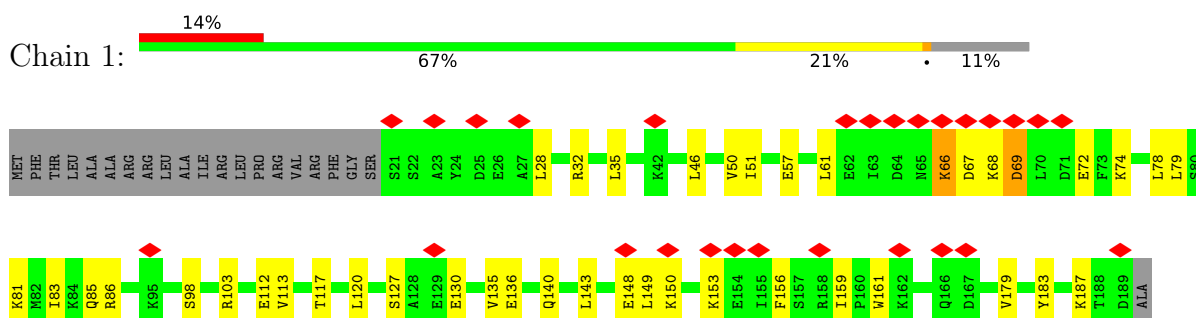


| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 51  | T     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 51  | U     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |

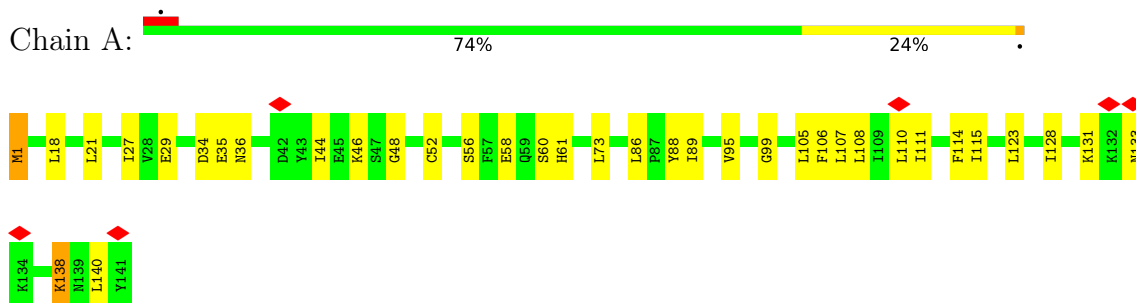
### 3 Residue-property plots [i](#)

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

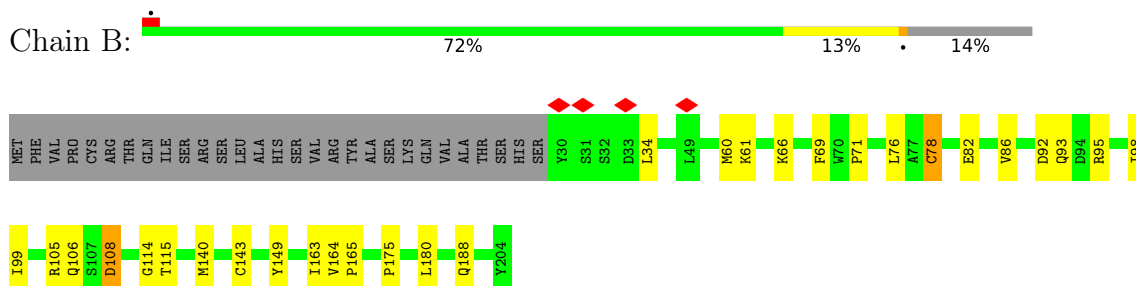
- Molecule 1: Altered inheritance of mitochondria protein 41, mitochondrial



- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

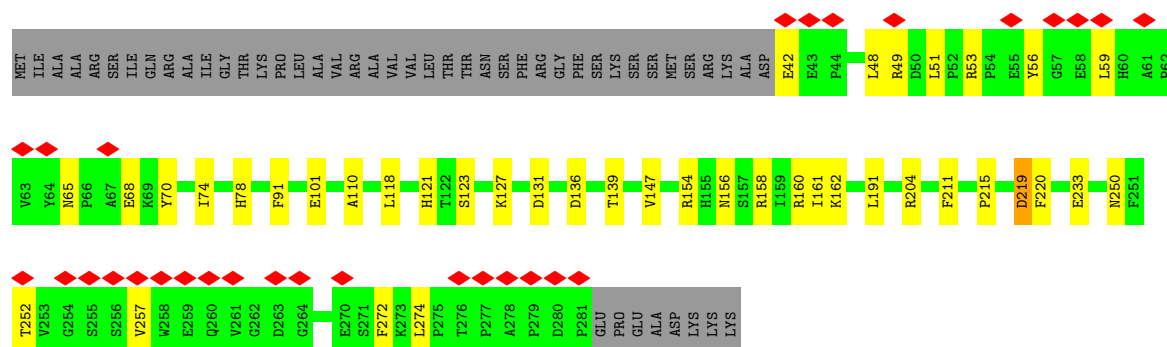


- Molecule 3: BA75\_00622T0



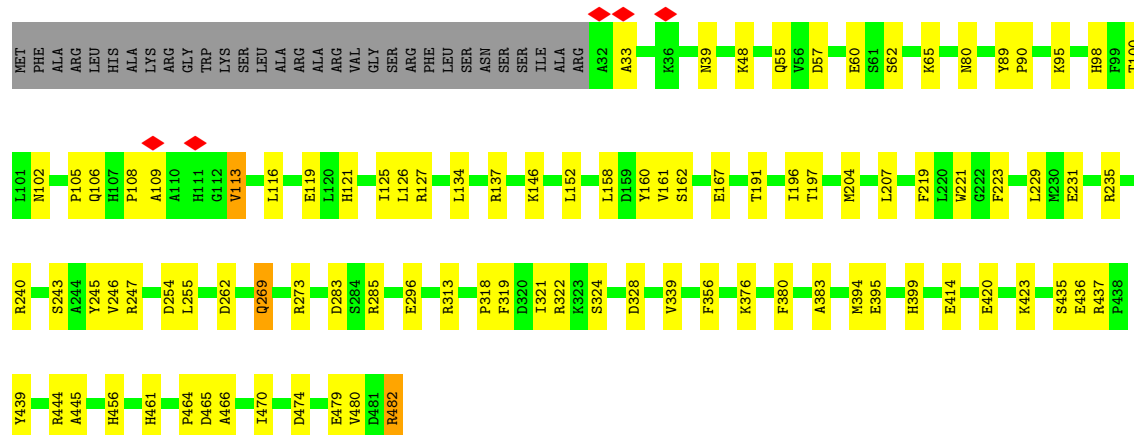
- Molecule 4: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)





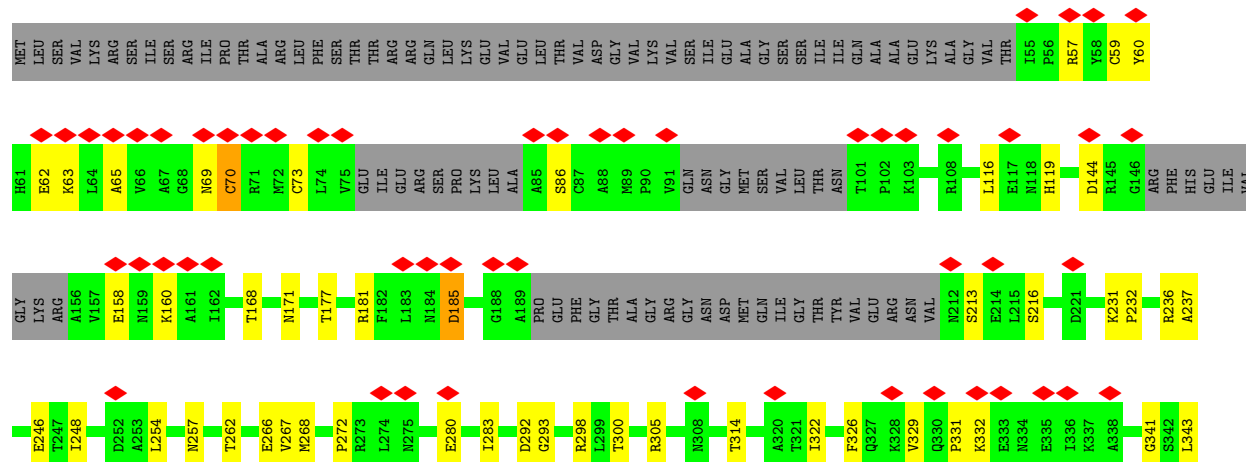
- Molecule 5: NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

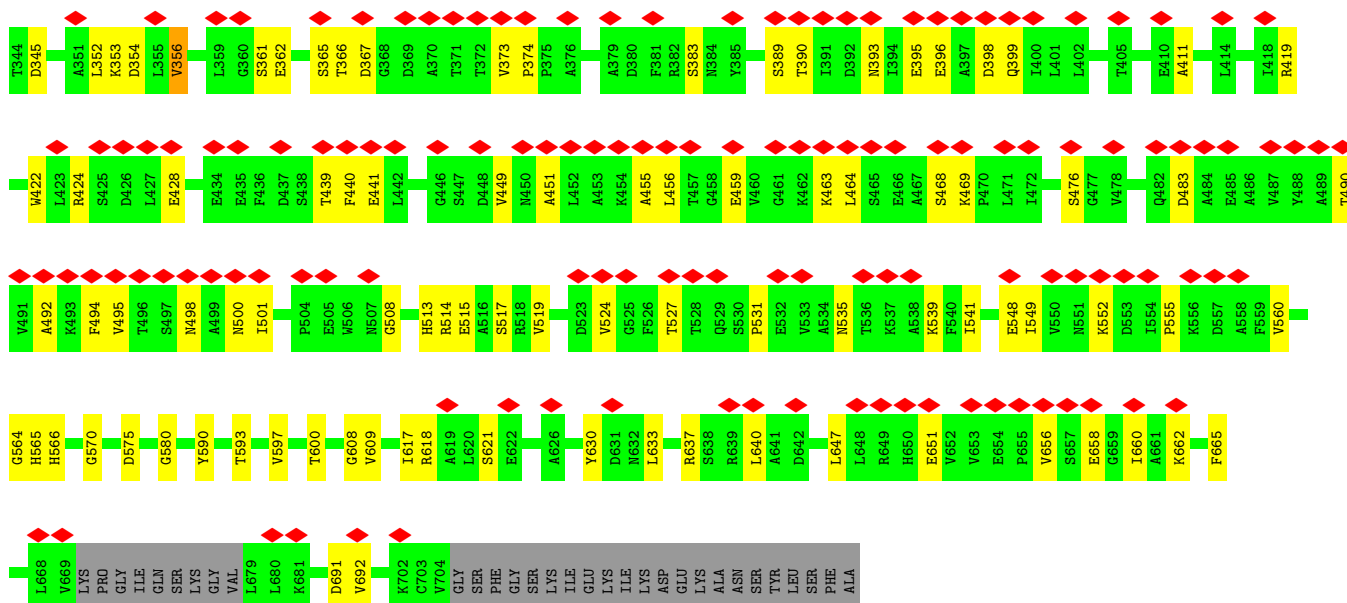
Chain D: 74% 19% 6%



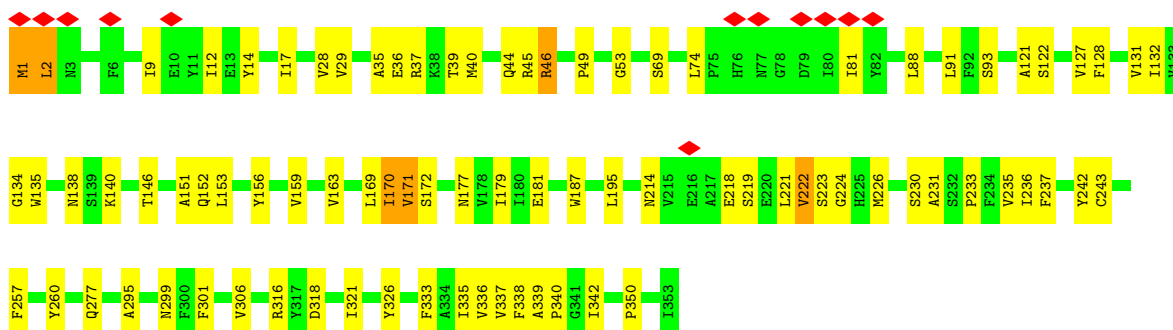
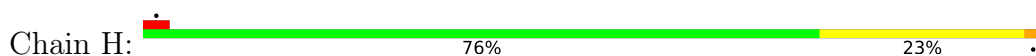
- Molecule 6: NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain G: 26% 62% 19% 18%

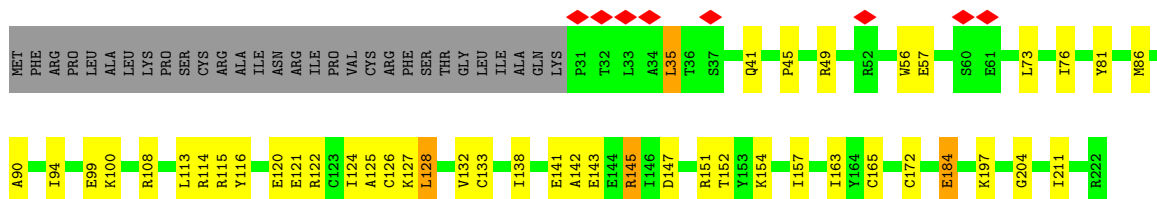




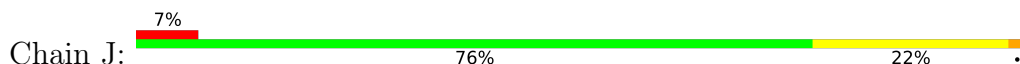
• Molecule 7: NADH-ubiquinone oxidoreductase chain 1

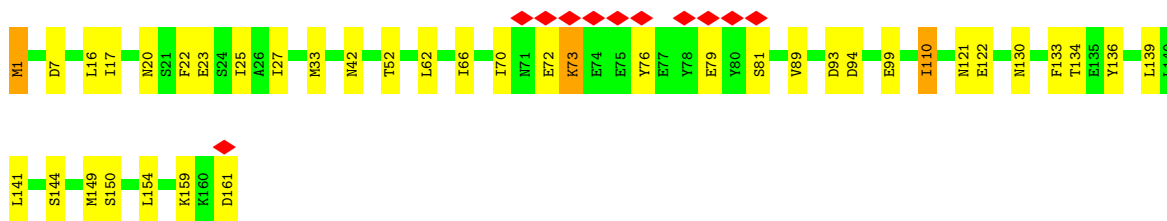


• Molecule 8: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

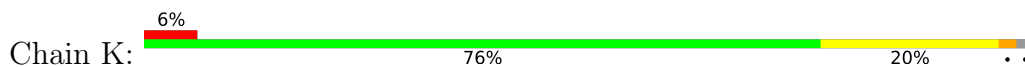


• Molecule 9: NADH-ubiquinone oxidoreductase chain 6

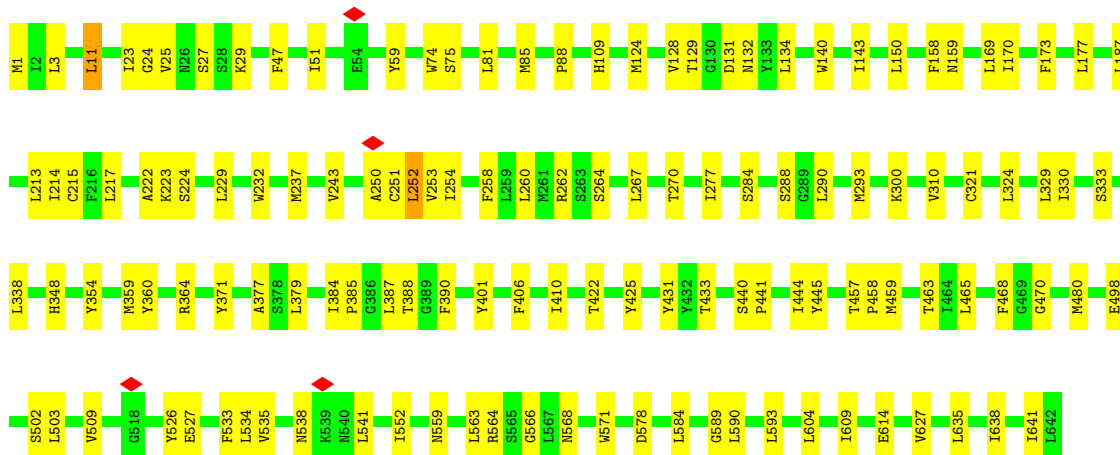
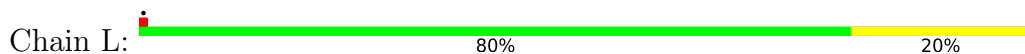




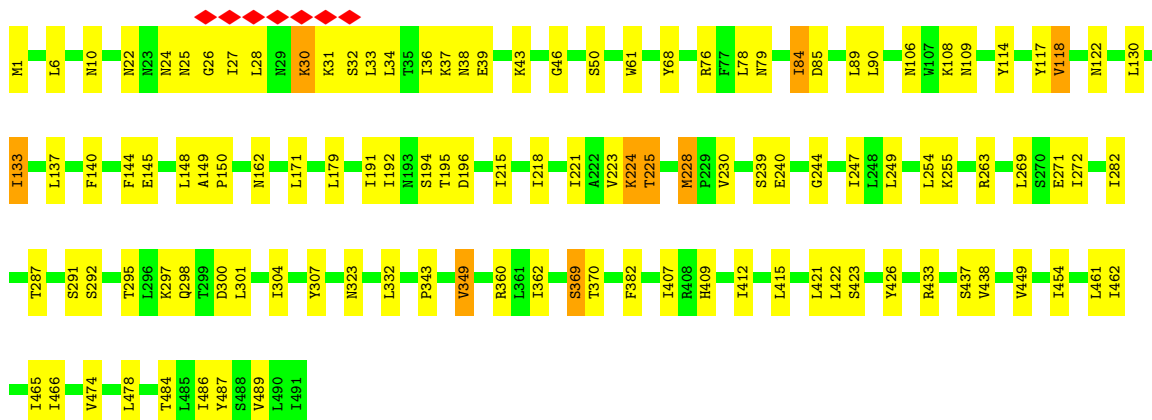
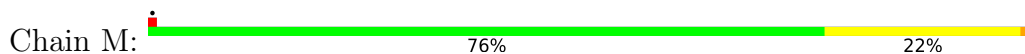
- Molecule 10: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



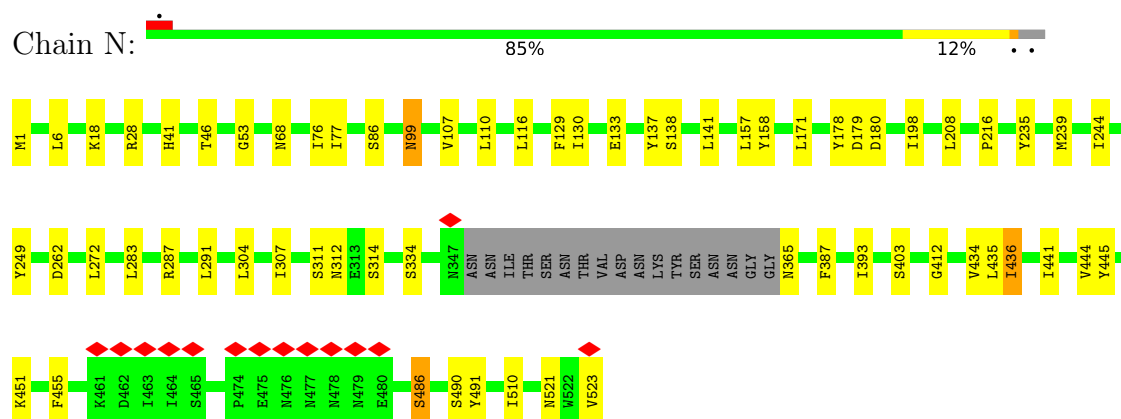
- Molecule 11: NADH-ubiquinone oxidoreductase chain 5



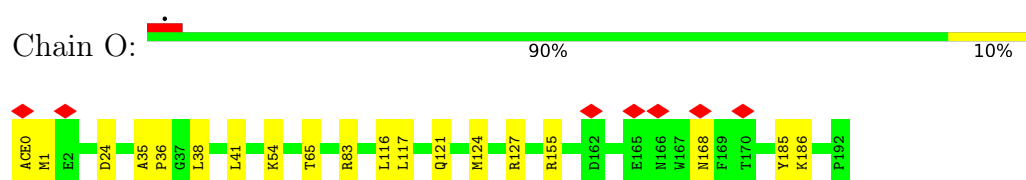
- Molecule 12: NADH-ubiquinone oxidoreductase chain 4



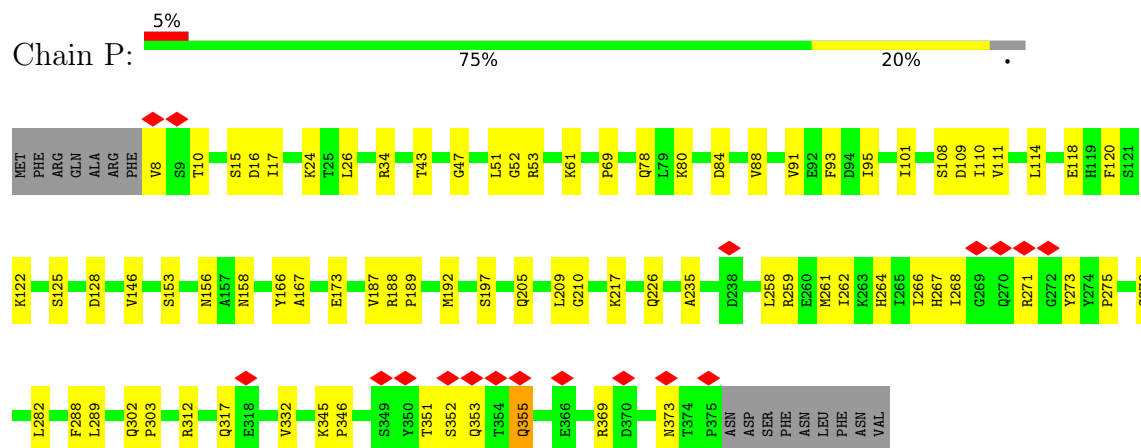
- Molecule 13: NADH-ubiquinone oxidoreductase chain 2



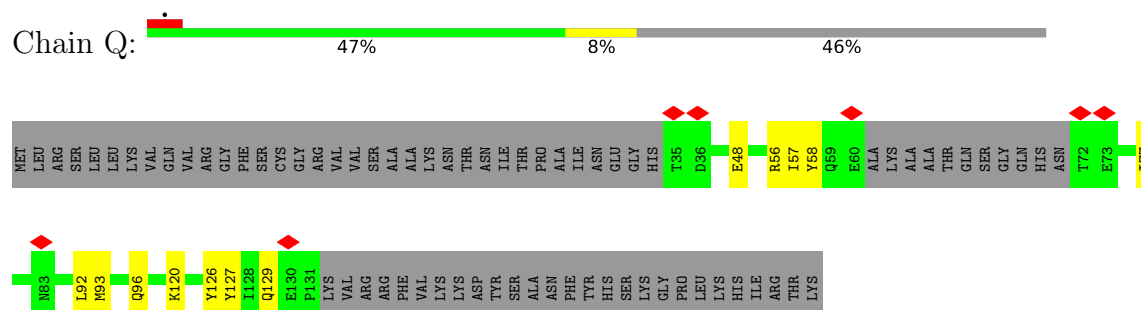
- Molecule 14: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 15: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)




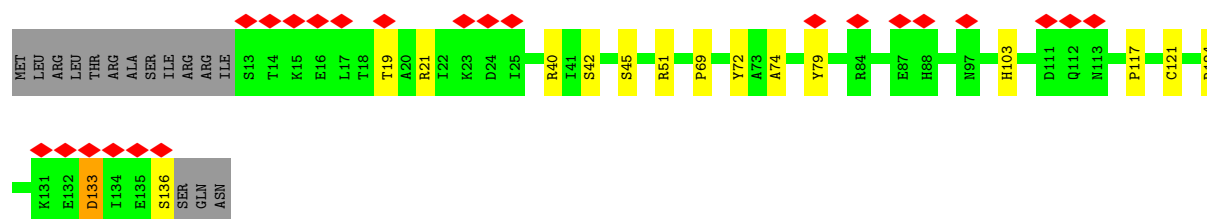
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial






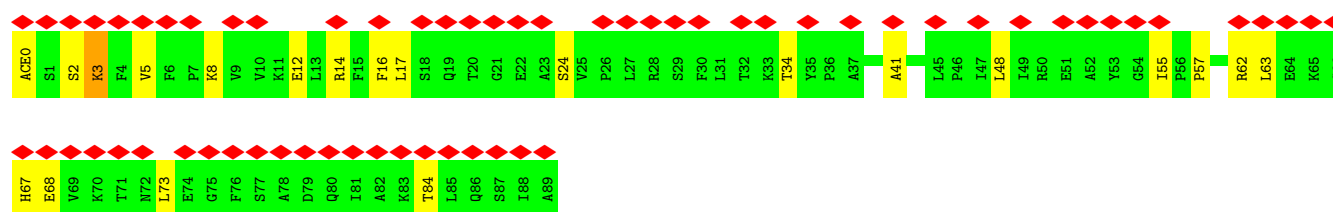
- Molecule 17: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain R: 



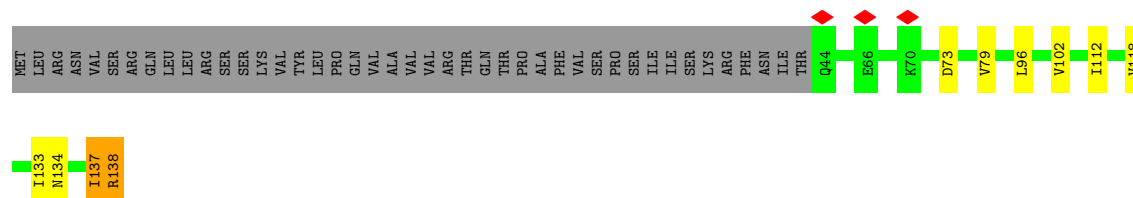
- Molecule 18: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain S: 



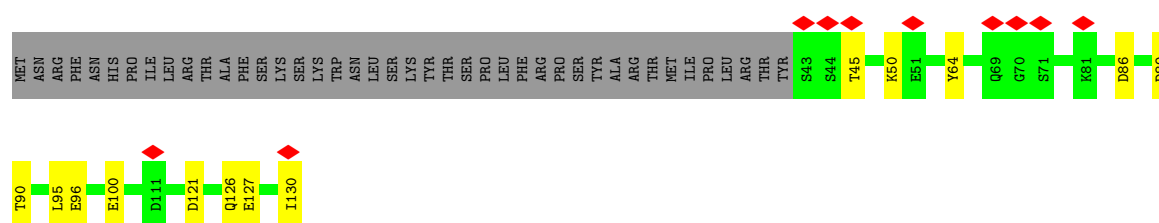
- Molecule 19: Acyl carrier protein

Chain T: 




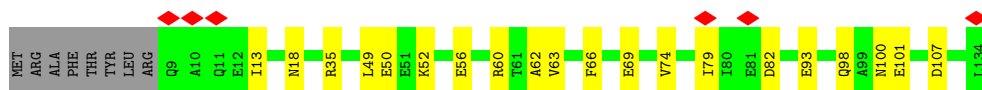
- Molecule 20: Acyl carrier protein

Chain U: 

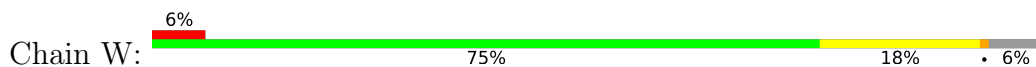


- Molecule 21: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain V: 



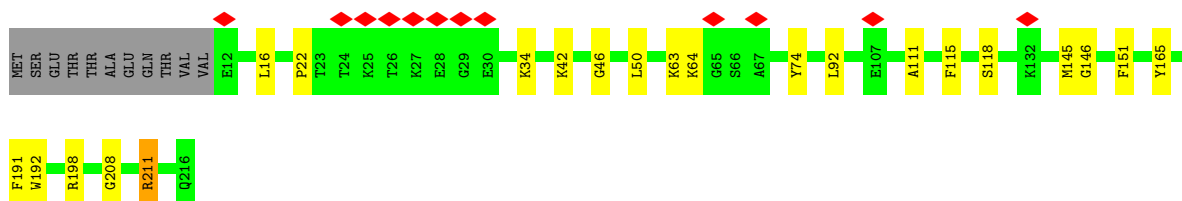
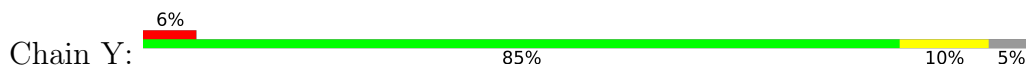
- Molecule 22: BA75\_04796T0



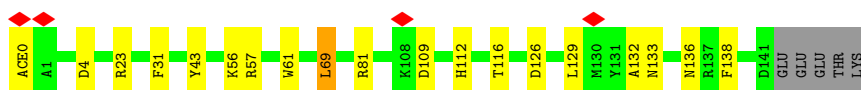
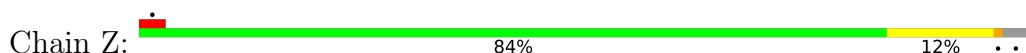
- Molecule 23: NADH-ubiquinone oxidoreductase



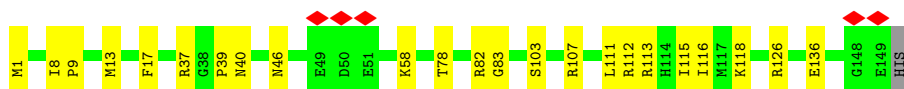
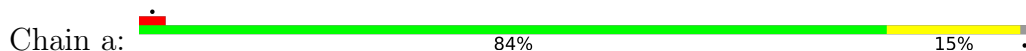
- Molecule 24: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



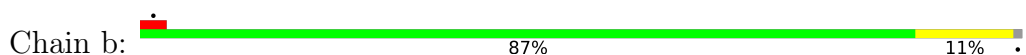
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

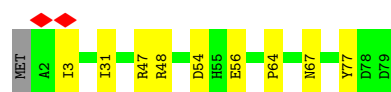


- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

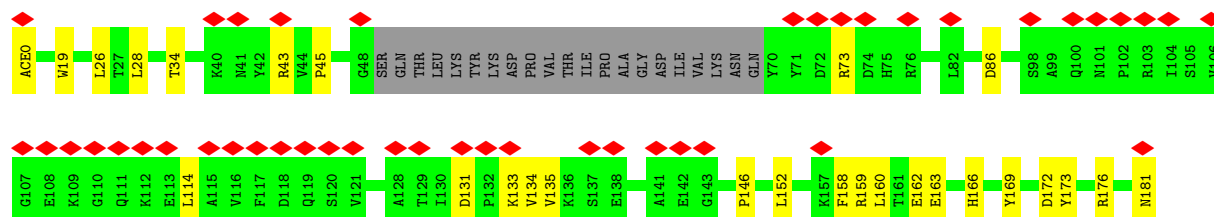
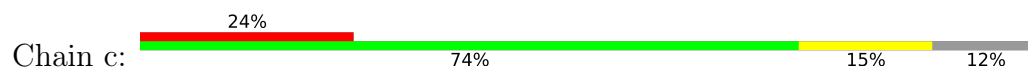


- Molecule 27: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

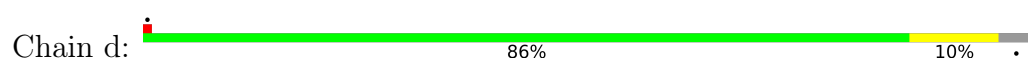




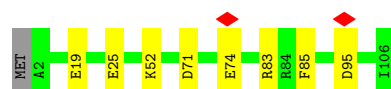
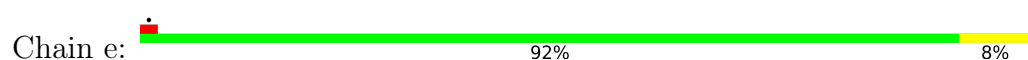
• Molecule 28: BA75\_00589T0



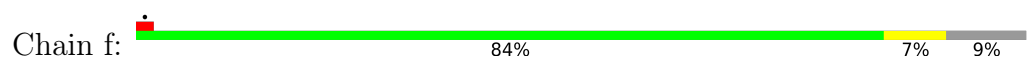
• Molecule 29: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM



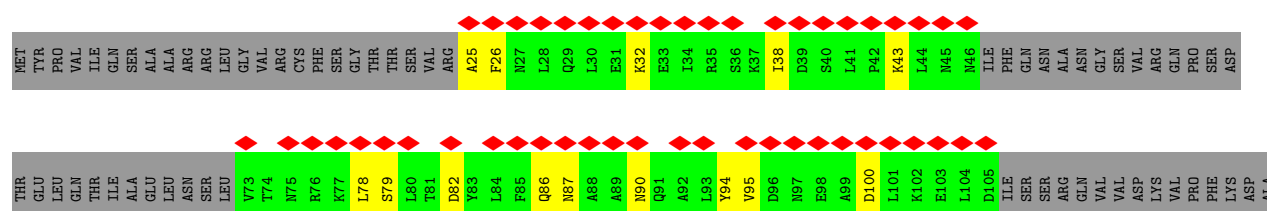
• Molecule 30: BA75\_05084T0

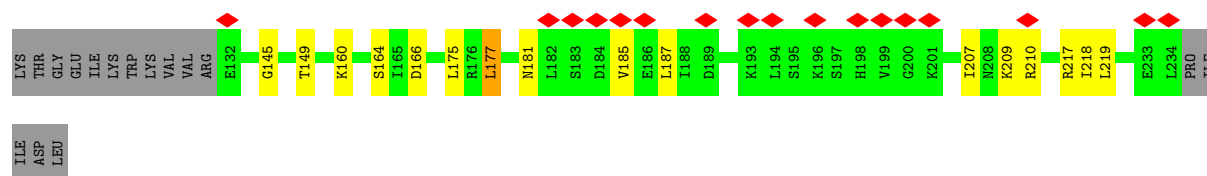


• Molecule 31: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

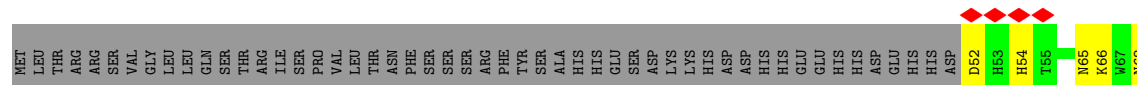


• Molecule 32: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

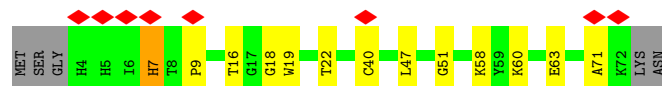
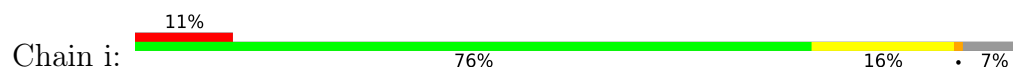




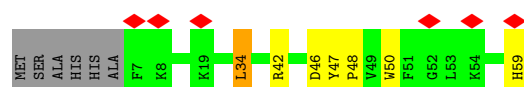
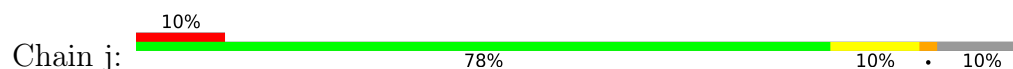
- Molecule 33: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



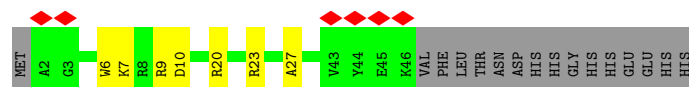
- Molecule 34: NUUM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 35: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

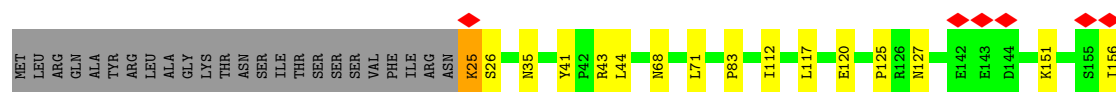


- Molecule 36: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

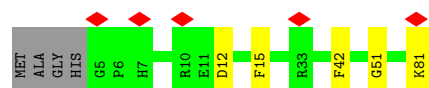
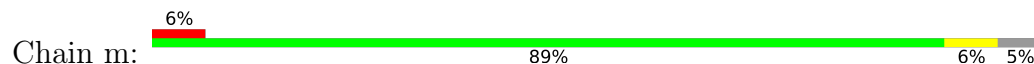


- Molecule 37: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

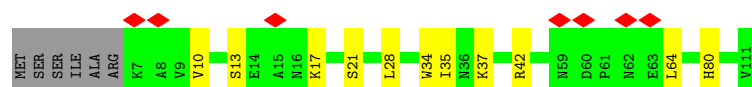
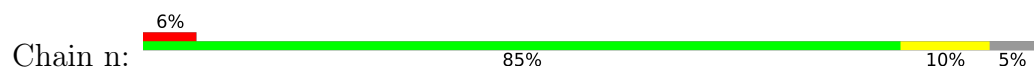




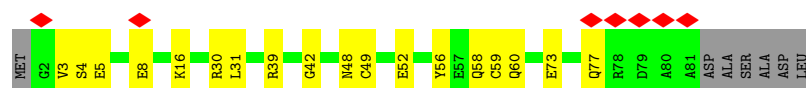
- Molecule 38: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



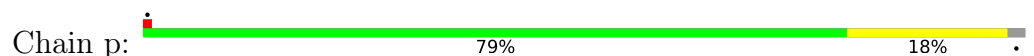
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



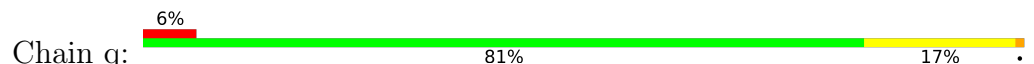
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 41: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



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



## 4 Experimental information

| Property                             | Value                   | Source    |
|--------------------------------------|-------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE         | Depositor |
| Imposed symmetry                     | POINT, C1               | Depositor |
| Number of particles used             | 61256                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF       | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY     | Depositor |
| Microscope                           | TFS KRIOS               | Depositor |
| Voltage (kV)                         | 300                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 47.79                   | Depositor |
| Minimum defocus (nm)                 | 600                     | Depositor |
| Maximum defocus (nm)                 | 1800                    | Depositor |
| Magnification                        | 130000                  | Depositor |
| Image detector                       | TFS FALCON 4i (4k x 4k) | Depositor |
| Maximum map value                    | 0.079                   | Depositor |
| Minimum map value                    | -0.036                  | Depositor |
| Average map value                    | -0.000                  | Depositor |
| Map value standard deviation         | 0.003                   | Depositor |
| Recommended contour level            | 0.0127                  | Depositor |
| Map size ( $\text{\AA}$ )            | 501.66, 501.66, 501.66  | wwPDB     |
| Map dimensions                       | 540, 540, 540           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.929, 0.929, 0.929     | 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: SF4, K, CDL, 3PE, PLC, FME, EHZ, NDP, ACE, ZN, FES, 2MR

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   | 1     | 0.11         | 0/1405        | 0.25        | 0/1896       |
| 2   | A     | 0.13         | 0/1151        | 0.23        | 0/1564       |
| 3   | B     | 0.16         | 0/1450        | 0.27        | 0/1969       |
| 4   | C     | 0.14         | 0/2033        | 0.26        | 0/2770       |
| 5   | D     | 0.14         | 0/3698        | 0.26        | 0/5007       |
| 6   | G     | 0.11         | 0/4642        | 0.27        | 0/6299       |
| 7   | H     | 0.15         | 0/2880        | 0.27        | 0/3939       |
| 8   | I     | 0.15         | 0/1596        | 0.28        | 0/2164       |
| 9   | J     | 0.14         | 0/1329        | 0.28        | 0/1816       |
| 10  | K     | 0.13         | 0/610         | 0.24        | 0/828        |
| 11  | L     | 0.14         | 0/5236        | 0.26        | 0/7128       |
| 12  | M     | 0.15         | 0/3940        | 0.27        | 0/5379       |
| 13  | N     | 0.14         | 0/4110        | 0.26        | 0/5609       |
| 14  | O     | 0.21         | 1/1621 (0.1%) | 0.28        | 0/2199       |
| 15  | P     | 0.13         | 0/2985        | 0.26        | 0/4035       |
| 16  | Q     | 0.13         | 0/726         | 0.24        | 0/979        |
| 17  | R     | 0.11         | 0/998         | 0.25        | 0/1350       |
| 18  | S     | 0.26         | 1/710 (0.1%)  | 0.32        | 1/961 (0.1%) |
| 19  | T     | 0.10         | 0/752         | 0.23        | 0/1021       |
| 20  | U     | 0.11         | 0/688         | 0.22        | 0/936        |
| 21  | V     | 0.12         | 0/1044        | 0.24        | 0/1411       |
| 22  | W     | 0.12         | 0/999         | 0.21        | 0/1340       |
| 23  | X     | 0.20         | 1/1475 (0.1%) | 0.25        | 0/1990       |
| 24  | Y     | 0.12         | 0/1615        | 0.24        | 0/2175       |
| 25  | Z     | 0.22         | 1/1210 (0.1%) | 0.24        | 0/1639       |
| 26  | a     | 0.13         | 0/1241        | 0.25        | 0/1670       |
| 27  | b     | 0.13         | 0/666         | 0.25        | 0/911        |
| 28  | c     | 0.21         | 1/1282 (0.1%) | 0.25        | 0/1736       |
| 29  | d     | 0.12         | 0/633         | 0.21        | 0/854        |
| 30  | e     | 0.13         | 0/865         | 0.24        | 0/1158       |
| 31  | f     | 0.12         | 0/663         | 0.20        | 0/896        |
| 32  | g     | 0.11         | 0/1293        | 0.24        | 0/1735       |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 33  | h     | 0.13         | 0/1114         | 0.27        | 0/1516         |
| 34  | i     | 0.14         | 0/571          | 0.31        | 0/777          |
| 35  | j     | 0.11         | 0/484          | 0.25        | 0/658          |
| 36  | k     | 0.12         | 0/382          | 0.23        | 0/514          |
| 37  | l     | 0.13         | 0/1119         | 0.27        | 0/1520         |
| 38  | m     | 0.12         | 0/661          | 0.23        | 0/893          |
| 39  | n     | 0.12         | 0/884          | 0.23        | 0/1197         |
| 40  | o     | 0.11         | 0/696          | 0.22        | 0/933          |
| 41  | p     | 0.13         | 0/756          | 0.25        | 0/1020         |
| 42  | q     | 0.22         | 1/1192 (0.1%)  | 0.29        | 0/1620         |
| All | All   | 0.14         | 6/63405 (0.0%) | 0.26        | 1/86012 (0.0%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 18  | S     | 0   | ACE  | C-N   | 6.21 | 1.45        | 1.33     |
| 14  | O     | 0   | ACE  | C-N   | 6.15 | 1.45        | 1.33     |
| 28  | c     | 0   | ACE  | C-N   | 6.14 | 1.45        | 1.33     |
| 25  | Z     | 0   | ACE  | C-N   | 6.13 | 1.45        | 1.33     |
| 42  | q     | 0   | ACE  | C-N   | 6.08 | 1.45        | 1.33     |
| 23  | X     | 0   | ACE  | C-N   | 5.96 | 1.45        | 1.33     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 18  | S     | 2   | SER  | CB-CA-C | -5.28 | 109.51      | 115.79   |

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   | 1     | 1383  | 0        | 1390     | 24      | 0            |
| 2   | A     | 1133  | 0        | 1167     | 32      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | B     | 1407  | 0        | 1372     | 28      | 0            |
| 4   | C     | 1970  | 0        | 1905     | 26      | 0            |
| 5   | D     | 3621  | 0        | 3531     | 62      | 0            |
| 6   | G     | 4563  | 0        | 4527     | 89      | 0            |
| 7   | H     | 2809  | 0        | 2880     | 60      | 0            |
| 8   | I     | 1556  | 0        | 1499     | 31      | 0            |
| 9   | J     | 1313  | 0        | 1320     | 36      | 0            |
| 10  | K     | 617   | 0        | 657      | 18      | 0            |
| 11  | L     | 5115  | 0        | 5338     | 90      | 0            |
| 12  | M     | 3868  | 0        | 4127     | 75      | 0            |
| 13  | N     | 4045  | 0        | 4327     | 42      | 0            |
| 14  | O     | 1575  | 0        | 1523     | 11      | 0            |
| 15  | P     | 2922  | 0        | 2915     | 53      | 0            |
| 16  | Q     | 711   | 0        | 679      | 9       | 0            |
| 17  | R     | 978   | 0        | 964      | 11      | 0            |
| 18  | S     | 697   | 0        | 736      | 12      | 0            |
| 19  | T     | 745   | 0        | 734      | 7       | 0            |
| 20  | U     | 681   | 0        | 664      | 7       | 0            |
| 21  | V     | 1025  | 0        | 1035     | 14      | 0            |
| 22  | W     | 979   | 0        | 980      | 15      | 0            |
| 23  | X     | 1450  | 0        | 1422     | 10      | 0            |
| 24  | Y     | 1578  | 0        | 1567     | 16      | 0            |
| 25  | Z     | 1176  | 0        | 1165     | 15      | 0            |
| 26  | a     | 1215  | 0        | 1197     | 19      | 0            |
| 27  | b     | 641   | 0        | 620      | 7       | 0            |
| 28  | c     | 1256  | 0        | 1281     | 20      | 0            |
| 29  | d     | 616   | 0        | 624      | 6       | 0            |
| 30  | e     | 848   | 0        | 830      | 9       | 0            |
| 31  | f     | 642   | 0        | 640      | 7       | 0            |
| 32  | g     | 1280  | 0        | 1302     | 19      | 0            |
| 33  | h     | 1078  | 0        | 1036     | 16      | 0            |
| 34  | i     | 552   | 0        | 540      | 11      | 0            |
| 35  | j     | 460   | 0        | 455      | 5       | 0            |
| 36  | k     | 368   | 0        | 348      | 6       | 0            |
| 37  | l     | 1082  | 0        | 1033     | 9       | 0            |
| 38  | m     | 642   | 0        | 635      | 5       | 0            |
| 39  | n     | 861   | 0        | 866      | 8       | 0            |
| 40  | o     | 682   | 0        | 677      | 9       | 0            |
| 41  | p     | 740   | 0        | 700      | 13      | 0            |
| 42  | q     | 1156  | 0        | 1115     | 20      | 0            |
| 43  | A     | 31    | 0        | 36       | 2       | 0            |
| 43  | B     | 31    | 0        | 36       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | D     | 42    | 0        | 64       | 2       | 0            |
| 43  | H     | 24    | 0        | 22       | 1       | 0            |
| 43  | L     | 109   | 0        | 146      | 9       | 0            |
| 43  | M     | 84    | 0        | 128      | 5       | 0            |
| 43  | P     | 31    | 0        | 36       | 4       | 0            |
| 43  | Y     | 72    | 0        | 98       | 5       | 0            |
| 43  | Z     | 42    | 0        | 64       | 0       | 0            |
| 43  | a     | 22    | 0        | 18       | 2       | 0            |
| 43  | b     | 39    | 0        | 55       | 1       | 0            |
| 43  | d     | 84    | 0        | 128      | 4       | 0            |
| 43  | g     | 39    | 0        | 55       | 3       | 0            |
| 43  | h     | 42    | 0        | 64       | 2       | 0            |
| 43  | q     | 78    | 0        | 113      | 4       | 0            |
| 44  | B     | 8     | 0        | 0        | 0       | 0            |
| 44  | G     | 16    | 0        | 0        | 1       | 0            |
| 44  | I     | 16    | 0        | 0        | 4       | 0            |
| 45  | G     | 4     | 0        | 0        | 0       | 0            |
| 46  | G     | 1     | 0        | 0        | 0       | 0            |
| 47  | H     | 31    | 0        | 36       | 0       | 0            |
| 47  | L     | 400   | 0        | 596      | 36      | 0            |
| 47  | M     | 35    | 0        | 44       | 1       | 0            |
| 47  | N     | 40    | 0        | 57       | 1       | 0            |
| 47  | O     | 66    | 0        | 80       | 2       | 0            |
| 47  | Y     | 26    | 0        | 26       | 2       | 0            |
| 47  | Z     | 36    | 0        | 46       | 3       | 0            |
| 47  | b     | 40    | 0        | 57       | 1       | 0            |
| 47  | f     | 51    | 0        | 82       | 6       | 0            |
| 47  | j     | 27    | 0        | 28       | 1       | 0            |
| 47  | m     | 60    | 0        | 68       | 2       | 0            |
| 48  | O     | 75    | 0        | 97       | 4       | 0            |
| 48  | P     | 42    | 0        | 28       | 1       | 0            |
| 48  | Z     | 49    | 0        | 42       | 0       | 0            |
| 48  | b     | 59    | 0        | 62       | 3       | 0            |
| 48  | c     | 60    | 0        | 64       | 3       | 0            |
| 49  | P     | 48    | 0        | 25       | 0       | 0            |
| 50  | R     | 1     | 0        | 0        | 0       | 0            |
| 51  | T     | 37    | 0        | 0        | 0       | 0            |
| 51  | U     | 37    | 0        | 0        | 1       | 0            |
| All | All   | 64071 | 0        | 64824    | 826     | 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 (826) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:R:103:HIS:CD2  | 17:R:121:CYS:SG   | 2.68                     | 0.87              |
| 12:M:24:ASN:HB3   | 12:M:30:LYS:HD2   | 1.65                     | 0.78              |
| 43:L:705:PLC:H42  | 34:i:18:GLY:HA2   | 1.64                     | 0.78              |
| 5:D:380:PHE:HB2   | 6:G:144:ASP:HB2   | 1.69                     | 0.73              |
| 5:D:121:HIS:HB2   | 5:D:126:LEU:HD11  | 1.71                     | 0.72              |
| 21:V:35:ARG:NH2   | 21:V:74:VAL:O     | 2.23                     | 0.72              |
| 8:I:115:ARG:NH2   | 17:R:72:TYR:O     | 2.23                     | 0.72              |
| 6:G:419:ARG:NH1   | 6:G:439:THR:O     | 2.23                     | 0.71              |
| 12:M:36:ILE:HG22  | 12:M:37:LYS:HG3   | 1.73                     | 0.71              |
| 16:Q:120:LYS:NZ   | 16:Q:126:TYR:OH   | 2.22                     | 0.71              |
| 25:Z:57:ARG:NH2   | 27:b:56:GLU:O     | 2.24                     | 0.71              |
| 35:j:42:ARG:NH2   | 35:j:46:ASP:OD2   | 2.24                     | 0.70              |
| 6:G:356:VAL:HG13  | 6:G:361:SER:HB3   | 1.74                     | 0.70              |
| 5:D:191:THR:OG1   | 5:D:328:ASP:O     | 2.10                     | 0.70              |
| 15:P:268:ILE:HG22 | 15:P:275:PRO:HG3  | 1.73                     | 0.69              |
| 15:P:353:GLN:NE2  | 22:W:41:ASN:OD1   | 2.25                     | 0.69              |
| 4:C:101:GLU:OE1   | 4:C:160:ARG:NH2   | 2.25                     | 0.69              |
| 6:G:59:CYS:HB3    | 6:G:70:CYS:HB3    | 1.73                     | 0.69              |
| 3:B:163:ILE:HG22  | 3:B:164:VAL:HG13  | 1.73                     | 0.69              |
| 11:L:223:LYS:HD3  | 11:L:252:LEU:HD12 | 1.75                     | 0.69              |
| 8:I:163:ILE:HG13  | 8:I:165:CYS:HB3   | 1.74                     | 0.69              |
| 32:g:160:LYS:HZ3  | 33:h:104:ILE:HD11 | 1.58                     | 0.69              |
| 2:A:138:LYS:NZ    | 21:V:100:ASN:OD1  | 2.26                     | 0.69              |
| 3:B:86:VAL:HG21   | 3:B:180:LEU:HD23  | 1.74                     | 0.68              |
| 6:G:65:ALA:O      | 6:G:181:ARG:NH1   | 2.27                     | 0.68              |
| 5:D:161:VAL:HG11  | 5:D:204:MET:HG2   | 1.76                     | 0.67              |
| 41:p:44:CYS:SG    | 41:p:69:LYS:NZ    | 2.67                     | 0.67              |
| 11:L:131:ASP:OD1  | 11:L:132:ASN:ND2  | 2.28                     | 0.67              |
| 15:P:24:LYS:NZ    | 15:P:109:ASP:OD1  | 2.26                     | 0.67              |
| 15:P:303:PRO:HA   | 43:P:502:PLC:H82  | 1.77                     | 0.67              |
| 6:G:246:GLU:OE1   | 16:Q:129:GLN:NE2  | 2.27                     | 0.67              |
| 47:L:712:3PE:H231 | 24:Y:46:GLY:HA3   | 1.76                     | 0.66              |
| 9:J:1:FME:O1      | 31:f:37:ARG:NH1   | 2.29                     | 0.66              |
| 12:M:84:ILE:HG13  | 12:M:133:ILE:HG22 | 1.78                     | 0.66              |
| 11:L:526:TYR:O    | 39:n:37:LYS:NZ    | 2.25                     | 0.66              |
| 10:K:74:ARG:HD3   | 19:T:133:ILE:HG22 | 1.78                     | 0.66              |
| 47:L:707:3PE:H241 | 47:L:707:3PE:H362 | 1.77                     | 0.66              |
| 2:A:128:ILE:HD11  | 10:K:78:GLU:HB3   | 1.76                     | 0.66              |
| 7:H:299:ASN:HD22  | 43:a:201:PLC:H41  | 1.60                     | 0.66              |
| 8:I:35:LEU:HD22   | 21:V:69:GLU:HG3   | 1.78                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:360:TYR:HD2  | 11:L:433:THR:HG22 | 1.60                     | 0.65              |
| 23:X:19:LYS:HB3   | 26:a:103:SER:HB3  | 1.77                     | 0.65              |
| 12:M:106:ASN:ND2  | 12:M:109:ASN:OD1  | 2.29                     | 0.65              |
| 7:H:221:LEU:O     | 7:H:223:SER:N     | 2.29                     | 0.65              |
| 11:L:440:SER:HB3  | 11:L:444:ILE:HD12 | 1.79                     | 0.65              |
| 21:V:50:GLU:HA    | 21:V:60:ARG:HH21  | 1.61                     | 0.65              |
| 6:G:531:PRO:O     | 6:G:535:ASN:ND2   | 2.30                     | 0.64              |
| 6:G:494:PHE:O     | 6:G:498:ASN:ND2   | 2.30                     | 0.64              |
| 12:M:130:LEU:HD23 | 12:M:133:ILE:HD11 | 1.78                     | 0.64              |
| 11:L:480:MET:O    | 40:o:39:ARG:NH2   | 2.27                     | 0.64              |
| 15:P:369:ARG:O    | 15:P:373:ASN:ND2  | 2.30                     | 0.64              |
| 47:L:711:3PE:H2H2 | 34:i:40:CYS:HB2   | 1.78                     | 0.64              |
| 17:R:21:ARG:O     | 17:R:40:ARG:NH2   | 2.26                     | 0.64              |
| 22:W:84:GLU:OE1   | 22:W:90:LYS:NZ    | 2.30                     | 0.64              |
| 15:P:226:GLN:NE2  | 15:P:332:VAL:O    | 2.31                     | 0.64              |
| 3:B:76:LEU:HB2    | 3:B:114:GLY:HA3   | 1.79                     | 0.63              |
| 4:C:127:LYS:NZ    | 21:V:101:GLU:OE1  | 2.30                     | 0.63              |
| 43:A:201:PLC:O2P  | 15:P:302:GLN:NE2  | 2.31                     | 0.63              |
| 18:S:73:LEU:HD21  | 18:S:84:THR:HG21  | 1.81                     | 0.63              |
| 6:G:555:PRO:O     | 42:q:138:ARG:NH2  | 2.32                     | 0.62              |
| 43:L:705:PLC:H61  | 12:M:370:THR:HA   | 1.81                     | 0.62              |
| 11:L:526:TYR:OH   | 43:L:702:PLC:O1P  | 2.15                     | 0.62              |
| 15:P:43:THR:OG1   | 15:P:108:SER:OG   | 2.17                     | 0.62              |
| 6:G:398:ASP:O     | 6:G:399:GLN:NE2   | 2.31                     | 0.62              |
| 2:A:133:ASN:HB3   | 21:V:18:ASN:HB2   | 1.81                     | 0.62              |
| 24:Y:16:LEU:HD11  | 43:Y:301:PLC:H2   | 1.82                     | 0.62              |
| 3:B:108:ASP:N     | 3:B:108:ASP:OD1   | 2.31                     | 0.62              |
| 6:G:476:SER:HB3   | 6:G:513:HIS:HA    | 1.82                     | 0.62              |
| 9:J:93:ASP:OD1    | 26:a:118:LYS:NZ   | 2.33                     | 0.62              |
| 6:G:63:LYS:NZ     | 6:G:280:GLU:OE2   | 2.31                     | 0.61              |
| 15:P:110:ILE:HD13 | 15:P:235:ALA:HB1  | 1.82                     | 0.61              |
| 15:P:173:GLU:OE1  | 15:P:188:ARG:NH2  | 2.33                     | 0.61              |
| 15:P:192:MET:O    | 15:P:197:SER:OG   | 2.18                     | 0.61              |
| 11:L:23:ILE:O     | 11:L:27:SER:OG    | 2.17                     | 0.61              |
| 21:V:62:ALA:HB1   | 28:c:146:PRO:HB3  | 1.81                     | 0.61              |
| 32:g:164:SER:OG   | 32:g:166:ASP:OD1  | 2.16                     | 0.61              |
| 1:l:140:GLN:NE2   | 37:l:35:ASN:OD1   | 2.33                     | 0.61              |
| 2:A:58:GLU:HG3    | 15:P:352:SER:HB3  | 1.81                     | 0.61              |
| 11:L:140:TRP:CZ2  | 11:L:223:LYS:HG3  | 2.36                     | 0.61              |
| 6:G:658:GLU:HG2   | 6:G:662:LYS:HE3   | 1.82                     | 0.61              |
| 11:L:124:MET:HE3  | 11:L:251:CYS:HA   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:140:MET:HG2   | 3:B:175:PRO:HG2   | 1.81                     | 0.61              |
| 6:G:343:LEU:HD11  | 6:G:691:ASP:HB2   | 1.83                     | 0.61              |
| 1:1:153:LYS:HA    | 1:1:156:PHE:HD2   | 1.67                     | 0.60              |
| 35:j:42:ARG:NH1   | 47:j:101:3PE:O12  | 2.35                     | 0.60              |
| 7:H:316:ARG:NH1   | 7:H:318:ASP:OD2   | 2.34                     | 0.60              |
| 9:J:81:SER:H      | 24:Y:63:LYS:HB3   | 1.64                     | 0.60              |
| 11:L:568:ASN:ND2  | 47:L:701:3PE:O22  | 2.34                     | 0.60              |
| 27:b:48:ARG:NH1   | 27:b:54:ASP:OD2   | 2.33                     | 0.60              |
| 12:M:323:ASN:ND2  | 12:M:487:TYR:O    | 2.35                     | 0.60              |
| 2:A:115:ILE:HG12  | 43:b:101:PLC:H4'1 | 1.84                     | 0.60              |
| 12:M:191:ILE:HG13 | 12:M:192:ILE:HG13 | 1.83                     | 0.60              |
| 2:A:29:GLU:OE1    | 3:B:61:LYS:NZ     | 2.35                     | 0.60              |
| 4:C:219:ASP:OD1   | 4:C:219:ASP:N     | 2.33                     | 0.60              |
| 9:J:22:PHE:HE2    | 9:J:70:ILE:HD12   | 1.67                     | 0.60              |
| 2:A:140:LEU:HD12  | 21:V:13:ILE:HD12  | 1.84                     | 0.59              |
| 5:D:80:ASN:O      | 13:N:287:ARG:NH2  | 2.34                     | 0.59              |
| 1:1:127:SER:OG    | 1:1:130:GLU:OE1   | 2.20                     | 0.59              |
| 2:A:86:LEU:HD23   | 2:A:89:ILE:HD12   | 1.83                     | 0.59              |
| 3:B:86:VAL:HG12   | 3:B:93:GLN:HB3    | 1.82                     | 0.59              |
| 6:G:177:THR:N     | 44:G:801:SF4:S4   | 2.74                     | 0.59              |
| 6:G:396:GLU:OE1   | 6:G:469:LYS:NZ    | 2.31                     | 0.59              |
| 11:L:187:LEU:HD13 | 12:M:407:ILE:HA   | 1.82                     | 0.59              |
| 42:q:30:LYS:HE2   | 42:q:47:VAL:HG21  | 1.84                     | 0.59              |
| 5:D:108:PRO:HG2   | 7:H:218:GLU:HG2   | 1.83                     | 0.59              |
| 37:l:25:LYS:HD3   | 37:l:26:SER:H     | 1.67                     | 0.59              |
| 11:L:11:LEU:HG    | 47:L:711:3PE:H2H1 | 1.85                     | 0.58              |
| 1:1:69:ASP:O      | 1:1:74:LYS:NZ     | 2.26                     | 0.58              |
| 17:R:51:ARG:NH2   | 17:R:69:PRO:O     | 2.35                     | 0.58              |
| 18:S:3:LYS:O      | 18:S:3:LYS:NZ     | 2.32                     | 0.58              |
| 6:G:354:ASP:OD2   | 6:G:630:TYR:OH    | 2.21                     | 0.58              |
| 18:S:12:GLU:OE2   | 18:S:14:ARG:NH1   | 2.31                     | 0.58              |
| 27:b:47:ARG:NH2   | 27:b:54:ASP:OD1   | 2.37                     | 0.58              |
| 6:G:329:VAL:HG23  | 6:G:331:PRO:HD3   | 1.86                     | 0.58              |
| 11:L:604:LEU:HD13 | 47:L:707:3PE:H352 | 1.84                     | 0.58              |
| 28:c:131:ASP:HB3  | 28:c:134:VAL:HG23 | 1.86                     | 0.58              |
| 7:H:121:ALA:HB1   | 9:J:52:THR:HB     | 1.85                     | 0.58              |
| 8:I:141:GLU:HB2   | 8:I:154:LYS:HB3   | 1.85                     | 0.58              |
| 1:1:86:ARG:NH1    | 1:1:112:GLU:OE1   | 2.36                     | 0.58              |
| 47:L:710:3PE:H252 | 47:L:711:3PE:H222 | 1.84                     | 0.58              |
| 13:N:129:PHE:O    | 13:N:133:GLU:HG2  | 2.04                     | 0.58              |
| 40:o:42:GLY:O     | 40:o:48:ASN:ND2   | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:c:162:GLU:OE1  | 28:c:162:GLU:N    | 2.37                     | 0.58              |
| 29:d:59:LEU:HD11  | 33:h:131:ILE:HD11 | 1.86                     | 0.58              |
| 40:o:4:SER:OG     | 40:o:5:GLU:OE1    | 2.20                     | 0.58              |
| 4:C:250:ASN:OD1   | 4:C:252:THR:OG1   | 2.16                     | 0.57              |
| 11:L:638:ILE:HG22 | 24:Y:145:MET:HE2  | 1.86                     | 0.57              |
| 9:J:94:ASP:OD1    | 26:a:113:ARG:NH1  | 2.38                     | 0.57              |
| 11:L:388:THR:HG22 | 11:L:470:GLY:H    | 1.69                     | 0.57              |
| 21:V:52:LYS:NZ    | 21:V:107:ASP:OD1  | 2.37                     | 0.57              |
| 25:Z:23:ARG:HG2   | 28:c:28:LEU:HD22  | 1.84                     | 0.57              |
| 22:W:31:TYR:HB3   | 22:W:55:ILE:HD13  | 1.87                     | 0.57              |
| 15:P:264:HIS:O    | 15:P:267:HIS:ND1  | 2.32                     | 0.57              |
| 1:1:143:LEU:HD13  | 1:1:149:LEU:HB2   | 1.85                     | 0.57              |
| 10:K:42:ASP:OD2   | 13:N:178:TYR:OH   | 2.21                     | 0.57              |
| 12:M:36:ILE:HD11  | 32:g:95:VAL:HG22  | 1.87                     | 0.57              |
| 9:J:17:ILE:O      | 15:P:271:ARG:NH2  | 2.37                     | 0.57              |
| 1:1:81:LYS:HE2    | 1:1:85:GLN:HE21   | 1.70                     | 0.57              |
| 13:N:116:LEU:HD11 | 13:N:239:MET:HB3  | 1.87                     | 0.56              |
| 6:G:514:ARG:HG3   | 6:G:515:GLU:HG3   | 1.86                     | 0.56              |
| 7:H:45:ARG:NH2    | 8:I:90:ALA:O      | 2.35                     | 0.56              |
| 11:L:538:ASN:HB3  | 11:L:541:LEU:HB2  | 1.87                     | 0.56              |
| 3:B:78:CYS:HB3    | 5:D:160:TYR:HB2   | 1.86                     | 0.56              |
| 6:G:519:VAL:HG21  | 6:G:593:THR:HA    | 1.88                     | 0.56              |
| 11:L:237:MET:HG3  | 11:L:300:LYS:HD3  | 1.87                     | 0.56              |
| 13:N:46:THR:HB    | 29:d:54:ARG:HH22  | 1.70                     | 0.56              |
| 12:M:61:TRP:CD1   | 12:M:89:LEU:HD21  | 2.40                     | 0.56              |
| 8:I:128:LEU:O     | 8:I:132:VAL:HG23  | 2.05                     | 0.56              |
| 47:L:709:3PE:H3D2 | 12:M:415:LEU:HD23 | 1.88                     | 0.56              |
| 4:C:48:LEU:O      | 4:C:53:ARG:NH2    | 2.39                     | 0.56              |
| 21:V:79:ILE:HG22  | 21:V:82:ASP:H     | 1.70                     | 0.56              |
| 3:B:69:PHE:HB3    | 3:B:98:ILE:HG12   | 1.87                     | 0.56              |
| 16:Q:57:ILE:HG12  | 16:Q:77:ILE:HG12  | 1.87                     | 0.56              |
| 14:O:41:LEU:HD11  | 43:d:101:PLC:H3A2 | 1.88                     | 0.56              |
| 42:q:24:GLN:C     | 43:q:202:PLC:H63  | 2.31                     | 0.56              |
| 9:J:42:ASN:HB2    | 23:X:18:LEU:HD13  | 1.88                     | 0.56              |
| 6:G:236:ARG:NH1   | 6:G:266:GLU:OE2   | 2.39                     | 0.55              |
| 8:I:114:ARG:HD3   | 8:I:211:ILE:HG21  | 1.87                     | 0.55              |
| 12:M:22:ASN:HD22  | 12:M:25:ASN:HD21  | 1.54                     | 0.55              |
| 22:W:91:GLN:OE1   | 22:W:91:GLN:N     | 2.36                     | 0.55              |
| 11:L:124:MET:HA   | 11:L:143:ILE:HD11 | 1.89                     | 0.55              |
| 3:B:105:ARG:HB3   | 7:H:230:SER:HB3   | 1.87                     | 0.55              |
| 8:I:73:LEU:HD22   | 8:I:76:ILE:HD12   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:L:571:TRP:HB2  | 12:M:297:LYS:HE2   | 1.88                     | 0.55              |
| 36:k:10:ASP:OD2   | 39:n:42:ARG:NE     | 2.39                     | 0.55              |
| 3:B:115:THR:HA    | 3:B:143:CYS:HB3    | 1.88                     | 0.55              |
| 22:W:84:GLU:HG2   | 22:W:90:LYS:HG3    | 1.89                     | 0.55              |
| 2:A:36:ASN:HB3    | 15:P:53:ARG:HH22   | 1.72                     | 0.55              |
| 7:H:277:GLN:NE2   | 23:X:166:LEU:O     | 2.39                     | 0.55              |
| 12:M:6:LEU:O      | 12:M:10:ASN:ND2    | 2.35                     | 0.55              |
| 14:O:185:TYR:O    | 27:b:67:ASN:ND2    | 2.39                     | 0.55              |
| 6:G:365:SER:OG    | 6:G:552:LYS:NZ     | 2.39                     | 0.55              |
| 9:J:62:LEU:HD11   | 10:K:16:ILE:HD11   | 1.88                     | 0.55              |
| 11:L:379:LEU:HD22 | 11:L:384:ILE:HG13  | 1.88                     | 0.55              |
| 15:P:24:LYS:HE2   | 15:P:26:LEU:HD21   | 1.88                     | 0.55              |
| 18:S:5:VAL:HG22   | 18:S:41:ALA:HB1    | 1.89                     | 0.55              |
| 11:L:24:GLY:HA3   | 34:i:22:THR:HG23   | 1.88                     | 0.55              |
| 12:M:465:ILE:HD13 | 43:h:201:PLC:HT'2  | 1.88                     | 0.54              |
| 5:D:221:TRP:CZ2   | 8:I:86:MET:HG3     | 2.43                     | 0.54              |
| 9:J:139:LEU:HD22  | 13:N:130:ILE:HD12  | 1.89                     | 0.54              |
| 41:p:30:LEU:HD23  | 41:p:82:PHE:HA     | 1.89                     | 0.54              |
| 6:G:637:ARG:HA    | 6:G:640:LEU:HG     | 1.89                     | 0.54              |
| 15:P:209:LEU:HD21 | 15:P:288:PHE:HE2   | 1.72                     | 0.54              |
| 25:Z:126:ASP:O    | 25:Z:133:ASN:ND2   | 2.41                     | 0.54              |
| 5:D:285:ARG:NH1   | 43:D:501:PLC:OB    | 2.39                     | 0.54              |
| 10:K:2:ASP:OD1    | 10:K:2:ASP:N       | 2.39                     | 0.54              |
| 11:L:590:LEU:HD12 | 43:M:1001:PLC:H3A2 | 1.89                     | 0.54              |
| 4:C:160:ARG:NH1   | 5:D:414:GLU:OE2    | 2.40                     | 0.54              |
| 7:H:172:SER:HB2   | 7:H:350:PRO:HG2    | 1.90                     | 0.54              |
| 29:d:4:SER:OG     | 43:d:102:PLC:O1P   | 2.26                     | 0.54              |
| 5:D:105:PRO:HG3   | 5:D:134:LEU:HD13   | 1.89                     | 0.54              |
| 7:H:44:GLN:OE1    | 7:H:46:ARG:NH1     | 2.40                     | 0.54              |
| 11:L:321:CYS:HB3  | 11:L:324:LEU:HG    | 1.90                     | 0.53              |
| 12:M:221:ILE:O    | 12:M:225:THR:HG22  | 2.08                     | 0.53              |
| 15:P:122:LYS:NZ   | 43:P:502:PLC:O2P   | 2.28                     | 0.53              |
| 5:D:283:ASP:OD1   | 28:c:173:TYR:OH    | 2.21                     | 0.53              |
| 6:G:399:GLN:HE22  | 6:G:428:GLU:HB2    | 1.73                     | 0.53              |
| 7:H:181:GLU:OE2   | 7:H:260:TYR:OH     | 2.26                     | 0.53              |
| 8:I:152:THR:O     | 8:I:197:LYS:NZ     | 2.42                     | 0.53              |
| 11:L:534:LEU:HD22 | 39:n:35:ILE:HG12   | 1.89                     | 0.53              |
| 25:Z:31:PHE:HZ    | 47:b:103:3PE:H371  | 1.73                     | 0.53              |
| 1:l:113:VAL:O     | 1:l:117:THR:OG1    | 2.23                     | 0.53              |
| 7:H:45:ARG:NH1    | 28:c:34:THR:O      | 2.32                     | 0.53              |
| 12:M:196:ASP:OD1  | 33:h:117:TYR:OH    | 2.25                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:D:55:GLN:NE2     | 5:D:57:ASP:OD2    | 2.39                     | 0.53              |
| 6:G:419:ARG:HB2    | 6:G:440:PHE:HD2   | 1.74                     | 0.53              |
| 10:K:15:ILE:HG13   | 19:T:134:ASN:HD22 | 1.74                     | 0.53              |
| 11:L:527:GLU:OE2   | 36:k:20:ARG:NE    | 2.42                     | 0.53              |
| 6:G:464:LEU:O      | 6:G:500:ASN:ND2   | 2.41                     | 0.53              |
| 7:H:151:ALA:HB1    | 7:H:321:ILE:HD11  | 1.90                     | 0.53              |
| 5:D:125:ILE:HD11   | 5:D:466:ALA:HB2   | 1.90                     | 0.53              |
| 10:K:55:ILE:HG21   | 13:N:133:GLU:HG3  | 1.91                     | 0.53              |
| 16:Q:48:GLU:N      | 16:Q:48:GLU:OE1   | 2.42                     | 0.53              |
| 22:W:111:ASP:OD1   | 22:W:111:ASP:N    | 2.40                     | 0.53              |
| 47:L:711:3PE:H232  | 34:i:47:LEU:HD13  | 1.91                     | 0.52              |
| 15:P:173:GLU:OE2   | 15:P:188:ARG:NE   | 2.42                     | 0.52              |
| 26:a:1:MET:HG3     | 42:q:0:ACE:H1     | 1.91                     | 0.52              |
| 11:L:290:LEU:HA    | 11:L:293:MET:HE2  | 1.89                     | 0.52              |
| 6:G:298:ARG:NH1    | 6:G:565:HIS:O     | 2.42                     | 0.52              |
| 12:M:85:ASP:CG     | 12:M:263:ARG:HH22 | 2.18                     | 0.52              |
| 40:o:8:GLU:O       | 40:o:30:ARG:NH1   | 2.38                     | 0.52              |
| 4:C:118:LEU:HD12   | 4:C:161:ILE:HD11  | 1.90                     | 0.52              |
| 5:D:456:HIS:HB2    | 22:W:2:THR:HG22   | 1.91                     | 0.52              |
| 8:I:121:GLU:O      | 8:I:151:ARG:NH1   | 2.42                     | 0.52              |
| 11:L:566:GLY:HA3   | 47:L:703:3PE:H371 | 1.91                     | 0.52              |
| 12:M:291:SER:O     | 12:M:295:THR:OG1  | 2.24                     | 0.52              |
| 15:P:15:SER:HA     | 22:W:119:LYS:HA   | 1.92                     | 0.52              |
| 15:P:153:SER:O     | 15:P:189:PRO:HD2  | 2.10                     | 0.52              |
| 5:D:480:VAL:O      | 5:D:482:ARG:NH1   | 2.42                     | 0.52              |
| 15:P:16:ASP:OD1    | 15:P:16:ASP:N     | 2.36                     | 0.52              |
| 43:M:1001:PLC:H3'1 | 13:N:444:VAL:HG21 | 1.92                     | 0.52              |
| 7:H:222:VAL:HG23   | 7:H:223:SER:H     | 1.75                     | 0.52              |
| 48:b:102:CDL:H322  | 48:b:102:CDL:H162 | 1.92                     | 0.52              |
| 2:A:131:LYS:NZ     | 5:D:296:GLU:OE1   | 2.43                     | 0.52              |
| 25:Z:112:HIS:NE2   | 30:e:19:GLU:OE2   | 2.43                     | 0.52              |
| 40:o:3:VAL:O       | 40:o:58:GLN:NE2   | 2.42                     | 0.52              |
| 2:A:73:LEU:HB3     | 9:J:154:LEU:HD13  | 1.90                     | 0.52              |
| 4:C:204:ARG:NH2    | 4:C:211:PHE:O     | 2.41                     | 0.52              |
| 5:D:376:LYS:HD3    | 5:D:383:ALA:HB1   | 1.92                     | 0.52              |
| 6:G:248:ILE:HG12   | 6:G:600:THR:HG22  | 1.92                     | 0.52              |
| 6:G:352:LEU:HB2    | 6:G:617:ILE:HD13  | 1.91                     | 0.52              |
| 43:L:705:PLC:H1A2  | 34:i:16:THR:HG23  | 1.92                     | 0.51              |
| 5:D:445:ALA:HB1    | 5:D:479:GLU:HG2   | 1.92                     | 0.51              |
| 12:M:449:VAL:HG12  | 12:M:454:ILE:HG13 | 1.92                     | 0.51              |
| 37:l:112:ILE:HG23  | 37:l:117:LEU:HB2  | 1.93                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:G:322:ILE:O      | 6:G:326:PHE:N     | 2.42                     | 0.51              |
| 10:K:13:LEU:HD23   | 19:T:138:ARG:HH21 | 1.75                     | 0.51              |
| 12:M:148:LEU:HD13  | 12:M:171:LEU:HD12 | 1.92                     | 0.51              |
| 13:N:486:SER:O     | 13:N:490:SER:OG   | 2.17                     | 0.51              |
| 7:H:171:VAL:HG21   | 7:H:179:ILE:HG12  | 1.92                     | 0.51              |
| 32:g:25:ALA:N      | 32:g:79:SER:HG    | 2.09                     | 0.51              |
| 6:G:366:THR:O      | 6:G:552:LYS:NZ    | 2.38                     | 0.51              |
| 15:P:166:TYR:OH    | 15:P:217:LYS:NZ   | 2.40                     | 0.51              |
| 1:1:148:GLU:OE1    | 1:1:150:LYS:NZ    | 2.29                     | 0.51              |
| 5:D:196:ILE:HG23   | 5:D:229:LEU:HD22  | 1.93                     | 0.51              |
| 47:L:707:3PE:H3C1  | 47:L:707:3PE:H341 | 1.93                     | 0.51              |
| 47:L:712:3PE:H32   | 47:L:712:3PE:H342 | 1.93                     | 0.51              |
| 12:M:90:LEU:HD13   | 12:M:474:VAL:HG13 | 1.91                     | 0.51              |
| 20:U:64:TYR:OH     | 20:U:89:ASP:OD1   | 2.28                     | 0.51              |
| 6:G:597:VAL:O      | 6:G:651:GLU:N     | 2.34                     | 0.51              |
| 9:J:110:ILE:HG22   | 25:Z:116:THR:HG22 | 1.92                     | 0.51              |
| 9:J:159:LYS:HE3    | 9:J:161:ASP:HB2   | 1.93                     | 0.51              |
| 11:L:563:LEU:HD21  | 47:L:703:3PE:H242 | 1.93                     | 0.51              |
| 47:L:712:3PE:H392  | 24:Y:50:LEU:HG    | 1.92                     | 0.51              |
| 5:D:235:ARG:NH2    | 5:D:262:ASP:OD2   | 2.37                     | 0.51              |
| 7:H:36:GLU:OE1     | 7:H:242:TYR:OH    | 2.15                     | 0.51              |
| 42:q:49:ASP:HB3    | 42:q:52:GLU:HG2   | 1.93                     | 0.51              |
| 6:G:331:PRO:HB3    | 6:G:539:LYS:HB2   | 1.92                     | 0.50              |
| 15:P:209:LEU:HD12  | 15:P:282:LEU:HB3  | 1.92                     | 0.50              |
| 17:R:133:ASP:O     | 17:R:136:SER:OG   | 2.28                     | 0.50              |
| 6:G:144:ASP:OD1    | 28:c:73:ARG:NH2   | 2.44                     | 0.50              |
| 31:f:11:VAL:HG23   | 47:f:101:3PE:H3C1 | 1.92                     | 0.50              |
| 5:D:62:SER:OG      | 13:N:283:LEU:O    | 2.25                     | 0.50              |
| 7:H:318:ASP:OD1    | 7:H:318:ASP:N     | 2.43                     | 0.50              |
| 13:N:180:ASP:OD1   | 26:a:126:ARG:NH2  | 2.44                     | 0.50              |
| 25:Z:136:ASN:ND2   | 25:Z:138:PHE:O    | 2.44                     | 0.50              |
| 7:H:28:VAL:HA      | 26:a:13:MET:HG2   | 1.92                     | 0.50              |
| 7:H:169:LEU:HD21   | 7:H:340:PRO:HG3   | 1.94                     | 0.50              |
| 11:L:224:SER:HB2   | 11:L:310:VAL:HG11 | 1.94                     | 0.50              |
| 6:G:395:GLU:HB3    | 6:G:424:ARG:NH2   | 2.26                     | 0.50              |
| 37:l:120:GLU:HB2   | 38:m:81:LYS:HE3   | 1.93                     | 0.50              |
| 43:M:1001:PLC:H6'2 | 13:N:441:ILE:HG12 | 1.94                     | 0.50              |
| 5:D:269:GLN:HG2    | 5:D:273:ARG:HH11  | 1.77                     | 0.50              |
| 12:M:179:LEU:HB3   | 13:N:436:ILE:HG12 | 1.93                     | 0.50              |
| 11:L:254:ILE:HB    | 11:L:329:LEU:HD11 | 1.91                     | 0.50              |
| 5:D:394:MET:HE2    | 6:G:119:HIS:HD2   | 1.77                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:75:SER:HB2   | 11:L:131:ASP:CG   | 2.37                     | 0.50              |
| 12:M:30:LYS:H     | 12:M:30:LYS:HD3   | 1.77                     | 0.50              |
| 21:V:49:LEU:HD22  | 21:V:60:ARG:HG3   | 1.94                     | 0.50              |
| 3:B:92:ASP:O      | 3:B:95:ARG:HG2    | 2.12                     | 0.49              |
| 15:P:302:GLN:O    | 43:P:502:PLC:H73  | 2.11                     | 0.49              |
| 23:X:89:ARG:NH1   | 27:b:77:TYR:O     | 2.44                     | 0.49              |
| 4:C:147:VAL:HG22  | 4:C:162:LYS:HG2   | 1.94                     | 0.49              |
| 5:D:321:ILE:HB    | 5:D:420:GLU:HB2   | 1.94                     | 0.49              |
| 2:A:111:ILE:HD13  | 48:b:102:CDL:H581 | 1.94                     | 0.49              |
| 6:G:293:GLY:O     | 6:G:566:HIS:NE2   | 2.33                     | 0.49              |
| 47:L:711:3PE:H3A1 | 33:h:75:LEU:HD23  | 1.92                     | 0.49              |
| 17:R:117:PRO:HA   | 17:R:124:ARG:HA   | 1.94                     | 0.49              |
| 6:G:660:ILE:HD11  | 18:S:17:LEU:HD11  | 1.95                     | 0.49              |
| 11:L:253:VAL:HG12 | 11:L:310:VAL:HG21 | 1.94                     | 0.49              |
| 13:N:510:ILE:HD11 | 43:d:102:PLC:H9'2 | 1.94                     | 0.49              |
| 30:e:25:GLU:OE2   | 33:h:174:ARG:NH2  | 2.44                     | 0.49              |
| 6:G:300:THR:HB    | 6:G:608:GLY:HA3   | 1.94                     | 0.49              |
| 11:L:169:LEU:HB2  | 47:L:703:3PE:H231 | 1.94                     | 0.49              |
| 11:L:354:TYR:O    | 11:L:360:TYR:OH   | 2.25                     | 0.49              |
| 15:P:120:PHE:HB2  | 15:P:125:SER:HA   | 1.93                     | 0.49              |
| 1:1:57:GLU:HB3    | 1:1:78:LEU:HD11   | 1.94                     | 0.49              |
| 2:A:106:PHE:CD1   | 9:J:144:SER:HB2   | 2.47                     | 0.49              |
| 22:W:116:LYS:O    | 22:W:121:ALA:N    | 2.46                     | 0.49              |
| 11:L:359:MET:O    | 11:L:440:SER:OG   | 2.30                     | 0.49              |
| 11:L:468:PHE:HZ   | 35:j:34:LEU:HD22  | 1.78                     | 0.49              |
| 12:M:32:SER:OG    | 12:M:33:LEU:N     | 2.46                     | 0.49              |
| 7:H:335:ILE:HA    | 7:H:338:PHE:HB3   | 1.94                     | 0.49              |
| 8:I:120:GLU:HA    | 17:R:74:ALA:HB1   | 1.93                     | 0.49              |
| 9:J:150:SER:O     | 9:J:154:LEU:HG    | 2.12                     | 0.49              |
| 2:A:36:ASN:O      | 15:P:53:ARG:NH1   | 2.43                     | 0.49              |
| 2:A:128:ILE:HD13  | 10:K:80:GLU:HG2   | 1.94                     | 0.49              |
| 7:H:338:PHE:O     | 7:H:342:ILE:HG12  | 2.12                     | 0.49              |
| 11:L:169:LEU:HD12 | 47:L:703:3PE:H222 | 1.95                     | 0.49              |
| 47:L:711:3PE:H3B1 | 43:g:301:PLC:H2'2 | 1.95                     | 0.49              |
| 3:B:69:PHE:O      | 3:B:98:ILE:HA     | 2.13                     | 0.48              |
| 11:L:533:PHE:CE1  | 43:L:702:PLC:H31  | 2.47                     | 0.48              |
| 11:L:627:VAL:HG21 | 13:N:262:ASP:HB3  | 1.94                     | 0.48              |
| 18:S:14:ARG:HG2   | 18:S:48:LEU:HB2   | 1.94                     | 0.48              |
| 1:1:156:PHE:HD1   | 1:1:161:TRP:HZ2   | 1.61                     | 0.48              |
| 5:D:126:LEU:HD22  | 10:K:80:GLU:HB2   | 1.95                     | 0.48              |
| 6:G:237:ALA:HB2   | 6:G:268:MET:HE2   | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:373:VAL:HB    | 6:G:374:PRO:HD3   | 1.96                     | 0.48              |
| 10:K:18:ILE:HG13  | 11:L:609:ILE:HG21 | 1.94                     | 0.48              |
| 13:N:451:LYS:HG3  | 13:N:455:PHE:CD2  | 2.48                     | 0.48              |
| 22:W:76:MET:HG2   | 22:W:80:MET:HE3   | 1.94                     | 0.48              |
| 42:q:69:ASP:HB3   | 42:q:72:GLU:HG3   | 1.94                     | 0.48              |
| 11:L:290:LEU:HD22 | 43:L:702:PLC:H7'2 | 1.95                     | 0.48              |
| 28:c:19:TRP:CE2   | 48:c:201:CDL:HB21 | 2.48                     | 0.48              |
| 6:G:367:ASP:HB2   | 6:G:548:GLU:HB2   | 1.94                     | 0.48              |
| 7:H:35:ALA:HB2    | 26:a:9:PRO:HB2    | 1.96                     | 0.48              |
| 11:L:222:ALA:HB2  | 11:L:229:LEU:HD13 | 1.95                     | 0.48              |
| 21:V:63:VAL:HA    | 21:V:66:PHE:CE2   | 2.49                     | 0.48              |
| 35:j:47:TYR:CD2   | 35:j:48:PRO:HD3   | 2.48                     | 0.48              |
| 7:H:91:LEU:HD22   | 7:H:236:ILE:HG23  | 1.94                     | 0.48              |
| 15:P:187:VAL:HG12 | 15:P:189:PRO:HD3  | 1.95                     | 0.48              |
| 23:X:107:ARG:HA   | 23:X:110:TRP:NE1  | 2.28                     | 0.48              |
| 32:g:218:ILE:HD12 | 41:p:43:VAL:HG11  | 1.94                     | 0.48              |
| 2:A:21:LEU:HD11   | 7:H:88:LEU:HD11   | 1.94                     | 0.48              |
| 3:B:69:PHE:O      | 3:B:71:PRO:HD3    | 2.13                     | 0.48              |
| 4:C:49:ARG:HD2    | 28:c:45:PRO:HG3   | 1.95                     | 0.48              |
| 8:I:127:LYS:N     | 44:I:302:SF4:S1   | 2.82                     | 0.48              |
| 11:L:81:LEU:HD23  | 11:L:262:ARG:HD2  | 1.95                     | 0.48              |
| 15:P:210:GLY:HA3  | 15:P:289:LEU:HD21 | 1.95                     | 0.48              |
| 19:T:96:LEU:HD13  | 19:T:118:VAL:HG11 | 1.95                     | 0.48              |
| 25:Z:61:TRP:CH2   | 27:b:64:PRO:HG2   | 2.49                     | 0.48              |
| 6:G:495:VAL:HG22  | 6:G:501:ILE:HG21  | 1.96                     | 0.48              |
| 6:G:618:ARG:O     | 6:G:621:SER:OG    | 2.25                     | 0.48              |
| 18:S:62:ARG:HA    | 18:S:68:GLU:HG2   | 1.94                     | 0.48              |
| 29:d:23:ARG:NH1   | 43:d:101:PLC:O1P  | 2.35                     | 0.48              |
| 29:d:27:PHE:O     | 29:d:34:TYR:OH    | 2.26                     | 0.48              |
| 11:L:284:SER:O    | 11:L:288:SER:OG   | 2.26                     | 0.48              |
| 11:L:388:THR:HG21 | 11:L:465:LEU:O    | 2.13                     | 0.48              |
| 14:O:1:MET:SD     | 33:h:179:ASN:ND2  | 2.87                     | 0.48              |
| 15:P:205:GLN:O    | 15:P:259:ARG:NH1  | 2.22                     | 0.48              |
| 5:D:158:LEU:O     | 5:D:479:GLU:N     | 2.47                     | 0.48              |
| 5:D:318:PRO:HB3   | 5:D:339:VAL:HG21  | 1.95                     | 0.48              |
| 5:D:461:HIS:HB3   | 5:D:465:ASP:HB2   | 1.95                     | 0.48              |
| 6:G:341:GLY:O     | 6:G:517:SER:OG    | 2.30                     | 0.48              |
| 13:N:76:ILE:HD12  | 47:N:601:3PE:H241 | 1.95                     | 0.48              |
| 3:B:82:GLU:OE1    | 5:D:240:ARG:NH2   | 2.38                     | 0.47              |
| 6:G:160:LYS:O     | 6:G:168:THR:OG1   | 2.32                     | 0.47              |
| 6:G:549:ILE:HD11  | 6:G:570:GLY:HA2   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:76:ARG:HH12  | 12:M:79:ASN:HD22  | 1.62                     | 0.47              |
| 51:U:201:EHZ:O2   | 51:U:201:EHZ:O1   | 2.28                     | 0.47              |
| 24:Y:151:PHE:HD1  | 43:Y:303:PLC:H4'1 | 1.79                     | 0.47              |
| 32:g:87:ASN:ND2   | 32:g:90:ASN:OD1   | 2.39                     | 0.47              |
| 6:G:213:SER:HB3   | 6:G:216:SER:HB3   | 1.95                     | 0.47              |
| 7:H:1:FME:HB2     | 7:H:2:LEU:H       | 1.46                     | 0.47              |
| 15:P:47:GLY:HA2   | 15:P:52:GLY:HA3   | 1.96                     | 0.47              |
| 6:G:57:ARG:HG3    | 6:G:60:TYR:HB3    | 1.97                     | 0.47              |
| 8:I:81:TYR:OH     | 28:c:26:LEU:O     | 2.28                     | 0.47              |
| 47:L:701:3PE:H352 | 38:m:42:PHE:HE1   | 1.79                     | 0.47              |
| 12:M:332:LEU:HD13 | 12:M:478:LEU:HD22 | 1.96                     | 0.47              |
| 28:c:172:ASP:OD1  | 28:c:172:ASP:N    | 2.46                     | 0.47              |
| 47:f:101:3PE:H221 | 47:f:101:3PE:H2   | 1.66                     | 0.47              |
| 11:L:401:TYR:HD1  | 11:L:503:LEU:HD22 | 1.80                     | 0.47              |
| 23:X:24:VAL:O     | 25:Z:81:ARG:NH2   | 2.47                     | 0.47              |
| 47:Z:203:3PE:H241 | 47:Z:203:3PE:H341 | 1.95                     | 0.47              |
| 41:p:83:LEU:HD22  | 41:p:87:LYS:HE3   | 1.97                     | 0.47              |
| 6:G:500:ASN:OD1   | 6:G:500:ASN:N     | 2.45                     | 0.47              |
| 7:H:93:SER:OG     | 7:H:122:SER:O     | 2.30                     | 0.47              |
| 7:H:153:LEU:HA    | 7:H:156:TYR:CE2   | 2.50                     | 0.47              |
| 9:J:66:ILE:HD11   | 10:K:16:ILE:HG12  | 1.95                     | 0.47              |
| 13:N:291:LEU:HD11 | 13:N:445:TYR:HB2  | 1.96                     | 0.47              |
| 1:1:81:LYS:HE2    | 1:1:85:GLN:NE2    | 2.27                     | 0.47              |
| 1:1:150:LYS:O     | 1:1:183:TYR:OH    | 2.22                     | 0.47              |
| 11:L:169:LEU:HB3  | 47:L:703:3PE:H252 | 1.96                     | 0.47              |
| 11:L:635:LEU:HD23 | 24:Y:92:LEU:HD23  | 1.97                     | 0.47              |
| 11:L:641:ILE:HG12 | 47:L:707:3PE:H231 | 1.96                     | 0.47              |
| 13:N:28:ARG:HG2   | 13:N:86:SER:OG    | 2.15                     | 0.47              |
| 16:Q:96:GLN:OE1   | 42:q:127:LYS:NZ   | 2.41                     | 0.47              |
| 22:W:26:ASN:OD1   | 22:W:29:ARG:NH2   | 2.44                     | 0.47              |
| 6:G:305:ARG:NH1   | 6:G:575:ASP:OD1   | 2.48                     | 0.47              |
| 9:J:79:GLU:HB2    | 15:P:271:ARG:HD3  | 1.97                     | 0.47              |
| 12:M:78:LEU:H     | 47:M:1003:3PE:HN3 | 1.62                     | 0.47              |
| 15:P:262:ILE:O    | 15:P:266:ILE:HG12 | 2.15                     | 0.47              |
| 5:D:254:ASP:OD1   | 5:D:255:LEU:N     | 2.46                     | 0.47              |
| 6:G:185:ASP:N     | 6:G:185:ASP:OD1   | 2.44                     | 0.47              |
| 7:H:14:TYR:HA     | 7:H:17:ILE:HD12   | 1.97                     | 0.47              |
| 7:H:39:THR:HB     | 7:H:306:VAL:HG11  | 1.97                     | 0.47              |
| 18:S:17:LEU:HB2   | 18:S:24:SER:HB3   | 1.95                     | 0.47              |
| 47:f:101:3PE:H3A1 | 47:f:101:3PE:H372 | 1.67                     | 0.47              |
| 3:B:106:GLN:NE2   | 7:H:226:MET:O     | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:76:TYR:CG     | 15:P:355:GLN:HG2  | 2.49                     | 0.47              |
| 38:m:12:ASP:HB3   | 38:m:15:PHE:HB2   | 1.97                     | 0.47              |
| 5:D:313:ARG:NH1   | 5:D:319:PHE:O     | 2.46                     | 0.46              |
| 11:L:459:MET:O    | 11:L:463:THR:OG1  | 2.29                     | 0.46              |
| 43:L:705:PLC:H63  | 34:i:19:TRP:CZ2   | 2.49                     | 0.46              |
| 2:A:48:GLY:O      | 3:B:105:ARG:NH2   | 2.48                     | 0.46              |
| 12:M:228:MET:HE3  | 12:M:287:THR:HG23 | 1.97                     | 0.46              |
| 12:M:486:ILE:HD12 | 41:p:79:ILE:HG22  | 1.97                     | 0.46              |
| 26:a:58:LYS:O     | 26:a:82:ARG:NH1   | 2.48                     | 0.46              |
| 31:f:8:ARG:HA     | 31:f:11:VAL:HG12  | 1.97                     | 0.46              |
| 32:g:145:GLY:O    | 32:g:149:THR:OG1  | 2.23                     | 0.46              |
| 39:n:17:LYS:O     | 39:n:21:SER:OG    | 2.29                     | 0.46              |
| 6:G:254:LEU:HD11  | 6:G:411:ALA:HB1   | 1.97                     | 0.46              |
| 6:G:362:GLU:OE2   | 18:S:62:ARG:NH1   | 2.39                     | 0.46              |
| 6:G:449:VAL:HG21  | 6:G:483:ASP:HB3   | 1.97                     | 0.46              |
| 6:G:353:LYS:NZ    | 6:G:524:VAL:O     | 2.38                     | 0.46              |
| 6:G:609:VAL:HG11  | 15:P:17:ILE:HB    | 1.97                     | 0.46              |
| 11:L:88:PRO:HG3   | 11:L:330:ILE:HG23 | 1.96                     | 0.46              |
| 32:g:207:ILE:HG22 | 32:g:209:LYS:HG2  | 1.98                     | 0.46              |
| 2:A:46:LYS:O      | 3:B:105:ARG:NH1   | 2.35                     | 0.46              |
| 2:A:95:VAL:HB     | 2:A:99:GLY:HA3    | 1.98                     | 0.46              |
| 6:G:314:THR:HG22  | 15:P:17:ILE:HG23  | 1.96                     | 0.46              |
| 12:M:50:SER:OG    | 12:M:122:ASN:OD1  | 2.33                     | 0.46              |
| 4:C:156:ASN:OD1   | 5:D:324:SER:HB2   | 2.16                     | 0.46              |
| 9:J:149:MET:SD    | 13:N:138:SER:OG   | 2.73                     | 0.46              |
| 11:L:217:LEU:HD13 | 11:L:277:ILE:HG12 | 1.97                     | 0.46              |
| 11:L:384:ILE:HB   | 11:L:387:LEU:HD12 | 1.98                     | 0.46              |
| 20:U:86:ASP:O     | 20:U:90:THR:OG1   | 2.27                     | 0.46              |
| 1:1:66:LYS:HE3    | 1:1:66:LYS:H      | 1.80                     | 0.46              |
| 2:A:34:ASP:CG     | 2:A:35:GLU:H      | 2.24                     | 0.46              |
| 11:L:134:LEU:HD23 | 11:L:134:LEU:HA   | 1.79                     | 0.46              |
| 11:L:170:ILE:HD12 | 11:L:232:TRP:HB3  | 1.97                     | 0.46              |
| 47:L:712:3PE:H321 | 47:L:712:3PE:H221 | 1.97                     | 0.46              |
| 30:e:71:ASP:HB3   | 30:e:74:GLU:HB2   | 1.98                     | 0.46              |
| 3:B:115:THR:OG1   | 3:B:143:CYS:SG    | 2.68                     | 0.46              |
| 7:H:128:PHE:O     | 7:H:132:ILE:HG12  | 2.16                     | 0.46              |
| 15:P:258:LEU:HD23 | 15:P:261:MET:HE3  | 1.97                     | 0.46              |
| 39:n:10:VAL:O     | 39:n:13:SER:OG    | 2.31                     | 0.46              |
| 3:B:165:PRO:HG3   | 15:P:78:GLN:HA    | 1.98                     | 0.46              |
| 5:D:105:PRO:HB3   | 5:D:113:VAL:HG12  | 1.98                     | 0.46              |
| 6:G:618:ARG:NE    | 6:G:630:TYR:O     | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:L:707:3PE:H391 | 13:N:216:PRO:HB3  | 1.97                     | 0.46              |
| 12:M:437:SER:OG   | 12:M:438:VAL:N    | 2.43                     | 0.46              |
| 14:O:24:ASP:OD2   | 14:O:83:ARG:NH1   | 2.46                     | 0.46              |
| 6:G:541:ILE:HB    | 6:G:560:VAL:HG22  | 1.97                     | 0.46              |
| 12:M:46:GLY:HA3   | 12:M:118:VAL:HG11 | 1.98                     | 0.46              |
| 12:M:239:SER:HB2  | 12:M:360:ARG:HH12 | 1.81                     | 0.46              |
| 11:L:109:HIS:CE1  | 43:L:705:PLC:H51  | 2.52                     | 0.45              |
| 11:L:441:PRO:HD2  | 11:L:444:ILE:HD12 | 1.98                     | 0.45              |
| 33:h:71:PRO:HG2   | 43:h:201:PLC:H3A2 | 1.98                     | 0.45              |
| 4:C:78:HIS:HB3    | 4:C:272:PHE:CZ    | 2.51                     | 0.45              |
| 5:D:152:LEU:HD22  | 5:D:247:ARG:HG2   | 1.98                     | 0.45              |
| 7:H:127:VAL:HG11  | 7:H:153:LEU:HD13  | 1.98                     | 0.45              |
| 7:H:257:PHE:CE1   | 7:H:301:PHE:HZ    | 2.33                     | 0.45              |
| 12:M:149:ALA:HB3  | 12:M:150:PRO:HD3  | 1.98                     | 0.45              |
| 26:a:40:ASN:ND2   | 30:e:95:ASP:HB3   | 2.31                     | 0.45              |
| 32:g:38:ILE:HG21  | 32:g:100:ASP:HB3  | 1.98                     | 0.45              |
| 4:C:136:ASP:O     | 5:D:439:TYR:OH    | 2.33                     | 0.45              |
| 33:h:85:ASP:OD2   | 33:h:89:ARG:NE    | 2.42                     | 0.45              |
| 5:D:167:GLU:HB2   | 5:D:246:VAL:HB    | 1.98                     | 0.45              |
| 15:P:95:ILE:HA    | 15:P:101:ILE:HD11 | 1.98                     | 0.45              |
| 43:g:301:PLC:H71  | 33:h:66:LYS:HE3   | 1.98                     | 0.45              |
| 42:q:75:PRO:HD3   | 42:q:107:HIS:CE1  | 2.51                     | 0.45              |
| 4:C:154:ARG:HH21  | 21:V:98:GLN:HE21  | 1.65                     | 0.45              |
| 9:J:141:LEU:HD13  | 48:O:201:CDL:H821 | 1.98                     | 0.45              |
| 11:L:11:LEU:HD11  | 47:L:711:3PE:H2E1 | 1.98                     | 0.45              |
| 12:M:43:LYS:HD3   | 12:M:114:TYR:CD1  | 2.51                     | 0.45              |
| 12:M:271:GLU:HG2  | 24:Y:198:ARG:HH21 | 1.81                     | 0.45              |
| 47:Y:302:3PE:H352 | 47:Y:302:3PE:H381 | 1.84                     | 0.45              |
| 5:D:322:ARG:HG3   | 5:D:420:GLU:HB3   | 1.98                     | 0.45              |
| 10:K:80:GLU:CD    | 10:K:80:GLU:H     | 2.24                     | 0.45              |
| 43:L:705:PLC:H71  | 12:M:369:SER:O    | 2.17                     | 0.45              |
| 25:Z:132:ALA:HB2  | 30:e:85:PHE:CD1   | 2.52                     | 0.45              |
| 26:a:136:GLU:OE1  | 30:e:52:LYS:NZ    | 2.33                     | 0.45              |
| 33:h:107:LYS:NZ   | 41:p:8:PRO:HG3    | 2.32                     | 0.45              |
| 34:i:7:HIS:HD2    | 34:i:9:PRO:HG3    | 1.81                     | 0.45              |
| 5:D:231:GLU:OE2   | 28:c:43:ARG:NH1   | 2.49                     | 0.45              |
| 6:G:272:PRO:HB3   | 6:G:283:ILE:HG23  | 1.99                     | 0.45              |
| 6:G:456:LEU:HD12  | 6:G:490:THR:HG22  | 1.99                     | 0.45              |
| 15:P:51:LEU:HD23  | 15:P:114:LEU:HD22 | 1.97                     | 0.45              |
| 20:U:86:ASP:OD1   | 20:U:86:ASP:N     | 2.50                     | 0.45              |
| 20:U:96:GLU:HG3   | 36:k:6:TRP:CZ2    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:Y:303:PLC:H4A2 | 43:Y:303:PLC:H7'2 | 1.98                     | 0.45              |
| 6:G:495:VAL:HA    | 6:G:501:ILE:HD12  | 1.98                     | 0.45              |
| 6:G:597:VAL:HG21  | 6:G:647:LEU:HA    | 1.98                     | 0.45              |
| 12:M:247:ILE:HG23 | 12:M:343:PRO:HB3  | 1.98                     | 0.45              |
| 33:h:52:ASP:O     | 33:h:54:HIS:ND1   | 2.50                     | 0.45              |
| 41:p:19:ASN:HB3   | 41:p:22:ASP:HB2   | 1.99                     | 0.45              |
| 1:1:46:LEU:O      | 1:1:50:VAL:HG23   | 2.17                     | 0.45              |
| 7:H:299:ASN:HB3   | 43:a:201:PLC:H83  | 1.99                     | 0.45              |
| 13:N:6:LEU:HD13   | 13:N:110:LEU:HB2  | 1.98                     | 0.45              |
| 23:X:16:ASP:OD2   | 30:e:83:ARG:HD2   | 2.17                     | 0.45              |
| 1:1:35:LEU:HB2    | 1:1:51:ILE:HG21   | 1.99                     | 0.44              |
| 12:M:249:LEU:O    | 12:M:254:LEU:HG   | 2.16                     | 0.44              |
| 18:S:63:LEU:N     | 18:S:67:HIS:O     | 2.50                     | 0.44              |
| 32:g:177:LEU:HD22 | 32:g:187:LEU:HD21 | 1.98                     | 0.44              |
| 47:m:101:3PE:O14  | 47:m:102:3PE:N    | 2.30                     | 0.44              |
| 8:I:138:ILE:HG12  | 8:I:157:ILE:HG12  | 2.00                     | 0.44              |
| 9:J:7:ASP:OD2     | 31:f:8:ARG:NH2    | 2.46                     | 0.44              |
| 12:M:34:LEU:O     | 12:M:39:GLU:HA    | 2.17                     | 0.44              |
| 16:Q:56:ARG:NE    | 16:Q:127:TYR:OH   | 2.49                     | 0.44              |
| 47:f:101:3PE:H381 | 47:f:101:3PE:H352 | 1.69                     | 0.44              |
| 42:q:47:VAL:HG11  | 42:q:52:GLU:HG3   | 1.99                     | 0.44              |
| 4:C:42:GLU:N      | 4:C:42:GLU:OE1    | 2.49                     | 0.44              |
| 7:H:163:VAL:HG22  | 7:H:195:LEU:HD22  | 1.98                     | 0.44              |
| 7:H:231:ALA:O     | 7:H:235:VAL:HG23  | 2.18                     | 0.44              |
| 8:I:49:ARG:NH1    | 21:V:93:GLU:OE2   | 2.36                     | 0.44              |
| 13:N:208:LEU:HD22 | 13:N:244:ILE:HG23 | 1.98                     | 0.44              |
| 6:G:691:ASP:OD1   | 6:G:691:ASP:N     | 2.51                     | 0.44              |
| 7:H:9:ILE:HA      | 7:H:12:ILE:HG22   | 2.00                     | 0.44              |
| 47:L:707:3PE:H222 | 47:L:707:3PE:H332 | 1.99                     | 0.44              |
| 12:M:462:ILE:HD11 | 43:g:301:PLC:H2   | 1.99                     | 0.44              |
| 13:N:235:TYR:CZ   | 13:N:239:MET:HG3  | 2.51                     | 0.44              |
| 15:P:345:LYS:NZ   | 22:W:45:ASP:OD1   | 2.39                     | 0.44              |
| 43:Y:303:PLC:H5'1 | 43:Y:303:PLC:H3A1 | 1.99                     | 0.44              |
| 1:1:79:LEU:HB2    | 1:1:120:LEU:HD13  | 1.99                     | 0.44              |
| 13:N:491:TYR:OH   | 29:d:41:TRP:NE1   | 2.47                     | 0.44              |
| 25:Z:43:TYR:HD1   | 47:Z:203:3PE:H242 | 1.81                     | 0.44              |
| 28:c:160:LEU:HD21 | 28:c:176:ARG:HH11 | 1.83                     | 0.44              |
| 3:B:99:ILE:HD11   | 7:H:37:ARG:CZ     | 2.48                     | 0.44              |
| 7:H:135:TRP:CZ2   | 9:J:22:PHE:HB3    | 2.53                     | 0.44              |
| 7:H:221:LEU:O     | 7:H:224:GLY:N     | 2.31                     | 0.44              |
| 12:M:137:LEU:HB2  | 12:M:195:THR:HB   | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:P:8:VAL:HG13   | 15:P:61:LYS:NZ    | 2.33                     | 0.44              |
| 47:f:101:3PE:H2I2 | 47:f:101:3PE:H371 | 1.99                     | 0.44              |
| 39:n:34:TRP:CD2   | 39:n:80:HIS:HD2   | 2.35                     | 0.44              |
| 12:M:423:SER:HA   | 12:M:426:TYR:CE2  | 2.52                     | 0.44              |
| 42:q:95:GLU:CD    | 42:q:95:GLU:H     | 2.26                     | 0.44              |
| 2:A:108:LEU:O     | 2:A:111:ILE:HG22  | 2.18                     | 0.44              |
| 5:D:464:PRO:HB2   | 7:H:316:ARG:HD3   | 1.99                     | 0.44              |
| 6:G:633:LEU:HD11  | 6:G:637:ARG:HE    | 1.83                     | 0.44              |
| 8:I:56:TRP:CE2    | 8:I:57:GLU:HG2    | 2.53                     | 0.44              |
| 11:L:564:ARG:NH2  | 37:l:83:PRO:O     | 2.51                     | 0.44              |
| 4:C:158:ARG:HG3   | 28:c:152:LEU:HD11 | 2.00                     | 0.44              |
| 7:H:170:ILE:HD11  | 7:H:339:ALA:HB1   | 1.99                     | 0.44              |
| 9:J:122:GLU:OE2   | 25:Z:56:LYS:NZ    | 2.49                     | 0.44              |
| 12:M:484:THR:HG22 | 41:p:31:LEU:HD11  | 1.99                     | 0.44              |
| 32:g:181:ASN:HB2  | 32:g:187:LEU:HD23 | 1.98                     | 0.44              |
| 5:D:395:GLU:HG2   | 6:G:116:LEU:HD13  | 2.00                     | 0.43              |
| 47:L:711:3PE:H2A1 | 47:L:711:3PE:H2D1 | 1.93                     | 0.43              |
| 12:M:362:ILE:HD11 | 12:M:433:ARG:HD3  | 1.99                     | 0.43              |
| 14:O:35:ALA:HB3   | 14:O:36:PRO:HD3   | 1.98                     | 0.43              |
| 18:S:16:PHE:O     | 18:S:57:PRO:HA    | 2.17                     | 0.43              |
| 27:b:31:ILE:HD13  | 48:b:102:CDL:H552 | 2.00                     | 0.43              |
| 42:q:47:VAL:HG12  | 42:q:49:ASP:H     | 1.82                     | 0.43              |
| 11:L:584:LEU:O    | 11:L:589:GLY:HA3  | 2.18                     | 0.43              |
| 47:L:708:3PE:H2G2 | 13:N:434:VAL:HG13 | 1.99                     | 0.43              |
| 12:M:30:LYS:HG2   | 12:M:32:SER:H     | 1.82                     | 0.43              |
| 12:M:269:LEU:HB3  | 12:M:272:ILE:HG22 | 2.00                     | 0.43              |
| 14:O:168:ASN:O    | 14:O:168:ASN:ND2  | 2.50                     | 0.43              |
| 24:Y:118:SER:HB2  | 24:Y:146:GLY:HA2  | 2.00                     | 0.43              |
| 47:Z:203:3PE:H321 | 47:Z:203:3PE:H232 | 2.00                     | 0.43              |
| 4:C:131:ASP:HB2   | 5:D:444:ARG:HG3   | 1.99                     | 0.43              |
| 12:M:382:PHE:CZ   | 12:M:461:LEU:HB2  | 2.54                     | 0.43              |
| 22:W:93:CYS:SG    | 22:W:94:HIS:ND1   | 2.84                     | 0.43              |
| 24:Y:111:ALA:N    | 43:Y:303:PLC:O2P  | 2.52                     | 0.43              |
| 3:B:95:ARG:HA     | 7:H:49:PRO:HA     | 1.99                     | 0.43              |
| 5:D:394:MET:HE2   | 6:G:119:HIS:CD2   | 2.52                     | 0.43              |
| 5:D:423:LYS:NZ    | 5:D:474:ASP:O     | 2.41                     | 0.43              |
| 6:G:332:LYS:HA    | 6:G:332:LYS:HD3   | 1.69                     | 0.43              |
| 11:L:385:PRO:HB2  | 35:j:50:TRP:CZ3   | 2.53                     | 0.43              |
| 48:O:201:CDL:H111 | 47:O:202:3PE:H332 | 1.99                     | 0.43              |
| 24:Y:115:PHE:CE2  | 47:Y:302:3PE:H341 | 2.53                     | 0.43              |
| 3:B:78:CYS:HB3    | 5:D:160:TYR:CB    | 2.47                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 47:f:101:3PE:H3C1 | 47:f:101:3PE:H392 | 1.75                     | 0.43              |
| 41:p:53:LYS:HA    | 41:p:53:LYS:HD3   | 1.76                     | 0.43              |
| 1:1:83:ILE:HG23   | 1:1:113:VAL:HG13  | 1.99                     | 0.43              |
| 1:1:156:PHE:HA    | 1:1:159:ILE:HD12  | 1.99                     | 0.43              |
| 6:G:389:SER:O     | 6:G:390:THR:OG1   | 2.28                     | 0.43              |
| 6:G:564:GLY:O     | 6:G:580:GLY:N     | 2.43                     | 0.43              |
| 8:I:116:TYR:CE2   | 8:I:122:ARG:HA    | 2.53                     | 0.43              |
| 11:L:422:THR:HA   | 11:L:425:TYR:CE2  | 2.52                     | 0.43              |
| 11:L:440:SER:HB2  | 11:L:445:TYR:CE1  | 2.54                     | 0.43              |
| 26:a:8:ILE:HG12   | 48:c:201:CDL:H601 | 1.99                     | 0.43              |
| 40:o:52:GLU:OE1   | 40:o:52:GLU:N     | 2.39                     | 0.43              |
| 4:C:215:PRO:HA    | 4:C:220:PHE:CD1   | 2.53                     | 0.43              |
| 11:L:74:TRP:CZ3   | 47:L:710:3PE:H2I2 | 2.54                     | 0.43              |
| 47:L:703:3PE:H31  | 37:l:83:PRO:HG3   | 2.00                     | 0.43              |
| 47:L:708:3PE:H272 | 47:L:708:3PE:H2A2 | 1.72                     | 0.43              |
| 28:c:169:TYR:HB3  | 28:c:173:TYR:CD1  | 2.53                     | 0.43              |
| 5:D:48:LYS:HB3    | 5:D:48:LYS:HE2    | 1.84                     | 0.43              |
| 5:D:435:SER:OG    | 5:D:436:GLU:N     | 2.52                     | 0.43              |
| 7:H:81:ILE:HG12   | 31:f:14:PHE:HB3   | 2.01                     | 0.43              |
| 7:H:134:GLY:HA3   | 7:H:146:THR:HG21  | 2.01                     | 0.43              |
| 12:M:140:PHE:O    | 12:M:144:PHE:HB2  | 2.19                     | 0.43              |
| 13:N:521:ASN:O    | 13:N:523:VAL:N    | 2.51                     | 0.43              |
| 1:1:98:SER:HB2    | 1:1:103:ARG:HA    | 2.01                     | 0.43              |
| 2:A:105:LEU:HD13  | 48:O:201:CDL:H802 | 2.00                     | 0.43              |
| 6:G:171:ASN:OD1   | 6:G:171:ASN:N     | 2.51                     | 0.43              |
| 7:H:187:TRP:N     | 43:H:401:PLC:O2P  | 2.35                     | 0.43              |
| 8:I:113:LEU:O     | 8:I:204:GLY:HA3   | 2.18                     | 0.43              |
| 9:J:136:TYR:HB3   | 9:J:139:LEU:HD12  | 2.01                     | 0.43              |
| 13:N:312:ASN:ND2  | 33:h:133:PHE:O    | 2.52                     | 0.43              |
| 17:R:79:TYR:CE1   | 17:R:124:ARG:HD3  | 2.54                     | 0.43              |
| 22:W:5:THR:OG1    | 22:W:83:GLN:NE2   | 2.52                     | 0.43              |
| 26:a:37:ARG:NH1   | 26:a:46:ASN:O     | 2.51                     | 0.43              |
| 28:c:163:GLU:HA   | 28:c:166:HIS:CE1  | 2.54                     | 0.43              |
| 32:g:82:ASP:O     | 32:g:86:GLN:HG2   | 2.19                     | 0.43              |
| 6:G:248:ILE:HD11  | 6:G:590:TYR:HB2   | 2.00                     | 0.43              |
| 6:G:398:ASP:OD2   | 6:G:468:SER:OG    | 2.24                     | 0.43              |
| 8:I:90:ALA:HB2    | 26:a:1:MET:HE1    | 2.01                     | 0.43              |
| 9:J:73:LYS:NZ     | 19:T:134:ASN:OD1  | 2.48                     | 0.43              |
| 9:J:134:THR:HB    | 14:O:124:MET:HE2  | 2.00                     | 0.43              |
| 11:L:85:MET:HG3   | 11:L:258:PHE:CD1  | 2.54                     | 0.43              |
| 11:L:385:PRO:HA   | 11:L:390:PHE:CG   | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:578:ASP:OD2  | 12:M:307:TYR:OH   | 2.34                     | 0.43              |
| 6:G:501:ILE:O     | 6:G:508:GLY:N     | 2.48                     | 0.42              |
| 7:H:29:VAL:HG21   | 7:H:243:CYS:SG    | 2.59                     | 0.42              |
| 7:H:230:SER:O     | 7:H:233:PRO:HD2   | 2.19                     | 0.42              |
| 9:J:154:LEU:HD22  | 10:K:65:SER:HB3   | 2.01                     | 0.42              |
| 12:M:162:ASN:HB2  | 12:M:240:GLU:CD   | 2.44                     | 0.42              |
| 13:N:77:ILE:HG22  | 13:N:239:MET:HE1  | 2.00                     | 0.42              |
| 32:g:175:LEU:HG   | 41:p:6:ARG:HH21   | 1.84                     | 0.42              |
| 34:i:58:LYS:HA    | 34:i:58:LYS:HD3   | 1.84                     | 0.42              |
| 1:1:61:LEU:HD22   | 1:1:78:LEU:HD22   | 2.00                     | 0.42              |
| 5:D:109:ALA:HB2   | 7:H:219:SER:O     | 2.19                     | 0.42              |
| 7:H:132:ILE:O     | 7:H:135:TRP:HB2   | 2.19                     | 0.42              |
| 12:M:298:GLN:HB2  | 12:M:304:ILE:HG12 | 2.00                     | 0.42              |
| 3:B:34:LEU:HD21   | 15:P:128:ASP:HB3  | 2.01                     | 0.42              |
| 11:L:250:ALA:HB2  | 11:L:333:SER:HB3  | 2.01                     | 0.42              |
| 12:M:145:GLU:OE1  | 12:M:148:LEU:HD12 | 2.20                     | 0.42              |
| 13:N:403:SER:O    | 13:N:412:GLY:HA3  | 2.19                     | 0.42              |
| 22:W:14:VAL:HB    | 22:W:20:MET:HE2   | 2.01                     | 0.42              |
| 24:Y:208:GLY:O    | 24:Y:211:ARG:NH2  | 2.51                     | 0.42              |
| 40:o:73:GLU:O     | 40:o:77:GLN:HG2   | 2.19                     | 0.42              |
| 2:A:44:ILE:HB     | 15:P:346:PRO:HB3  | 2.01                     | 0.42              |
| 2:A:60:SER:HB2    | 7:H:138:ASN:HA    | 2.01                     | 0.42              |
| 4:C:191:LEU:HA    | 4:C:215:PRO:HD2   | 2.00                     | 0.42              |
| 7:H:333:PHE:O     | 7:H:336:VAL:HG12  | 2.19                     | 0.42              |
| 47:L:707:3PE:H3D2 | 47:L:707:3PE:H3A2 | 1.75                     | 0.42              |
| 15:P:158:ASN:O    | 15:P:167:ALA:HA   | 2.19                     | 0.42              |
| 24:Y:22:PRO:HD3   | 24:Y:191:PHE:CZ   | 2.54                     | 0.42              |
| 42:q:30:LYS:NZ    | 42:q:56:ARG:HB3   | 2.35                     | 0.42              |
| 3:B:61:LYS:HE3    | 7:H:69:SER:HB2    | 2.02                     | 0.42              |
| 5:D:60:GLU:HG2    | 5:D:65:LYS:HG2    | 2.01                     | 0.42              |
| 6:G:459:GLU:HG3   | 6:G:463:LYS:HE3   | 2.01                     | 0.42              |
| 28:c:86:ASP:OD1   | 28:c:86:ASP:N     | 2.44                     | 0.42              |
| 2:A:1:FME:SD      | 23:X:2:SER:HB3    | 2.60                     | 0.42              |
| 5:D:116:LEU:HD22  | 5:D:470:ILE:HD11  | 2.02                     | 0.42              |
| 12:M:68:TYR:HE1   | 33:h:107:LYS:HG3  | 1.84                     | 0.42              |
| 15:P:118:GLU:CD   | 15:P:312:ARG:HH12 | 2.28                     | 0.42              |
| 39:n:64:LEU:HA    | 39:n:64:LEU:HD12  | 1.80                     | 0.42              |
| 42:q:88:PRO:HB2   | 42:q:90:ASN:OD1   | 2.19                     | 0.42              |
| 4:C:91:PHE:HB3    | 4:C:110:ALA:HB1   | 2.01                     | 0.42              |
| 6:G:451:ALA:O     | 6:G:455:ALA:N     | 2.42                     | 0.42              |
| 12:M:30:LYS:NZ    | 12:M:32:SER:HB2   | 2.35                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:38:ASN:HB3   | 12:M:114:TYR:CE2  | 2.55                     | 0.42              |
| 13:N:99:ASN:OD1   | 13:N:99:ASN:N     | 2.52                     | 0.42              |
| 13:N:137:TYR:O    | 13:N:141:LEU:HG   | 2.20                     | 0.42              |
| 13:N:249:TYR:HD2  | 13:N:307:ILE:HG12 | 1.84                     | 0.42              |
| 18:S:16:PHE:HB3   | 18:S:55:ILE:HD12  | 2.01                     | 0.42              |
| 20:U:50:LYS:NZ    | 20:U:121:ASP:OD1  | 2.43                     | 0.42              |
| 32:g:26:PHE:CZ    | 32:g:90:ASN:HB3   | 2.55                     | 0.42              |
| 5:D:119:GLU:CD    | 5:D:127:ARG:HH21  | 2.27                     | 0.42              |
| 5:D:146:LYS:O     | 5:D:437:ARG:HG2   | 2.19                     | 0.42              |
| 11:L:431:TYR:CE2  | 11:L:526:TYR:HB3  | 2.54                     | 0.42              |
| 13:N:272:LEU:HD12 | 13:N:434:VAL:HG11 | 2.02                     | 0.42              |
| 15:P:111:VAL:HG23 | 15:P:146:VAL:HG11 | 2.01                     | 0.42              |
| 3:B:60:MET:HE3    | 43:q:201:PLC:H7A2 | 2.02                     | 0.42              |
| 10:K:64:LEU:HD23  | 10:K:64:LEU:HA    | 1.90                     | 0.42              |
| 47:L:707:3PE:H3B2 | 47:L:712:3PE:H2I1 | 2.00                     | 0.42              |
| 12:M:26:GLY:O     | 12:M:28:LEU:HD12  | 2.20                     | 0.42              |
| 13:N:53:GLY:O     | 33:h:145:ARG:NH1  | 2.53                     | 0.42              |
| 26:a:115:ILE:HG23 | 26:a:116:ILE:HG13 | 2.02                     | 0.42              |
| 33:h:65:ASN:OD1   | 33:h:68:ASN:ND2   | 2.52                     | 0.42              |
| 34:i:60:LYS:HB2   | 34:i:63:GLU:HG3   | 2.00                     | 0.42              |
| 2:A:56:SER:HB3    | 5:D:102:ASN:ND2   | 2.35                     | 0.42              |
| 4:C:56:TYR:HB3    | 4:C:59:LEU:HD11   | 2.01                     | 0.42              |
| 11:L:25:VAL:O     | 11:L:29:LYS:HG3   | 2.20                     | 0.42              |
| 11:L:338:LEU:HD23 | 11:L:377:ALA:HB2  | 2.02                     | 0.42              |
| 5:D:162:SER:HA    | 5:D:197:THR:HG23  | 2.02                     | 0.41              |
| 6:G:395:GLU:HB3   | 6:G:424:ARG:HH22  | 1.84                     | 0.41              |
| 9:J:17:ILE:HD12   | 15:P:273:TYR:OH   | 2.20                     | 0.41              |
| 10:K:15:ILE:HD11  | 19:T:137:ILE:HG23 | 2.02                     | 0.41              |
| 15:P:80:LYS:HD2   | 15:P:88:VAL:HB    | 2.02                     | 0.41              |
| 23:X:98:LEU:HD23  | 23:X:138:MET:HE1  | 2.02                     | 0.41              |
| 26:a:78:THR:OG1   | 26:a:83:GLY:HA3   | 2.20                     | 0.41              |
| 2:A:18:LEU:HD21   | 31:f:10:ALA:HA    | 2.02                     | 0.41              |
| 43:D:501:PLC:H63  | 43:D:501:PLC:H41  | 1.86                     | 0.41              |
| 7:H:128:PHE:CZ    | 7:H:132:ILE:HD11  | 2.54                     | 0.41              |
| 8:I:125:ALA:HB1   | 8:I:142:ALA:HB2   | 2.02                     | 0.41              |
| 47:L:706:3PE:H241 | 47:L:706:3PE:H2   | 2.02                     | 0.41              |
| 43:P:502:PLC:H3A2 | 48:P:503:CDL:HB62 | 2.02                     | 0.41              |
| 32:g:217:ARG:HA   | 32:g:217:ARG:HD3  | 1.84                     | 0.41              |
| 5:D:243:SER:O     | 5:D:245:TYR:N     | 2.50                     | 0.41              |
| 11:L:371:TYR:OH   | 36:k:27:ALA:O     | 2.22                     | 0.41              |
| 12:M:33:LEU:HD21  | 32:g:94:TYR:HB3   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:6:LEU:HD11   | 13:N:107:VAL:HG13 | 2.01                     | 0.41              |
| 26:a:39:PRO:HG2   | 30:e:95:ASP:HB2   | 2.03                     | 0.41              |
| 5:D:89:TYR:HA     | 5:D:90:PRO:HD3    | 1.94                     | 0.41              |
| 6:G:248:ILE:HG22  | 6:G:257:ASN:ND2   | 2.35                     | 0.41              |
| 6:G:292:ASP:OD1   | 6:G:292:ASP:N     | 2.54                     | 0.41              |
| 11:L:260:LEU:HD13 | 11:L:277:ILE:HD13 | 2.02                     | 0.41              |
| 11:L:559:ASN:O    | 11:L:564:ARG:HG2  | 2.20                     | 0.41              |
| 32:g:210:ARG:HD3  | 32:g:210:ARG:HA   | 1.84                     | 0.41              |
| 1:1:28:LEU:HB3    | 1:1:32:ARG:NH1    | 2.35                     | 0.41              |
| 7:H:152:GLN:HE21  | 7:H:214:ASN:HB2   | 1.86                     | 0.41              |
| 7:H:295:ALA:HB2   | 26:a:17:PHE:HB2   | 2.02                     | 0.41              |
| 8:I:184:GLU:OE2   | 42:q:78:HIS:NE2   | 2.42                     | 0.41              |
| 9:J:99:GLU:HG3    | 26:a:107:ARG:HD2  | 2.03                     | 0.41              |
| 12:M:194:SER:HB2  | 33:h:125:ALA:HB2  | 2.03                     | 0.41              |
| 12:M:282:ILE:CD1  | 38:m:51:GLY:HA2   | 2.51                     | 0.41              |
| 14:O:117:LEU:HB3  | 14:O:121:GLN:HB2  | 2.02                     | 0.41              |
| 20:U:95:LEU:HD12  | 39:n:28:LEU:HD12  | 2.02                     | 0.41              |
| 37:l:125:PRO:HG2  | 37:l:151:LYS:NZ   | 2.36                     | 0.41              |
| 9:J:20:ASN:ND2    | 9:J:23:GLU:OE2    | 2.54                     | 0.41              |
| 11:L:177:LEU:O    | 11:L:215:CYS:HB3  | 2.20                     | 0.41              |
| 11:L:213:LEU:HD13 | 11:L:267:LEU:HA   | 2.02                     | 0.41              |
| 11:L:593:LEU:HB2  | 47:L:708:3PE:H342 | 2.03                     | 0.41              |
| 13:N:304:LEU:HD23 | 13:N:307:ILE:HD12 | 2.03                     | 0.41              |
| 17:R:103:HIS:HD2  | 17:R:121:CYS:SG   | 2.30                     | 0.41              |
| 25:Z:109:ASP:OD1  | 25:Z:109:ASP:N    | 2.42                     | 0.41              |
| 41:p:78:ARG:O     | 41:p:80:GLN:NE2   | 2.41                     | 0.41              |
| 6:G:262:THR:HG22  | 6:G:267:VAL:HG22  | 2.02                     | 0.41              |
| 6:G:383:SER:HB3   | 6:G:656:VAL:HG21  | 2.02                     | 0.41              |
| 11:L:85:MET:O     | 11:L:88:PRO:HD2   | 2.20                     | 0.41              |
| 12:M:409:HIS:CG   | 12:M:412:ILE:HG22 | 2.55                     | 0.41              |
| 12:M:462:ILE:O    | 12:M:466:ILE:HG12 | 2.21                     | 0.41              |
| 13:N:311:SER:H    | 13:N:314:SER:HB2  | 1.86                     | 0.41              |
| 25:Z:132:ALA:HB2  | 30:e:85:PHE:CG    | 2.56                     | 0.41              |
| 2:A:52:CYS:HA     | 5:D:106:GLN:HB3   | 2.01                     | 0.41              |
| 5:D:100:THR:O     | 7:H:140:LYS:NZ    | 2.47                     | 0.41              |
| 6:G:345:ASP:OD1   | 6:G:345:ASP:N     | 2.49                     | 0.41              |
| 10:K:11:VAL:HG11  | 10:K:18:ILE:HD13  | 2.03                     | 0.41              |
| 11:L:173:PHE:HD1  | 12:M:421:LEU:HD22 | 1.86                     | 0.41              |
| 11:L:457:THR:HB   | 11:L:458:PRO:HD3  | 2.03                     | 0.41              |
| 11:L:527:GLU:OE1  | 36:k:23:ARG:NH2   | 2.54                     | 0.41              |
| 12:M:300:ASP:OD2  | 12:M:360:ARG:NH1  | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:O:38:LEU:HD23   | 14:O:38:LEU:HA     | 1.92                     | 0.41              |
| 48:O:201:CDL:H541  | 48:O:201:CDL:H512  | 1.54                     | 0.41              |
| 17:R:19:THR:O      | 17:R:42:SER:HB2    | 2.21                     | 0.41              |
| 32:g:219:LEU:HB3   | 34:i:71:ALA:HB2    | 2.02                     | 0.41              |
| 47:m:102:3PE:H2B2  | 47:m:102:3PE:H282  | 1.88                     | 0.41              |
| 41:p:44:CYS:SG     | 41:p:73:MET:HE1    | 2.61                     | 0.41              |
| 43:A:201:PLC:H82   | 43:A:201:PLC:H41   | 1.95                     | 0.41              |
| 4:C:65:ASN:HB3     | 4:C:68:GLU:HG2     | 2.02                     | 0.41              |
| 5:D:207:LEU:HB3    | 5:D:219:PHE:HA     | 2.02                     | 0.41              |
| 6:G:73:CYS:SG      | 6:G:86:SER:N       | 2.94                     | 0.41              |
| 6:G:422:TRP:CZ2    | 6:G:441:GLU:HB2    | 2.56                     | 0.41              |
| 8:I:145:ARG:HB3    | 8:I:147:ASP:OD1    | 2.21                     | 0.41              |
| 8:I:172:CYS:HA     | 44:I:302:SF4:S2    | 2.61                     | 0.41              |
| 9:J:16:LEU:O       | 24:Y:64:LYS:HD3    | 2.21                     | 0.41              |
| 12:M:215:ILE:HA    | 12:M:218:ILE:HG22  | 2.02                     | 0.41              |
| 12:M:239:SER:HB2   | 12:M:360:ARG:NH1   | 2.35                     | 0.41              |
| 12:M:301:LEU:HB3   | 12:M:349:VAL:HG13  | 2.01                     | 0.41              |
| 15:P:34:ARG:HG2    | 15:P:84:ASP:HB2    | 2.03                     | 0.41              |
| 15:P:156:ASN:HD21  | 15:P:317:GLN:HA    | 1.86                     | 0.41              |
| 15:P:279:GLY:HA2   | 31:f:21:ILE:HD13   | 2.03                     | 0.41              |
| 28:c:159:ARG:HB3   | 28:c:181:ASN:HB2   | 2.03                     | 0.41              |
| 32:g:78:LEU:HD23   | 32:g:78:LEU:HA     | 1.92                     | 0.41              |
| 40:o:56:TYR:OH     | 40:o:60:GLN:NE2    | 2.49                     | 0.41              |
| 4:C:48:LEU:HA      | 4:C:51:LEU:HG      | 2.04                     | 0.41              |
| 6:G:389:SER:O      | 6:G:393:ASN:HB2    | 2.21                     | 0.41              |
| 8:I:94:ILE:HG21    | 42:q:55:MET:HB2    | 2.02                     | 0.41              |
| 11:L:47:PHE:CE1    | 11:L:51:ILE:HG13   | 2.56                     | 0.41              |
| 11:L:59:TYR:CE2    | 34:i:51:GLY:HA3    | 2.56                     | 0.41              |
| 12:M:33:LEU:HD23   | 12:M:33:LEU:HA     | 1.83                     | 0.41              |
| 12:M:292:SER:HB3   | 12:M:422:LEU:HB3   | 2.03                     | 0.41              |
| 43:M:1002:PLC:H7'1 | 43:M:1002:PLC:HT'2 | 1.87                     | 0.41              |
| 19:T:73:ASP:OD1    | 19:T:73:ASP:N      | 2.53                     | 0.41              |
| 24:Y:165:TYR:HD1   | 24:Y:192:TRP:HB3   | 1.86                     | 0.41              |
| 42:q:27:ASN:OD1    | 43:q:202:PLC:H61   | 2.21                     | 0.41              |
| 1:l:136:GLU:OE2    | 37:l:43:ARG:NH1    | 2.54                     | 0.40              |
| 2:A:88:TYR:HB2     | 9:J:133:PHE:CZ     | 2.56                     | 0.40              |
| 4:C:70:TYR:O       | 4:C:74:ILE:HG13    | 2.21                     | 0.40              |
| 4:C:121:HIS:CD2    | 4:C:123:SER:HB2    | 2.57                     | 0.40              |
| 5:D:399:HIS:CE1    | 6:G:144:ASP:HA     | 2.57                     | 0.40              |
| 6:G:231:LYS:HB3    | 6:G:232:PRO:HD3    | 2.03                     | 0.40              |
| 8:I:45:PRO:HB3     | 28:c:158:PHE:O     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:99:GLU:OE2    | 42:q:26:TYR:OH    | 2.32                     | 0.40              |
| 11:L:150:LEU:HD22 | 11:L:243:VAL:HG22 | 2.03                     | 0.40              |
| 11:L:177:LEU:HD13 | 11:L:177:LEU:HA   | 1.93                     | 0.40              |
| 13:N:129:PHE:CE1  | 13:N:171:LEU:HB2  | 2.56                     | 0.40              |
| 13:N:235:TYR:CE2  | 13:N:239:MET:HG3  | 2.56                     | 0.40              |
| 14:O:124:MET:HE3  | 14:O:124:MET:HB3  | 1.99                     | 0.40              |
| 16:Q:56:ARG:HG2   | 16:Q:58:TYR:HD1   | 1.85                     | 0.40              |
| 37:l:41:TYR:OH    | 37:l:71:LEU:O     | 2.33                     | 0.40              |
| 41:p:69:LYS:HG2   | 41:p:73:MET:HE2   | 2.03                     | 0.40              |
| 2:A:107:LEU:HD13  | 7:H:337:VAL:HG22  | 2.03                     | 0.40              |
| 4:C:274:LEU:HD23  | 4:C:274:LEU:HA    | 1.91                     | 0.40              |
| 7:H:53:GLY:C      | 43:q:202:PLC:H41  | 2.45                     | 0.40              |
| 8:I:143:GLU:OE2   | 17:R:45:SER:OG    | 2.33                     | 0.40              |
| 11:L:214:ILE:HD13 | 11:L:214:ILE:HA   | 1.96                     | 0.40              |
| 47:L:712:3PE:H12  | 24:Y:42:LYS:HD2   | 2.03                     | 0.40              |
| 12:M:144:PHE:CZ   | 12:M:224:LYS:HD2  | 2.56                     | 0.40              |
| 14:O:65:THR:HB    | 47:O:203:3PE:H282 | 2.03                     | 0.40              |
| 16:Q:92:LEU:HG    | 16:Q:93:MET:HG2   | 2.03                     | 0.40              |
| 23:X:40:VAL:HG21  | 25:Z:69:LEU:HD13  | 2.02                     | 0.40              |
| 3:B:82:GLU:O      | 3:B:86:VAL:HG23   | 2.21                     | 0.40              |
| 9:J:23:GLU:O      | 9:J:27:ILE:HG12   | 2.21                     | 0.40              |
| 11:L:128:VAL:HG23 | 11:L:129:THR:HG23 | 2.03                     | 0.40              |
| 11:L:406:PHE:O    | 11:L:410:ILE:HG12 | 2.21                     | 0.40              |
| 11:L:498:GLU:O    | 11:L:502:SER:OG   | 2.21                     | 0.40              |
| 12:M:117:TYR:OH   | 12:M:244:GLY:HA3  | 2.22                     | 0.40              |
| 13:N:41:HIS:NE2   | 13:N:68:ASN:OD1   | 2.44                     | 0.40              |
| 16:Q:93:MET:SD    | 42:q:120:PRO:HB2  | 2.62                     | 0.40              |
| 20:U:100:GLU:HG2  | 36:k:9:ARG:HH22   | 1.85                     | 0.40              |
| 40:o:31:LEU:HD12  | 40:o:59:CYS:HB2   | 2.02                     | 0.40              |
| 42:q:77:TRP:CE2   | 42:q:89:PRO:HG2   | 2.57                     | 0.40              |
| 1:l:135:VAL:HG11  | 1:l:179:VAL:HG22  | 2.04                     | 0.40              |
| 2:A:61:HIS:HB2    | 9:J:72:GLU:CD     | 2.47                     | 0.40              |
| 3:B:66:LYS:HG3    | 3:B:188:GLN:HB3   | 2.04                     | 0.40              |
| 5:D:39:ASN:O      | 5:D:95:LYS:NZ     | 2.45                     | 0.40              |
| 8:I:163:ILE:HG12  | 44:I:301:SF4:S3   | 2.62                     | 0.40              |
| 9:J:130:ASN:O     | 9:J:134:THR:OG1   | 2.30                     | 0.40              |
| 10:K:36:SER:OG    | 13:N:179:ASP:OD1  | 2.24                     | 0.40              |
| 28:c:19:TRP:CD2   | 48:c:201:CDL:HB21 | 2.56                     | 0.40              |
| 2:A:123:LEU:HD12  | 7:H:326:TYR:HE1   | 1.86                     | 0.40              |
| 5:D:243:SER:HA    | 8:I:108:ARG:HH22  | 1.87                     | 0.40              |
| 6:G:492:ALA:HB1   | 6:G:665:PHE:O     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:I:133:CYS:HA    | 44:I:301:SF4:S4    | 2.61                     | 0.40              |
| 9:J:99:GLU:OE1    | 26:a:112:ARG:HD3   | 2.22                     | 0.40              |
| 47:L:708:3PE:H3D2 | 43:M:1001:PLC:HE'2 | 2.02                     | 0.40              |
| 12:M:223:VAL:HG22 | 12:M:230:VAL:HB    | 2.04                     | 0.40              |
| 12:M:282:ILE:HD13 | 38:m:51:GLY:HA2    | 2.02                     | 0.40              |
| 15:P:69:PRO:HA    | 15:P:91:VAL:O      | 2.22                     | 0.40              |
| 42:q:28:ASP:OD2   | 42:q:56:ARG:NH2    | 2.48                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 167/190 (88%)  | 158 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 2   | A     | 139/141 (99%)  | 135 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 3   | B     | 173/204 (85%)  | 168 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 4   | C     | 238/289 (82%)  | 231 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 5   | D     | 448/482 (93%)  | 432 (96%) | 15 (3%) | 1 (0%)   | 44          | 73  |
| 6   | G     | 580/726 (80%)  | 562 (97%) | 18 (3%) | 0        | 100         | 100 |
| 7   | H     | 351/353 (99%)  | 338 (96%) | 11 (3%) | 2 (1%)   | 22          | 52  |
| 8   | I     | 190/222 (86%)  | 186 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 9   | J     | 159/161 (99%)  | 156 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 10  | K     | 78/82 (95%)    | 78 (100%) | 0       | 0        | 100         | 100 |
| 11  | L     | 640/642 (100%) | 626 (98%) | 13 (2%) | 1 (0%)   | 44          | 73  |
| 12  | M     | 489/491 (100%) | 475 (97%) | 14 (3%) | 0        | 100         | 100 |
| 13  | N     | 502/523 (96%)  | 490 (98%) | 12 (2%) | 0        | 100         | 100 |
| 14  | O     | 191/193 (99%)  | 186 (97%) | 5 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 15  | P     | 366/384 (95%)   | 355 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 16  | Q     | 82/159 (52%)    | 82 (100%)  | 0        | 0        | 100         | 100 |
| 17  | R     | 122/139 (88%)   | 120 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 18  | S     | 88/90 (98%)     | 85 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 19  | T     | 93/138 (67%)    | 91 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 20  | U     | 86/130 (66%)    | 81 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 21  | V     | 124/134 (92%)   | 121 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 22  | W     | 111/122 (91%)   | 110 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 23  | X     | 182/184 (99%)   | 182 (100%) | 0        | 0        | 100         | 100 |
| 24  | Y     | 203/216 (94%)   | 194 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 25  | Z     | 140/147 (95%)   | 137 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 26  | a     | 147/150 (98%)   | 144 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 27  | b     | 76/79 (96%)     | 74 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 28  | c     | 157/182 (86%)   | 153 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 29  | d     | 73/78 (94%)     | 72 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 30  | e     | 103/106 (97%)   | 101 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 31  | f     | 76/86 (88%)     | 76 (100%)  | 0        | 0        | 100         | 100 |
| 32  | g     | 152/239 (64%)   | 146 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 33  | h     | 129/182 (71%)   | 124 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 34  | i     | 67/74 (90%)     | 62 (92%)   | 5 (8%)   | 0        | 100         | 100 |
| 35  | j     | 51/59 (86%)     | 49 (96%)   | 2 (4%)   | 0        | 100         | 100 |
| 36  | k     | 43/61 (70%)     | 42 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 37  | l     | 130/156 (83%)   | 127 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 38  | m     | 75/81 (93%)     | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 39  | n     | 103/111 (93%)   | 103 (100%) | 0        | 0        | 100         | 100 |
| 40  | o     | 78/87 (90%)     | 75 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 41  | p     | 88/92 (96%)     | 86 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 42  | q     | 138/140 (99%)   | 133 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| All | All   | 7628/8505 (90%) | 7420 (97%) | 204 (3%) | 4 (0%)   | 50          | 77  |

All (4) Ramachandran outliers are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | H     | 222 | VAL  |
| 7   | H     | 2   | LEU  |
| 5   | D     | 33  | ALA  |
| 11  | L     | 552 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 1   | 1     | 152/168 (90%)  | 146 (96%) | 6 (4%)   | 27          | 62  |
| 2   | A     | 128/128 (100%) | 124 (97%) | 4 (3%)   | 35          | 70  |
| 3   | B     | 154/180 (86%)  | 151 (98%) | 3 (2%)   | 52          | 81  |
| 4   | C     | 214/254 (84%)  | 210 (98%) | 4 (2%)   | 52          | 81  |
| 5   | D     | 384/408 (94%)  | 378 (98%) | 6 (2%)   | 58          | 84  |
| 6   | G     | 498/610 (82%)  | 490 (98%) | 8 (2%)   | 58          | 84  |
| 7   | H     | 307/307 (100%) | 298 (97%) | 9 (3%)   | 37          | 72  |
| 8   | I     | 166/192 (86%)  | 158 (95%) | 8 (5%)   | 21          | 54  |
| 9   | J     | 149/149 (100%) | 143 (96%) | 6 (4%)   | 27          | 61  |
| 10  | K     | 70/72 (97%)    | 65 (93%)  | 5 (7%)   | 12          | 36  |
| 11  | L     | 576/576 (100%) | 564 (98%) | 12 (2%)  | 48          | 78  |
| 12  | M     | 439/439 (100%) | 425 (97%) | 14 (3%)  | 34          | 69  |
| 13  | N     | 474/489 (97%)  | 462 (98%) | 12 (2%)  | 42          | 75  |
| 14  | O     | 169/169 (100%) | 164 (97%) | 5 (3%)   | 36          | 71  |
| 15  | P     | 317/332 (96%)  | 313 (99%) | 4 (1%)   | 65          | 88  |
| 16  | Q     | 74/135 (55%)   | 74 (100%) | 0        | 100         | 100 |
| 17  | R     | 104/118 (88%)  | 103 (99%) | 1 (1%)   | 73          | 91  |
| 18  | S     | 77/77 (100%)   | 74 (96%)  | 3 (4%)   | 27          | 62  |
| 19  | T     | 87/128 (68%)   | 82 (94%)  | 5 (6%)   | 17          | 47  |
| 20  | U     | 80/120 (67%)   | 76 (95%)  | 4 (5%)   | 20          | 52  |
| 21  | V     | 112/119 (94%)  | 111 (99%) | 1 (1%)   | 75          | 92  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 22  | W     | 107/114 (94%)   | 105 (98%)  | 2 (2%)   | 52          | 81  |
| 23  | X     | 165/165 (100%)  | 163 (99%)  | 2 (1%)   | 67          | 89  |
| 24  | Y     | 163/173 (94%)   | 160 (98%)  | 3 (2%)   | 54          | 82  |
| 25  | Z     | 123/128 (96%)   | 120 (98%)  | 3 (2%)   | 44          | 76  |
| 26  | a     | 128/129 (99%)   | 127 (99%)  | 1 (1%)   | 79          | 93  |
| 27  | b     | 66/67 (98%)     | 65 (98%)   | 1 (2%)   | 60          | 85  |
| 28  | c     | 140/159 (88%)   | 137 (98%)  | 3 (2%)   | 48          | 78  |
| 29  | d     | 62/65 (95%)     | 61 (98%)   | 1 (2%)   | 58          | 84  |
| 30  | e     | 91/92 (99%)     | 91 (100%)  | 0        | 100         | 100 |
| 31  | f     | 64/71 (90%)     | 64 (100%)  | 0        | 100         | 100 |
| 32  | g     | 143/215 (66%)   | 139 (97%)  | 4 (3%)   | 38          | 73  |
| 33  | h     | 118/167 (71%)   | 117 (99%)  | 1 (1%)   | 79          | 93  |
| 34  | i     | 59/63 (94%)     | 58 (98%)   | 1 (2%)   | 56          | 83  |
| 35  | j     | 46/50 (92%)     | 44 (96%)   | 2 (4%)   | 25          | 57  |
| 36  | k     | 32/47 (68%)     | 31 (97%)   | 1 (3%)   | 35          | 70  |
| 37  | l     | 116/137 (85%)   | 111 (96%)  | 5 (4%)   | 25          | 57  |
| 38  | m     | 64/66 (97%)     | 64 (100%)  | 0        | 100         | 100 |
| 39  | n     | 95/100 (95%)    | 95 (100%)  | 0        | 100         | 100 |
| 40  | o     | 74/79 (94%)     | 72 (97%)   | 2 (3%)   | 40          | 73  |
| 41  | p     | 83/85 (98%)     | 83 (100%)  | 0        | 100         | 100 |
| 42  | q     | 125/125 (100%)  | 122 (98%)  | 3 (2%)   | 44          | 76  |
| All | All   | 6795/7467 (91%) | 6640 (98%) | 155 (2%) | 46          | 77  |

All (155) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 66  | LYS  |
| 1   | 1     | 67  | ASP  |
| 1   | 1     | 68  | LYS  |
| 1   | 1     | 69  | ASP  |
| 1   | 1     | 72  | GLU  |
| 1   | 1     | 187 | LYS  |
| 2   | A     | 27  | ILE  |
| 2   | A     | 110 | LEU  |
| 2   | A     | 114 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 138 | LYS  |
| 3   | B     | 78  | CYS  |
| 3   | B     | 108 | ASP  |
| 3   | B     | 149 | TYR  |
| 4   | C     | 139 | THR  |
| 4   | C     | 219 | ASP  |
| 4   | C     | 233 | GLU  |
| 4   | C     | 257 | VAL  |
| 5   | D     | 98  | HIS  |
| 5   | D     | 113 | VAL  |
| 5   | D     | 223 | PHE  |
| 5   | D     | 269 | GLN  |
| 5   | D     | 356 | PHE  |
| 5   | D     | 482 | ARG  |
| 6   | G     | 62  | GLU  |
| 6   | G     | 69  | ASN  |
| 6   | G     | 70  | CYS  |
| 6   | G     | 158 | GLU  |
| 6   | G     | 185 | ASP  |
| 6   | G     | 356 | VAL  |
| 6   | G     | 527 | THR  |
| 6   | G     | 692 | VAL  |
| 7   | H     | 40  | MET  |
| 7   | H     | 46  | ARG  |
| 7   | H     | 74  | LEU  |
| 7   | H     | 131 | VAL  |
| 7   | H     | 159 | VAL  |
| 7   | H     | 170 | ILE  |
| 7   | H     | 171 | VAL  |
| 7   | H     | 177 | ASN  |
| 7   | H     | 237 | PHE  |
| 8   | I     | 35  | LEU  |
| 8   | I     | 41  | GLN  |
| 8   | I     | 100 | LYS  |
| 8   | I     | 124 | ILE  |
| 8   | I     | 126 | CYS  |
| 8   | I     | 128 | LEU  |
| 8   | I     | 145 | ARG  |
| 8   | I     | 184 | GLU  |
| 9   | J     | 25  | ILE  |
| 9   | J     | 33  | MET  |
| 9   | J     | 73  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | J     | 89  | VAL  |
| 9   | J     | 110 | ILE  |
| 9   | J     | 121 | ASN  |
| 10  | K     | 2   | ASP  |
| 10  | K     | 5   | LEU  |
| 10  | K     | 35  | TYR  |
| 10  | K     | 74  | ARG  |
| 10  | K     | 75  | ASN  |
| 11  | L     | 3   | LEU  |
| 11  | L     | 11  | LEU  |
| 11  | L     | 158 | PHE  |
| 11  | L     | 159 | ASN  |
| 11  | L     | 252 | LEU  |
| 11  | L     | 264 | SER  |
| 11  | L     | 270 | THR  |
| 11  | L     | 348 | HIS  |
| 11  | L     | 364 | ARG  |
| 11  | L     | 509 | VAL  |
| 11  | L     | 535 | VAL  |
| 11  | L     | 614 | GLU  |
| 12  | M     | 27  | ILE  |
| 12  | M     | 30  | LYS  |
| 12  | M     | 31  | LYS  |
| 12  | M     | 84  | ILE  |
| 12  | M     | 108 | LYS  |
| 12  | M     | 118 | VAL  |
| 12  | M     | 133 | ILE  |
| 12  | M     | 224 | LYS  |
| 12  | M     | 225 | THR  |
| 12  | M     | 228 | MET  |
| 12  | M     | 255 | LYS  |
| 12  | M     | 349 | VAL  |
| 12  | M     | 369 | SER  |
| 12  | M     | 489 | VAL  |
| 13  | N     | 18  | LYS  |
| 13  | N     | 99  | ASN  |
| 13  | N     | 157 | LEU  |
| 13  | N     | 158 | TYR  |
| 13  | N     | 198 | ILE  |
| 13  | N     | 334 | SER  |
| 13  | N     | 365 | ASN  |
| 13  | N     | 387 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 393 | ILE  |
| 13  | N     | 435 | LEU  |
| 13  | N     | 436 | ILE  |
| 13  | N     | 486 | SER  |
| 14  | O     | 54  | LYS  |
| 14  | O     | 116 | LEU  |
| 14  | O     | 127 | ARG  |
| 14  | O     | 155 | ARG  |
| 14  | O     | 186 | LYS  |
| 15  | P     | 10  | THR  |
| 15  | P     | 93  | PHE  |
| 15  | P     | 351 | THR  |
| 15  | P     | 355 | GLN  |
| 17  | R     | 133 | ASP  |
| 18  | S     | 3   | LYS  |
| 18  | S     | 8   | LYS  |
| 18  | S     | 34  | THR  |
| 19  | T     | 79  | VAL  |
| 19  | T     | 102 | VAL  |
| 19  | T     | 112 | ILE  |
| 19  | T     | 137 | ILE  |
| 19  | T     | 138 | ARG  |
| 20  | U     | 45  | THR  |
| 20  | U     | 126 | GLN  |
| 20  | U     | 127 | GLU  |
| 20  | U     | 130 | ILE  |
| 21  | V     | 56  | GLU  |
| 22  | W     | 109 | LYS  |
| 22  | W     | 111 | ASP  |
| 23  | X     | 1   | SER  |
| 23  | X     | 183 | ILE  |
| 24  | Y     | 34  | LYS  |
| 24  | Y     | 74  | TYR  |
| 24  | Y     | 211 | ARG  |
| 25  | Z     | 4   | ASP  |
| 25  | Z     | 69  | LEU  |
| 25  | Z     | 129 | LEU  |
| 26  | a     | 111 | LEU  |
| 27  | b     | 3   | ILE  |
| 28  | c     | 114 | LEU  |
| 28  | c     | 133 | LYS  |
| 28  | c     | 135 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | d     | 61  | LYS  |
| 32  | g     | 32  | LYS  |
| 32  | g     | 43  | LYS  |
| 32  | g     | 177 | LEU  |
| 32  | g     | 185 | VAL  |
| 33  | h     | 104 | ILE  |
| 34  | i     | 7   | HIS  |
| 35  | j     | 34  | LEU  |
| 35  | j     | 59  | HIS  |
| 36  | k     | 7   | LYS  |
| 37  | l     | 25  | LYS  |
| 37  | l     | 44  | LEU  |
| 37  | l     | 68  | ASN  |
| 37  | l     | 127 | ASN  |
| 37  | l     | 156 | ILE  |
| 40  | o     | 16  | LYS  |
| 40  | o     | 49  | CYS  |
| 42  | q     | 1   | SER  |
| 42  | q     | 27  | ASN  |
| 42  | q     | 37  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 85  | GLN  |
| 2   | A     | 130 | HIS  |
| 3   | B     | 93  | GLN  |
| 3   | B     | 118 | ASN  |
| 4   | C     | 142 | ASN  |
| 5   | D     | 107 | HIS  |
| 5   | D     | 269 | GLN  |
| 6   | G     | 175 | HIS  |
| 6   | G     | 297 | GLN  |
| 6   | G     | 482 | GLN  |
| 7   | H     | 76  | HIS  |
| 9   | J     | 101 | ASN  |
| 11  | L     | 109 | HIS  |
| 11  | L     | 439 | ASN  |
| 11  | L     | 451 | ASN  |
| 11  | L     | 550 | GLN  |
| 11  | L     | 574 | ASN  |
| 11  | L     | 608 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | M     | 22  | ASN  |
| 12  | M     | 193 | ASN  |
| 12  | M     | 238 | HIS  |
| 12  | M     | 329 | ASN  |
| 12  | M     | 338 | HIS  |
| 12  | M     | 363 | ASN  |
| 13  | N     | 17  | ASN  |
| 13  | N     | 256 | ASN  |
| 13  | N     | 331 | ASN  |
| 13  | N     | 390 | ASN  |
| 14  | O     | 184 | GLN  |
| 15  | P     | 18  | ASN  |
| 15  | P     | 78  | GLN  |
| 16  | Q     | 86  | ASN  |
| 17  | R     | 34  | GLN  |
| 17  | R     | 57  | ASN  |
| 18  | S     | 72  | ASN  |
| 18  | S     | 80  | GLN  |
| 21  | V     | 77  | ASN  |
| 23  | X     | 158 | ASN  |
| 24  | Y     | 55  | HIS  |
| 24  | Y     | 109 | GLN  |
| 24  | Y     | 189 | GLN  |
| 25  | Z     | 65  | HIS  |
| 25  | Z     | 77  | ASN  |
| 25  | Z     | 133 | ASN  |
| 27  | b     | 12  | GLN  |
| 27  | b     | 20  | HIS  |
| 29  | d     | 20  | GLN  |
| 30  | e     | 10  | HIS  |
| 30  | e     | 21  | GLN  |
| 30  | e     | 64  | HIS  |
| 31  | f     | 48  | HIS  |
| 32  | g     | 181 | ASN  |
| 33  | h     | 118 | GLN  |
| 33  | h     | 140 | HIS  |
| 34  | i     | 4   | HIS  |
| 37  | l     | 63  | ASN  |
| 38  | m     | 16  | GLN  |
| 40  | o     | 18  | ASN  |
| 40  | o     | 36  | ASN  |
| 40  | o     | 77  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 41  | p     | 19  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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 | $\# Z  > 2$ |
| 2   | FME  | A     | 1   | 2    | 8,9,10       | 1.53 | 1 (12%)     | 7,9,11      | 1.76 | 2 (28%)     |
| 7   | FME  | H     | 1   | 7    | 8,9,10       | 1.53 | 1 (12%)     | 7,9,11      | 1.56 | 1 (14%)     |
| 12  | FME  | M     | 1   | 12   | 8,9,10       | 1.51 | 1 (12%)     | 7,9,11      | 1.55 | 1 (14%)     |
| 10  | FME  | K     | 1   | 10   | 8,9,10       | 1.50 | 1 (12%)     | 7,9,11      | 1.56 | 1 (14%)     |
| 9   | FME  | J     | 1   | 9    | 8,9,10       | 1.49 | 1 (12%)     | 7,9,11      | 1.64 | 2 (28%)     |
| 5   | 2MR  | D     | 137 | 5    | 10,12,13     | 2.36 | 2 (20%)     | 5,13,15     | 1.91 | 1 (20%)     |
| 11  | FME  | L     | 1   | 11   | 8,9,10       | 1.49 | 1 (12%)     | 7,9,11      | 1.62 | 2 (28%)     |
| 13  | FME  | N     | 1   | 13   | 8,9,10       | 1.49 | 1 (12%)     | 7,9,11      | 1.52 | 1 (14%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 2   | FME  | A     | 1   | 2    | -       | 5/7/9/11 | -     |
| 7   | FME  | H     | 1   | 7    | -       | 5/7/9/11 | -     |
| 12  | FME  | M     | 1   | 12   | -       | 1/7/9/11 | -     |
| 10  | FME  | K     | 1   | 10   | -       | 2/7/9/11 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 9   | FME  | J     | 1   | 9    | -       | 3/7/9/11   | -     |
| 5   | 2MR  | D     | 137 | 5    | -       | 0/10/13/15 | -     |
| 11  | FME  | L     | 1   | 11   | -       | 0/7/9/11   | -     |
| 13  | FME  | N     | 1   | 13   | -       | 0/7/9/11   | -     |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 5   | D     | 137 | 2MR  | CZ-NH2 | 5.24 | 1.45        | 1.33     |
| 5   | D     | 137 | 2MR  | CZ-NE  | 4.87 | 1.44        | 1.34     |
| 7   | H     | 1   | FME  | CN-N   | 3.74 | 1.45        | 1.33     |
| 2   | A     | 1   | FME  | CN-N   | 3.71 | 1.45        | 1.33     |
| 12  | M     | 1   | FME  | CN-N   | 3.71 | 1.45        | 1.33     |
| 10  | K     | 1   | FME  | CN-N   | 3.66 | 1.45        | 1.33     |
| 9   | J     | 1   | FME  | CN-N   | 3.62 | 1.45        | 1.33     |
| 13  | N     | 1   | FME  | CN-N   | 3.59 | 1.45        | 1.33     |
| 11  | L     | 1   | FME  | CN-N   | 3.59 | 1.45        | 1.33     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | D     | 137 | 2MR  | CD-NE-CZ | -3.50 | 116.86      | 123.41   |
| 2   | A     | 1   | FME  | CE-SD-CG | 2.99  | 110.67      | 100.40   |
| 12  | M     | 1   | FME  | CE-SD-CG | 2.77  | 109.93      | 100.40   |
| 7   | H     | 1   | FME  | CE-SD-CG | 2.66  | 109.55      | 100.40   |
| 10  | K     | 1   | FME  | CE-SD-CG | 2.66  | 109.53      | 100.40   |
| 11  | L     | 1   | FME  | CE-SD-CG | 2.59  | 109.31      | 100.40   |
| 13  | N     | 1   | FME  | CE-SD-CG | 2.50  | 108.99      | 100.40   |
| 9   | J     | 1   | FME  | CE-SD-CG | 2.36  | 108.50      | 100.40   |
| 2   | A     | 1   | FME  | CA-N-CN  | -2.23 | 119.40      | 122.82   |
| 9   | J     | 1   | FME  | O1-CN-N  | -2.08 | 119.78      | 125.27   |
| 11  | L     | 1   | FME  | O1-CN-N  | -2.05 | 119.88      | 125.27   |

There are no chirality outliers.

All (16) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms      |
|-----|-------|-----|------|------------|
| 2   | A     | 1   | FME  | O1-CN-N-CA |
| 2   | A     | 1   | FME  | CB-CA-N-CN |
| 2   | A     | 1   | FME  | N-CA-CB-CG |
| 2   | A     | 1   | FME  | C-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | H     | 1   | FME  | N-CA-CB-CG  |
| 7   | H     | 1   | FME  | C-CA-CB-CG  |
| 7   | H     | 1   | FME  | O-C-CA-CB   |
| 9   | J     | 1   | FME  | C-CA-CB-CG  |
| 10  | K     | 1   | FME  | C-CA-CB-CG  |
| 2   | A     | 1   | FME  | CB-CG-SD-CE |
| 10  | K     | 1   | FME  | N-CA-CB-CG  |
| 7   | H     | 1   | FME  | CA-CB-CG-SD |
| 7   | H     | 1   | FME  | CB-CG-SD-CE |
| 12  | M     | 1   | FME  | CB-CG-SD-CE |
| 9   | J     | 1   | FME  | N-CA-CB-CG  |
| 9   | J     | 1   | FME  | CB-CA-N-CN  |

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | A     | 1   | FME  | 1       | 0            |
| 7   | H     | 1   | FME  | 1       | 0            |
| 9   | J     | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 2 are monoatomic - leaving 56 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 | $\# Z  > 2$ |
| 43  | PLC  | D     | 501 | -    | 41,41,41     | 0.50 | 0           | 47,49,49    | 0.57 | 1 (2%)      |
| 47  | 3PE  | L     | 707 | -    | 50,50,50     | 0.86 | 4 (8%)      | 53,55,55    | 1.10 | 2 (3%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 47  | 3PE  | j     | 101  | -    | 26,26,50     | 1.16 | 4 (15%)  | 29,31,55    | 1.17 | 2 (6%)   |
| 48  | CDL  | b     | 102  | -    | 58,58,99     | 1.11 | 8 (13%)  | 64,70,111   | 1.22 | 4 (6%)   |
| 48  | CDL  | Z     | 202  | -    | 48,48,99     | 1.22 | 8 (16%)  | 54,60,111   | 1.27 | 4 (7%)   |
| 48  | CDL  | c     | 201  | -    | 59,59,99     | 1.10 | 8 (13%)  | 65,71,111   | 1.17 | 4 (6%)   |
| 47  | 3PE  | Z     | 203  | -    | 35,35,50     | 1.01 | 4 (11%)  | 38,40,55    | 1.13 | 2 (5%)   |
| 47  | 3PE  | m     | 102  | -    | 34,34,50     | 1.03 | 4 (11%)  | 37,39,55    | 1.10 | 2 (5%)   |
| 43  | PLC  | q     | 202  | -    | 35,35,41     | 0.55 | 0        | 41,43,49    | 0.63 | 0        |
| 47  | 3PE  | f     | 101  | -    | 50,50,50     | 0.86 | 4 (8%)   | 53,55,55    | 1.11 | 2 (3%)   |
| 47  | 3PE  | m     | 101  | -    | 24,24,50     | 1.21 | 4 (16%)  | 27,29,55    | 1.38 | 2 (7%)   |
| 47  | 3PE  | L     | 711  | -    | 45,45,50     | 0.90 | 4 (8%)   | 48,50,55    | 1.11 | 2 (4%)   |
| 47  | 3PE  | N     | 601  | -    | 39,39,50     | 0.97 | 4 (10%)  | 42,44,55    | 1.16 | 2 (4%)   |
| 44  | SF4  | I     | 302  | 8    | 0,12,12      | -    | -        | -           | -    | -        |
| 47  | 3PE  | L     | 703  | -    | 41,41,50     | 0.95 | 3 (7%)   | 44,46,55    | 1.15 | 2 (4%)   |
| 43  | PLC  | L     | 702  | -    | 34,34,41     | 0.56 | 0        | 40,42,49    | 0.63 | 1 (2%)   |
| 43  | PLC  | d     | 102  | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.51 | 0        |
| 44  | SF4  | B     | 301  | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 44  | SF4  | G     | 802  | 6    | 0,12,12      | -    | -        | -           | -    | -        |
| 43  | PLC  | h     | 201  | -    | 41,41,41     | 0.51 | 0        | 47,49,49    | 0.52 | 0        |
| 43  | PLC  | d     | 101  | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.54 | 0        |
| 51  | EHZ  | T     | 201  | 19   | 29,36,37     | 1.68 | 5 (17%)  | 35,44,47    | 1.58 | 7 (20%)  |
| 43  | PLC  | Y     | 301  | -    | 35,35,41     | 0.55 | 0        | 41,43,49    | 0.51 | 0        |
| 44  | SF4  | I     | 301  | 8    | 0,12,12      | -    | -        | -           | -    | -        |
| 47  | 3PE  | L     | 708  | -    | 50,50,50     | 0.85 | 4 (8%)   | 53,55,55    | 1.11 | 2 (3%)   |
| 47  | 3PE  | L     | 710  | -    | 50,50,50     | 0.86 | 4 (8%)   | 53,55,55    | 1.11 | 2 (3%)   |
| 47  | 3PE  | L     | 712  | -    | 50,50,50     | 0.86 | 4 (8%)   | 53,55,55    | 1.12 | 2 (3%)   |
| 43  | PLC  | P     | 502  | -    | 30,30,41     | 0.58 | 0        | 36,38,49    | 0.60 | 0        |
| 47  | 3PE  | Y     | 302  | -    | 25,25,50     | 1.18 | 4 (16%)  | 28,30,55    | 1.29 | 3 (10%)  |
| 47  | 3PE  | L     | 709  | -    | 45,45,50     | 0.90 | 4 (8%)   | 48,50,55    | 1.10 | 2 (4%)   |
| 51  | EHZ  | U     | 201  | 20   | 29,36,37     | 1.68 | 5 (17%)  | 35,44,47    | 1.61 | 8 (22%)  |
| 43  | PLC  | a     | 201  | -    | 21,21,41     | 0.68 | 0        | 27,29,49    | 0.65 | 0        |
| 47  | 3PE  | H     | 402  | -    | 30,30,50     | 1.08 | 4 (13%)  | 33,35,55    | 1.16 | 2 (6%)   |
| 43  | PLC  | L     | 705  | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.65 | 1 (2%)   |
| 48  | CDL  | O     | 201  | -    | 74,74,99     | 0.99 | 7 (9%)   | 80,86,111   | 1.13 | 5 (6%)   |
| 43  | PLC  | M     | 1002 | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.50 | 0        |
| 43  | PLC  | b     | 101  | -    | 38,38,41     | 0.53 | 0        | 44,46,49    | 0.54 | 0        |
| 43  | PLC  | H     | 401  | -    | 23,23,41     | 0.68 | 0        | 29,31,49    | 0.61 | 1 (3%)   |
| 43  | PLC  | M     | 1001 | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.52 | 0        |
| 43  | PLC  | q     | 201  | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.52 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 48  | CDL  | P     | 503  | -    | 41,41,99     | 1.27 | 7 (17%)  | 47,53,111   | 1.32 | 4 (8%)   |
| 49  | NDP  | P     | 501  | -    | 45,52,52     | 4.28 | 23 (51%) | 53,80,80    | 2.11 | 5 (9%)   |
| 43  | PLC  | A     | 201  | -    | 30,30,41     | 0.60 | 0        | 36,38,49    | 0.53 | 0        |
| 43  | PLC  | L     | 704  | -    | 31,31,41     | 0.55 | 0        | 37,39,49    | 0.57 | 0        |
| 43  | PLC  | B     | 302  | -    | 30,30,41     | 0.59 | 0        | 36,38,49    | 0.55 | 0        |
| 47  | 3PE  | M     | 1003 | -    | 34,34,50     | 1.02 | 4 (11%)  | 37,39,55    | 1.16 | 2 (5%)   |
| 44  | SF4  | G     | 801  | 6    | 0,12,12      | -    | -        | -           | -    | -        |
| 47  | 3PE  | L     | 706  | -    | 32,32,50     | 1.06 | 4 (12%)  | 35,37,55    | 1.18 | 2 (5%)   |
| 47  | 3PE  | O     | 202  | -    | 30,30,50     | 1.08 | 4 (13%)  | 33,35,55    | 1.12 | 2 (6%)   |
| 43  | PLC  | g     | 301  | -    | 38,38,41     | 0.53 | 0        | 44,46,49    | 0.53 | 0        |
| 47  | 3PE  | b     | 103  | -    | 39,39,50     | 0.96 | 4 (10%)  | 42,44,55    | 1.12 | 2 (4%)   |
| 47  | 3PE  | O     | 203  | -    | 34,34,50     | 1.04 | 4 (11%)  | 37,39,55    | 1.17 | 2 (5%)   |
| 43  | PLC  | Z     | 201  | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.53 | 0        |
| 47  | 3PE  | L     | 701  | -    | 28,28,50     | 1.13 | 4 (14%)  | 31,33,55    | 1.15 | 2 (6%)   |
| 43  | PLC  | Y     | 303  | -    | 35,35,41     | 0.53 | 0        | 41,43,49    | 0.58 | 0        |
| 45  | FES  | G     | 803  | 6    | 0,4,4        | -    | -        | -           | -    | -        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 43  | PLC  | D     | 501 | -    | -       | 18/45/45/45  | -       |
| 47  | 3PE  | L     | 707 | -    | -       | 33/54/54/54  | -       |
| 47  | 3PE  | j     | 101 | -    | -       | 12/30/30/54  | -       |
| 48  | CDL  | b     | 102 | -    | -       | 32/69/69/110 | -       |
| 48  | CDL  | Z     | 202 | -    | -       | 27/58/58/110 | -       |
| 48  | CDL  | c     | 201 | -    | -       | 35/70/70/110 | -       |
| 47  | 3PE  | Z     | 203 | -    | -       | 22/39/39/54  | -       |
| 47  | 3PE  | m     | 102 | -    | -       | 12/38/38/54  | -       |
| 43  | PLC  | q     | 202 | -    | -       | 13/39/39/45  | -       |
| 47  | 3PE  | f     | 101 | -    | -       | 26/54/54/54  | -       |
| 47  | 3PE  | m     | 101 | -    | -       | 15/27/27/54  | -       |
| 47  | 3PE  | L     | 711 | -    | -       | 28/49/49/54  | -       |
| 47  | 3PE  | N     | 601 | -    | -       | 20/43/43/54  | -       |
| 44  | SF4  | I     | 302 | 8    | -       | -            | 0/6/5/5 |
| 47  | 3PE  | L     | 703 | -    | -       | 22/45/45/54  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|------|------|---------|--------------|---------|
| 43  | PLC  | L     | 702  | -    | -       | 18/38/38/45  | -       |
| 43  | PLC  | d     | 102  | -    | -       | 19/45/45/45  | -       |
| 44  | SF4  | B     | 301  | 3    | -       | -            | 0/6/5/5 |
| 44  | SF4  | G     | 802  | 6    | -       | -            | 0/6/5/5 |
| 43  | PLC  | h     | 201  | -    | -       | 21/45/45/45  | -       |
| 43  | PLC  | d     | 101  | -    | -       | 14/45/45/45  | -       |
| 51  | EHZ  | T     | 201  | 19   | -       | 22/42/44/45  | -       |
| 43  | PLC  | Y     | 301  | -    | -       | 8/39/39/45   | -       |
| 47  | 3PE  | L     | 708  | -    | -       | 20/54/54/54  | -       |
| 44  | SF4  | I     | 301  | 8    | -       | -            | 0/6/5/5 |
| 47  | 3PE  | L     | 710  | -    | -       | 23/54/54/54  | -       |
| 47  | 3PE  | L     | 712  | -    | -       | 29/54/54/54  | -       |
| 43  | PLC  | P     | 502  | -    | -       | 11/34/34/45  | -       |
| 47  | 3PE  | Y     | 302  | -    | -       | 12/28/28/54  | -       |
| 47  | 3PE  | L     | 709  | -    | -       | 23/49/49/54  | -       |
| 51  | EHZ  | U     | 201  | 20   | -       | 15/42/44/45  | -       |
| 43  | PLC  | a     | 201  | -    | -       | 7/23/23/45   | -       |
| 47  | 3PE  | H     | 402  | -    | -       | 18/34/34/54  | -       |
| 43  | PLC  | L     | 705  | -    | -       | 21/45/45/45  | -       |
| 48  | CDL  | O     | 201  | -    | -       | 45/85/85/110 | -       |
| 43  | PLC  | M     | 1002 | -    | -       | 15/45/45/45  | -       |
| 43  | PLC  | b     | 101  | -    | -       | 14/42/42/45  | -       |
| 43  | PLC  | H     | 401  | -    | -       | 8/26/26/45   | -       |
| 43  | PLC  | M     | 1001 | -    | -       | 14/45/45/45  | -       |
| 43  | PLC  | q     | 201  | -    | -       | 20/45/45/45  | -       |
| 48  | CDL  | P     | 503  | -    | -       | 21/50/50/110 | -       |
| 49  | NDP  | P     | 501  | -    | -       | 11/30/77/77  | 0/5/5/5 |
| 43  | PLC  | A     | 201  | -    | -       | 9/34/34/45   | -       |
| 43  | PLC  | L     | 704  | -    | -       | 17/35/35/45  | -       |
| 43  | PLC  | B     | 302  | -    | -       | 14/34/34/45  | -       |
| 47  | 3PE  | M     | 1003 | -    | -       | 15/38/38/54  | -       |
| 44  | SF4  | G     | 801  | 6    | -       | -            | 0/6/5/5 |
| 47  | 3PE  | L     | 706  | -    | -       | 16/36/36/54  | -       |
| 47  | 3PE  | O     | 202  | -    | -       | 21/34/34/54  | -       |
| 43  | PLC  | g     | 301  | -    | -       | 16/42/42/45  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 47  | 3PE  | b     | 103 | -    | -       | 29/43/43/54 | -       |
| 47  | 3PE  | O     | 203 | -    | -       | 21/38/38/54 | -       |
| 43  | PLC  | Z     | 201 | -    | -       | 16/45/45/45 | -       |
| 47  | 3PE  | L     | 701 | -    | -       | 14/32/32/54 | -       |
| 43  | PLC  | Y     | 303 | -    | -       | 17/39/39/45 | -       |
| 45  | FES  | G     | 803 | 6    | -       | -           | 0/1/1/1 |

All (154) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | P     | 501 | NDP  | O4B-C1B | 14.86 | 1.61        | 1.41     |
| 49  | P     | 501 | NDP  | C6N-C5N | 12.21 | 1.55        | 1.33     |
| 49  | P     | 501 | NDP  | C7N-N7N | 8.27  | 1.55        | 1.33     |
| 49  | P     | 501 | NDP  | O4D-C1D | 8.02  | 1.61        | 1.42     |
| 49  | P     | 501 | NDP  | C2D-C1D | -7.21 | 1.30        | 1.53     |
| 49  | P     | 501 | NDP  | O4D-C4D | -6.51 | 1.30        | 1.45     |
| 49  | P     | 501 | NDP  | P2B-O2B | 5.53  | 1.69        | 1.59     |
| 51  | T     | 201 | EHZ  | C15-N2  | 5.40  | 1.45        | 1.33     |
| 51  | U     | 201 | EHZ  | C15-N2  | 5.33  | 1.45        | 1.33     |
| 51  | U     | 201 | EHZ  | C12-N1  | 5.27  | 1.45        | 1.33     |
| 51  | T     | 201 | EHZ  | C12-N1  | 5.25  | 1.45        | 1.33     |
| 49  | P     | 501 | NDP  | O4B-C4B | -5.20 | 1.33        | 1.45     |
| 49  | P     | 501 | NDP  | C2N-C3N | 4.69  | 1.48        | 1.34     |
| 49  | P     | 501 | NDP  | O7N-C7N | -4.07 | 1.14        | 1.24     |
| 49  | P     | 501 | NDP  | O2D-C2D | 3.95  | 1.52        | 1.43     |
| 49  | P     | 501 | NDP  | C6A-N6A | 3.84  | 1.48        | 1.34     |
| 49  | P     | 501 | NDP  | C5A-C4A | -3.60 | 1.31        | 1.40     |
| 49  | P     | 501 | NDP  | C4N-C3N | 3.26  | 1.56        | 1.49     |
| 49  | P     | 501 | NDP  | C2A-N3A | 2.76  | 1.36        | 1.32     |
| 49  | P     | 501 | NDP  | C4N-C5N | 2.71  | 1.56        | 1.48     |
| 48  | O     | 201 | CDL  | OB6-CB4 | -2.70 | 1.39        | 1.46     |
| 49  | P     | 501 | NDP  | O3B-C3B | -2.68 | 1.36        | 1.43     |
| 48  | c     | 201 | CDL  | OB6-CB4 | -2.63 | 1.40        | 1.46     |
| 47  | b     | 103 | 3PE  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 47  | L     | 703 | 3PE  | O21-C2  | -2.61 | 1.40        | 1.46     |
| 47  | L     | 712 | 3PE  | O21-C2  | -2.60 | 1.40        | 1.46     |
| 48  | b     | 102 | CDL  | OA6-CA4 | -2.59 | 1.40        | 1.46     |
| 48  | b     | 102 | CDL  | OB6-CB4 | -2.57 | 1.40        | 1.46     |
| 47  | L     | 708 | 3PE  | O21-C2  | -2.57 | 1.40        | 1.46     |
| 47  | j     | 101 | 3PE  | O21-C2  | -2.56 | 1.40        | 1.46     |
| 49  | P     | 501 | NDP  | O3D-C3D | -2.56 | 1.37        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 47  | m     | 102  | 3PE  | O21-C2  | -2.55 | 1.40        | 1.46     |
| 48  | P     | 503  | CDL  | OB6-CB4 | -2.55 | 1.40        | 1.46     |
| 47  | L     | 707  | 3PE  | O21-C2  | -2.55 | 1.40        | 1.46     |
| 48  | Z     | 202  | CDL  | OB6-CB4 | -2.54 | 1.40        | 1.46     |
| 47  | L     | 710  | 3PE  | O21-C2  | -2.53 | 1.40        | 1.46     |
| 47  | Y     | 302  | 3PE  | O21-C2  | -2.53 | 1.40        | 1.46     |
| 47  | L     | 711  | 3PE  | O21-C2  | -2.53 | 1.40        | 1.46     |
| 47  | f     | 101  | 3PE  | O21-C2  | -2.52 | 1.40        | 1.46     |
| 48  | P     | 503  | CDL  | OA6-CA4 | -2.51 | 1.40        | 1.46     |
| 47  | Z     | 203  | 3PE  | O21-C2  | -2.50 | 1.40        | 1.46     |
| 47  | L     | 701  | 3PE  | O21-C2  | -2.49 | 1.40        | 1.46     |
| 47  | M     | 1003 | 3PE  | O21-C2  | -2.48 | 1.40        | 1.46     |
| 47  | O     | 202  | 3PE  | O31-C31 | 2.48  | 1.40        | 1.33     |
| 48  | O     | 201  | CDL  | OA8-CA7 | 2.48  | 1.40        | 1.33     |
| 47  | H     | 402  | 3PE  | O21-C2  | -2.48 | 1.40        | 1.46     |
| 48  | c     | 201  | CDL  | OB8-CB7 | 2.48  | 1.40        | 1.33     |
| 47  | O     | 203  | 3PE  | O21-C2  | -2.44 | 1.40        | 1.46     |
| 49  | P     | 501  | NDP  | C6N-N1N | 2.44  | 1.43        | 1.37     |
| 48  | b     | 102  | CDL  | OB8-CB7 | 2.43  | 1.40        | 1.33     |
| 48  | c     | 201  | CDL  | OA6-CA4 | -2.43 | 1.40        | 1.46     |
| 47  | m     | 101  | 3PE  | O21-C21 | 2.42  | 1.40        | 1.35     |
| 47  | L     | 703  | 3PE  | O31-C31 | 2.42  | 1.40        | 1.33     |
| 48  | Z     | 202  | CDL  | OA8-CA7 | 2.42  | 1.40        | 1.33     |
| 47  | N     | 601  | 3PE  | O21-C2  | -2.41 | 1.40        | 1.46     |
| 47  | m     | 102  | 3PE  | O31-C31 | 2.41  | 1.40        | 1.33     |
| 48  | b     | 102  | CDL  | OA8-CA7 | 2.39  | 1.40        | 1.33     |
| 48  | P     | 503  | CDL  | OA8-CA7 | 2.38  | 1.40        | 1.33     |
| 48  | Z     | 202  | CDL  | OA6-CA5 | 2.38  | 1.40        | 1.35     |
| 48  | Z     | 202  | CDL  | OB8-CB7 | 2.38  | 1.40        | 1.33     |
| 47  | M     | 1003 | 3PE  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 47  | Y     | 302  | 3PE  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 47  | L     | 701  | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 47  | m     | 101  | 3PE  | O31-C31 | 2.36  | 1.40        | 1.33     |
| 51  | U     | 201  | EHZ  | C9-S1   | 2.36  | 1.81        | 1.76     |
| 47  | L     | 706  | 3PE  | O31-C31 | 2.35  | 1.40        | 1.33     |
| 47  | Z     | 203  | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 47  | O     | 203  | 3PE  | O31-C31 | 2.34  | 1.40        | 1.33     |
| 47  | j     | 101  | 3PE  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 47  | N     | 601  | 3PE  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 47  | H     | 402  | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 47  | L     | 711  | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |
| 47  | L     | 709  | 3PE  | O31-C31 | 2.32  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 48  | O     | 201 | CDL  | OA6-CA4 | -2.31 | 1.40        | 1.46     |
| 47  | b     | 103 | 3PE  | O31-C31 | 2.31  | 1.40        | 1.33     |
| 47  | f     | 101 | 3PE  | O31-C31 | 2.31  | 1.40        | 1.33     |
| 47  | L     | 707 | 3PE  | O31-C3  | -2.30 | 1.39        | 1.45     |
| 47  | L     | 706 | 3PE  | O21-C21 | 2.29  | 1.40        | 1.34     |
| 49  | P     | 501 | NDP  | C7N-C3N | 2.29  | 1.53        | 1.48     |
| 47  | L     | 706 | 3PE  | O21-C2  | -2.29 | 1.40        | 1.46     |
| 47  | L     | 710 | 3PE  | O31-C31 | 2.28  | 1.40        | 1.33     |
| 48  | O     | 201 | CDL  | OB8-CB6 | -2.28 | 1.40        | 1.45     |
| 51  | T     | 201 | EHZ  | O4-C15  | -2.27 | 1.18        | 1.23     |
| 47  | L     | 708 | 3PE  | O31-C31 | 2.27  | 1.40        | 1.33     |
| 47  | L     | 712 | 3PE  | O31-C3  | -2.27 | 1.40        | 1.45     |
| 48  | c     | 201 | CDL  | OA8-CA7 | 2.27  | 1.40        | 1.33     |
| 48  | P     | 503 | CDL  | OB6-CB5 | 2.27  | 1.40        | 1.35     |
| 47  | L     | 709 | 3PE  | O21-C2  | -2.26 | 1.40        | 1.46     |
| 48  | O     | 201 | CDL  | OB8-CB7 | 2.26  | 1.39        | 1.33     |
| 51  | T     | 201 | EHZ  | O3-C12  | -2.26 | 1.18        | 1.23     |
| 47  | m     | 101 | 3PE  | O21-C2  | -2.24 | 1.41        | 1.46     |
| 49  | P     | 501 | NDP  | PA-O5B  | 2.24  | 1.68        | 1.59     |
| 47  | L     | 712 | 3PE  | O31-C31 | 2.23  | 1.39        | 1.33     |
| 47  | Z     | 203 | 3PE  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 47  | O     | 203 | 3PE  | O31-C3  | -2.23 | 1.40        | 1.45     |
| 51  | T     | 201 | EHZ  | C9-S1   | 2.23  | 1.81        | 1.76     |
| 48  | c     | 201 | CDL  | OA8-CA6 | -2.22 | 1.40        | 1.45     |
| 51  | U     | 201 | EHZ  | O4-C15  | -2.22 | 1.19        | 1.23     |
| 47  | N     | 601 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 48  | O     | 201 | CDL  | OA6-CA5 | 2.22  | 1.40        | 1.34     |
| 47  | L     | 708 | 3PE  | O31-C3  | -2.21 | 1.40        | 1.45     |
| 47  | L     | 709 | 3PE  | O21-C21 | 2.21  | 1.40        | 1.34     |
| 47  | O     | 203 | 3PE  | O21-C21 | 2.20  | 1.40        | 1.34     |
| 47  | L     | 710 | 3PE  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 49  | P     | 501 | NDP  | P2B-O1X | 2.20  | 1.57        | 1.50     |
| 47  | O     | 202 | 3PE  | O21-C2  | -2.20 | 1.41        | 1.46     |
| 47  | H     | 402 | 3PE  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 47  | b     | 103 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 51  | U     | 201 | EHZ  | O3-C12  | -2.19 | 1.18        | 1.23     |
| 47  | L     | 709 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 47  | f     | 101 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 47  | Y     | 302 | 3PE  | O21-C21 | 2.19  | 1.40        | 1.35     |
| 48  | Z     | 202 | CDL  | OA6-CA4 | -2.18 | 1.41        | 1.46     |
| 48  | c     | 201 | CDL  | OA6-CA5 | 2.17  | 1.40        | 1.34     |
| 48  | P     | 503 | CDL  | OA8-CA6 | -2.17 | 1.40        | 1.45     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 47  | M     | 1003 | 3PE  | O31-C3  | -2.17 | 1.40        | 1.45     |
| 47  | O     | 202  | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 47  | N     | 601  | 3PE  | O21-C21 | 2.17  | 1.40        | 1.34     |
| 47  | L     | 711  | 3PE  | O31-C3  | -2.16 | 1.40        | 1.45     |
| 48  | P     | 503  | CDL  | OB8-CB6 | -2.16 | 1.40        | 1.45     |
| 47  | L     | 711  | 3PE  | O21-C21 | 2.16  | 1.40        | 1.34     |
| 47  | Y     | 302  | 3PE  | O31-C3  | -2.15 | 1.40        | 1.45     |
| 48  | Z     | 202  | CDL  | OB6-CB5 | 2.15  | 1.40        | 1.34     |
| 47  | m     | 101  | 3PE  | O31-C3  | -2.15 | 1.40        | 1.45     |
| 48  | Z     | 202  | CDL  | OB8-CB6 | -2.15 | 1.40        | 1.45     |
| 47  | L     | 701  | 3PE  | O31-C3  | -2.15 | 1.40        | 1.45     |
| 47  | L     | 707  | 3PE  | O31-C31 | 2.15  | 1.39        | 1.33     |
| 47  | j     | 101  | 3PE  | O31-C3  | -2.14 | 1.40        | 1.45     |
| 47  | H     | 402  | 3PE  | O21-C21 | 2.14  | 1.40        | 1.34     |
| 47  | L     | 703  | 3PE  | O31-C3  | -2.13 | 1.40        | 1.45     |
| 48  | b     | 102  | CDL  | OB8-CB6 | -2.12 | 1.40        | 1.45     |
| 48  | c     | 201  | CDL  | OB8-CB6 | -2.12 | 1.40        | 1.45     |
| 48  | P     | 503  | CDL  | OA6-CA5 | 2.11  | 1.40        | 1.34     |
| 47  | Z     | 203  | 3PE  | O21-C21 | 2.11  | 1.40        | 1.34     |
| 47  | L     | 701  | 3PE  | O21-C21 | 2.11  | 1.40        | 1.34     |
| 47  | m     | 102  | 3PE  | O31-C3  | -2.11 | 1.40        | 1.45     |
| 47  | L     | 706  | 3PE  | O31-C3  | -2.10 | 1.40        | 1.45     |
| 47  | f     | 101  | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 48  | b     | 102  | CDL  | OA8-CA6 | -2.10 | 1.40        | 1.45     |
| 48  | Z     | 202  | CDL  | OA8-CA6 | -2.10 | 1.40        | 1.45     |
| 47  | M     | 1003 | 3PE  | O21-C21 | 2.10  | 1.40        | 1.34     |
| 47  | L     | 707  | 3PE  | O21-C21 | 2.09  | 1.40        | 1.34     |
| 47  | j     | 101  | 3PE  | O21-C21 | 2.09  | 1.40        | 1.34     |
| 47  | O     | 202  | 3PE  | O31-C3  | -2.08 | 1.40        | 1.45     |
| 47  | L     | 710  | 3PE  | O21-C21 | 2.08  | 1.40        | 1.34     |
| 48  | b     | 102  | CDL  | OB6-CB5 | 2.06  | 1.40        | 1.34     |
| 47  | m     | 102  | 3PE  | O21-C21 | 2.06  | 1.40        | 1.34     |
| 47  | L     | 712  | 3PE  | O21-C21 | 2.04  | 1.40        | 1.34     |
| 49  | P     | 501  | NDP  | C5B-C4B | 2.02  | 1.57        | 1.51     |
| 48  | O     | 201  | CDL  | OA8-CA6 | -2.02 | 1.40        | 1.45     |
| 48  | b     | 102  | CDL  | OA6-CA5 | 2.02  | 1.40        | 1.34     |
| 47  | b     | 103  | 3PE  | O21-C21 | 2.01  | 1.40        | 1.34     |
| 48  | c     | 201  | CDL  | OB6-CB5 | 2.01  | 1.40        | 1.34     |
| 47  | L     | 708  | 3PE  | O21-C21 | 2.00  | 1.40        | 1.34     |

All (88) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | P     | 501  | NDP  | C5A-C6A-N6A | 8.56  | 133.36      | 120.35   |
| 49  | P     | 501  | NDP  | C1B-N9A-C4A | -7.78 | 112.97      | 126.64   |
| 49  | P     | 501  | NDP  | N6A-C6A-N1A | -6.02 | 106.09      | 118.57   |
| 49  | P     | 501  | NDP  | N3A-C2A-N1A | -5.57 | 119.97      | 128.68   |
| 51  | U     | 201  | EHZ  | C8-C9-S1    | 5.34  | 120.24      | 113.63   |
| 47  | m     | 101  | 3PE  | O21-C21-C22 | 5.19  | 120.64      | 111.09   |
| 51  | T     | 201  | EHZ  | C8-C9-S1    | 5.18  | 120.03      | 113.63   |
| 48  | P     | 503  | CDL  | OB6-CB5-C51 | 4.90  | 120.10      | 111.09   |
| 47  | Y     | 302  | 3PE  | O21-C21-C22 | 4.84  | 120.00      | 111.09   |
| 48  | Z     | 202  | CDL  | OA6-CA5-C11 | 4.77  | 119.86      | 111.09   |
| 47  | L     | 706  | 3PE  | O21-C21-C22 | 4.64  | 121.50      | 111.50   |
| 47  | N     | 601  | 3PE  | O21-C21-C22 | 4.35  | 120.88      | 111.50   |
| 47  | L     | 712  | 3PE  | O21-C21-C22 | 4.30  | 120.76      | 111.50   |
| 47  | L     | 703  | 3PE  | O21-C21-C22 | 4.26  | 120.69      | 111.50   |
| 47  | f     | 101  | 3PE  | O21-C21-C22 | 4.16  | 120.46      | 111.50   |
| 47  | L     | 710  | 3PE  | O21-C21-C22 | 4.15  | 120.44      | 111.50   |
| 48  | Z     | 202  | CDL  | OB6-CB5-C51 | 4.10  | 120.34      | 111.50   |
| 47  | H     | 402  | 3PE  | O21-C21-C22 | 4.03  | 120.20      | 111.50   |
| 47  | L     | 708  | 3PE  | O21-C21-C22 | 4.03  | 120.19      | 111.50   |
| 47  | L     | 711  | 3PE  | O21-C21-C22 | 4.02  | 120.17      | 111.50   |
| 48  | b     | 102  | CDL  | OB6-CB5-C51 | 4.02  | 120.16      | 111.50   |
| 47  | M     | 1003 | 3PE  | O21-C21-C22 | 4.01  | 120.15      | 111.50   |
| 47  | O     | 203  | 3PE  | O21-C21-C22 | 4.00  | 120.13      | 111.50   |
| 47  | L     | 707  | 3PE  | O21-C21-C22 | 3.99  | 120.11      | 111.50   |
| 48  | c     | 201  | CDL  | OB6-CB5-C51 | 3.96  | 120.04      | 111.50   |
| 48  | P     | 503  | CDL  | OA6-CA5-C11 | 3.96  | 120.03      | 111.50   |
| 47  | m     | 102  | 3PE  | O21-C21-C22 | 3.91  | 119.92      | 111.50   |
| 47  | L     | 701  | 3PE  | O21-C21-C22 | 3.87  | 119.83      | 111.50   |
| 47  | Z     | 203  | 3PE  | O21-C21-C22 | 3.87  | 119.83      | 111.50   |
| 48  | b     | 102  | CDL  | OA6-CA5-C11 | 3.86  | 119.83      | 111.50   |
| 47  | j     | 101  | 3PE  | O21-C21-C22 | 3.86  | 119.82      | 111.50   |
| 48  | O     | 201  | CDL  | OB6-CB5-C51 | 3.81  | 119.72      | 111.50   |
| 47  | L     | 709  | 3PE  | O21-C21-C22 | 3.81  | 119.70      | 111.50   |
| 47  | b     | 103  | 3PE  | O21-C21-C22 | 3.78  | 119.64      | 111.50   |
| 48  | c     | 201  | CDL  | OA6-CA5-C11 | 3.77  | 119.64      | 111.50   |
| 48  | O     | 201  | CDL  | OA6-CA5-C11 | 3.68  | 119.42      | 111.50   |
| 47  | O     | 202  | 3PE  | O21-C21-C22 | 3.63  | 119.33      | 111.50   |
| 48  | b     | 102  | CDL  | OB8-CB7-C71 | 3.35  | 120.16      | 111.38   |
| 47  | O     | 203  | 3PE  | O31-C31-C32 | 2.88  | 120.96      | 111.91   |
| 49  | P     | 501  | NDP  | PN-O3-PA    | -2.79 | 123.27      | 132.83   |
| 48  | c     | 201  | CDL  | OB8-CB7-C71 | 2.77  | 120.60      | 111.91   |
| 47  | L     | 703  | 3PE  | O31-C31-C32 | 2.76  | 120.58      | 111.91   |
| 47  | O     | 202  | 3PE  | O31-C31-C32 | 2.76  | 120.56      | 111.91   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 47  | L     | 711  | 3PE  | O31-C31-C32 | 2.74  | 120.52      | 111.91   |
| 48  | O     | 201  | CDL  | OB8-CB7-C71 | 2.71  | 120.42      | 111.91   |
| 47  | m     | 101  | 3PE  | O31-C31-C32 | 2.69  | 120.34      | 111.91   |
| 48  | Z     | 202  | CDL  | OB8-CB7-C71 | 2.69  | 120.34      | 111.91   |
| 48  | b     | 102  | CDL  | OA8-CA7-C31 | 2.66  | 120.24      | 111.91   |
| 47  | j     | 101  | 3PE  | O31-C31-C32 | 2.65  | 120.24      | 111.91   |
| 47  | L     | 707  | 3PE  | O31-C31-C32 | 2.65  | 120.22      | 111.91   |
| 47  | N     | 601  | 3PE  | O31-C31-C32 | 2.65  | 120.21      | 111.91   |
| 48  | P     | 503  | CDL  | OA8-CA7-C31 | 2.62  | 120.13      | 111.91   |
| 47  | L     | 701  | 3PE  | O31-C31-C32 | 2.61  | 120.11      | 111.91   |
| 47  | L     | 709  | 3PE  | O31-C31-C32 | 2.61  | 120.10      | 111.91   |
| 47  | L     | 706  | 3PE  | O31-C31-C32 | 2.61  | 120.09      | 111.91   |
| 47  | f     | 101  | 3PE  | O31-C31-C32 | 2.59  | 120.04      | 111.91   |
| 47  | b     | 103  | 3PE  | O31-C31-C32 | 2.58  | 120.02      | 111.91   |
| 47  | Z     | 203  | 3PE  | O31-C31-C32 | 2.58  | 120.01      | 111.91   |
| 48  | c     | 201  | CDL  | OA8-CA7-C31 | 2.58  | 120.00      | 111.91   |
| 51  | U     | 201  | EHZ  | C14-C13-C12 | -2.57 | 108.07      | 112.36   |
| 48  | O     | 201  | CDL  | OA8-CA7-C31 | 2.55  | 119.92      | 111.91   |
| 47  | m     | 102  | 3PE  | O31-C31-C32 | 2.53  | 119.86      | 111.91   |
| 47  | L     | 710  | 3PE  | O31-C31-C32 | 2.50  | 119.75      | 111.91   |
| 47  | L     | 712  | 3PE  | O31-C31-C32 | 2.50  | 119.74      | 111.91   |
| 47  | M     | 1003 | 3PE  | O31-C31-C32 | 2.50  | 119.74      | 111.91   |
| 47  | L     | 708  | 3PE  | O31-C31-C32 | 2.48  | 119.68      | 111.91   |
| 48  | Z     | 202  | CDL  | OA8-CA7-C31 | 2.47  | 119.65      | 111.91   |
| 47  | H     | 402  | 3PE  | O31-C31-C32 | 2.45  | 119.60      | 111.91   |
| 51  | T     | 201  | EHZ  | C13-C12-N1  | 2.44  | 120.54      | 116.42   |
| 51  | U     | 201  | EHZ  | C10-S1-C9   | 2.41  | 109.36      | 101.87   |
| 47  | Y     | 302  | 3PE  | O31-C31-C32 | 2.34  | 119.24      | 111.91   |
| 51  | T     | 201  | EHZ  | C11-N1-C12  | -2.32 | 118.54      | 122.84   |
| 51  | T     | 201  | EHZ  | O2-C9-S1    | -2.31 | 119.61      | 122.61   |
| 43  | L     | 702  | PLC  | C3-C2-C1    | 2.30  | 117.24      | 111.79   |
| 51  | U     | 201  | EHZ  | C13-C12-N1  | 2.28  | 120.26      | 116.42   |
| 43  | D     | 501  | PLC  | C2-O2-C'    | 2.26  | 123.36      | 117.79   |
| 51  | U     | 201  | EHZ  | C7-C8-C9    | -2.16 | 108.97      | 113.89   |
| 48  | P     | 503  | CDL  | CB4-OB6-CB5 | -2.12 | 113.94      | 117.90   |
| 51  | U     | 201  | EHZ  | C13-C14-N2  | -2.08 | 107.70      | 111.90   |
| 48  | O     | 201  | CDL  | CB4-OB6-CB5 | -2.06 | 112.72      | 117.79   |
| 51  | T     | 201  | EHZ  | C14-C13-C12 | -2.06 | 108.93      | 112.36   |
| 47  | Y     | 302  | 3PE  | C2-O21-C21  | -2.06 | 114.06      | 117.90   |
| 43  | L     | 705  | PLC  | C3-C2-C1    | 2.05  | 116.65      | 111.79   |
| 51  | T     | 201  | EHZ  | C10-S1-C9   | 2.04  | 108.23      | 101.87   |
| 51  | U     | 201  | EHZ  | O2-C9-S1    | -2.03 | 119.98      | 122.61   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 51  | U     | 201 | EHZ  | C5-C6-C7 | -2.02 | 109.04      | 114.85   |
| 51  | T     | 201 | EHZ  | C7-C8-C9 | -2.02 | 109.28      | 113.89   |
| 43  | H     | 401 | PLC  | C3-C2-C1 | 2.02  | 116.56      | 111.79   |

There are no chirality outliers.

All (949) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 43  | A     | 201  | PLC  | O4P-C4-C5-N  |
| 43  | A     | 201  | PLC  | C1'-C'-O2-C2 |
| 43  | A     | 201  | PLC  | O'-C'-O2-C2  |
| 43  | A     | 201  | PLC  | C4-O4P-P-O3P |
| 43  | B     | 302  | PLC  | O4P-C4-C5-N  |
| 43  | B     | 302  | PLC  | C1-O3P-P-O2P |
| 43  | D     | 501  | PLC  | C3-C2-O2-C'  |
| 43  | D     | 501  | PLC  | O4P-C4-C5-N  |
| 43  | D     | 501  | PLC  | C1'-C'-O2-C2 |
| 43  | H     | 401  | PLC  | C1-O3P-P-O4P |
| 43  | H     | 401  | PLC  | C4-O4P-P-O1P |
| 43  | H     | 401  | PLC  | C4-O4P-P-O2P |
| 43  | L     | 702  | PLC  | O4P-C4-C5-N  |
| 43  | L     | 704  | PLC  | C1-O3P-P-O1P |
| 43  | L     | 704  | PLC  | C1-O3P-P-O2P |
| 43  | L     | 704  | PLC  | C1-O3P-P-O4P |
| 43  | L     | 705  | PLC  | C1-O3P-P-O1P |
| 43  | L     | 705  | PLC  | C1-O3P-P-O2P |
| 43  | L     | 705  | PLC  | C1-O3P-P-O4P |
| 43  | M     | 1002 | PLC  | O4P-C4-C5-N  |
| 43  | P     | 502  | PLC  | O2-C2-C3-O3  |
| 43  | Y     | 301  | PLC  | O4P-C4-C5-N  |
| 43  | Y     | 301  | PLC  | C1'-C'-O2-C2 |
| 43  | Y     | 303  | PLC  | O'-C'-O2-C2  |
| 43  | Y     | 303  | PLC  | C1-O3P-P-O1P |
| 43  | Z     | 201  | PLC  | O2-C2-C3-O3  |
| 43  | Z     | 201  | PLC  | O4P-C4-C5-N  |
| 43  | Z     | 201  | PLC  | C4-O4P-P-O1P |
| 43  | a     | 201  | PLC  | O4P-C4-C5-N  |
| 43  | b     | 101  | PLC  | C1-O3P-P-O1P |
| 43  | b     | 101  | PLC  | C1-O3P-P-O2P |
| 43  | b     | 101  | PLC  | C4-O4P-P-O1P |
| 43  | d     | 101  | PLC  | C1-O3P-P-O2P |
| 43  | d     | 101  | PLC  | C4-O4P-P-O1P |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 43  | d     | 101 | PLC  | C4-O4P-P-O2P   |
| 43  | d     | 102 | PLC  | O4P-C4-C5-N    |
| 43  | g     | 301 | PLC  | C1'-C'-O2-C2   |
| 43  | g     | 301 | PLC  | O'-C'-O2-C2    |
| 43  | h     | 201 | PLC  | O3P-C1-C2-O2   |
| 43  | h     | 201 | PLC  | C2-C1-O3P-P    |
| 43  | h     | 201 | PLC  | C1-O3P-P-O1P   |
| 43  | h     | 201 | PLC  | C1-O3P-P-O2P   |
| 43  | h     | 201 | PLC  | C1-O3P-P-O4P   |
| 43  | h     | 201 | PLC  | C4-O4P-P-O1P   |
| 43  | h     | 201 | PLC  | C4-O4P-P-O3P   |
| 43  | q     | 201 | PLC  | C1-O3P-P-O4P   |
| 43  | q     | 202 | PLC  | O4P-C4-C5-N    |
| 43  | q     | 202 | PLC  | C1'-C'-O2-C2   |
| 47  | H     | 402 | 3PE  | C1-O11-P-O12   |
| 47  | H     | 402 | 3PE  | C1-O11-P-O14   |
| 47  | H     | 402 | 3PE  | C11-O13-P-O11  |
| 47  | H     | 402 | 3PE  | C11-O13-P-O12  |
| 47  | H     | 402 | 3PE  | C11-O13-P-O14  |
| 47  | H     | 402 | 3PE  | C22-C21-O21-C2 |
| 47  | L     | 701 | 3PE  | O13-C11-C12-N  |
| 47  | L     | 703 | 3PE  | C1-O11-P-O12   |
| 47  | L     | 703 | 3PE  | C11-O13-P-O11  |
| 47  | L     | 703 | 3PE  | C11-O13-P-O14  |
| 47  | L     | 703 | 3PE  | C32-C31-O31-C3 |
| 47  | L     | 706 | 3PE  | C1-O11-P-O12   |
| 47  | L     | 706 | 3PE  | C1-O11-P-O14   |
| 47  | L     | 706 | 3PE  | C22-C21-O21-C2 |
| 47  | L     | 707 | 3PE  | C11-O13-P-O12  |
| 47  | L     | 707 | 3PE  | C11-O13-P-O14  |
| 47  | L     | 707 | 3PE  | C22-C21-O21-C2 |
| 47  | L     | 708 | 3PE  | C1-O11-P-O13   |
| 47  | L     | 708 | 3PE  | C1-O11-P-O14   |
| 47  | L     | 709 | 3PE  | C1-O11-P-O12   |
| 47  | L     | 709 | 3PE  | C1-O11-P-O13   |
| 47  | L     | 709 | 3PE  | C1-O11-P-O14   |
| 47  | L     | 709 | 3PE  | C11-O13-P-O12  |
| 47  | L     | 710 | 3PE  | O22-C21-O21-C2 |
| 47  | L     | 710 | 3PE  | C22-C21-O21-C2 |
| 47  | L     | 711 | 3PE  | C11-O13-P-O11  |
| 47  | L     | 711 | 3PE  | C11-O13-P-O12  |
| 47  | L     | 711 | 3PE  | C11-O13-P-O14  |

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| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 47  | L     | 711  | 3PE  | O13-C11-C12-N  |
| 47  | L     | 711  | 3PE  | C22-C21-O21-C2 |
| 47  | L     | 712  | 3PE  | C1-O11-P-O12   |
| 47  | L     | 712  | 3PE  | C1-O11-P-O14   |
| 47  | L     | 712  | 3PE  | C11-O13-P-O12  |
| 47  | L     | 712  | 3PE  | C11-O13-P-O14  |
| 47  | L     | 712  | 3PE  | O22-C21-O21-C2 |
| 47  | M     | 1003 | 3PE  | O13-C11-C12-N  |
| 47  | N     | 601  | 3PE  | C12-C11-O13-P  |
| 47  | N     | 601  | 3PE  | O13-C11-C12-N  |
| 47  | N     | 601  | 3PE  | C22-C21-O21-C2 |
| 47  | O     | 202  | 3PE  | C1-O11-P-O14   |
| 47  | O     | 202  | 3PE  | O32-C31-O31-C3 |
| 47  | O     | 202  | 3PE  | C32-C31-O31-C3 |
| 47  | O     | 203  | 3PE  | C1-O11-P-O12   |
| 47  | O     | 203  | 3PE  | C1-O11-P-O14   |
| 47  | O     | 203  | 3PE  | C11-O13-P-O12  |
| 47  | O     | 203  | 3PE  | C11-O13-P-O14  |
| 47  | Y     | 302  | 3PE  | C1-O11-P-O13   |
| 47  | Y     | 302  | 3PE  | C1-O11-P-O14   |
| 47  | Y     | 302  | 3PE  | O22-C21-O21-C2 |
| 47  | Y     | 302  | 3PE  | C22-C21-O21-C2 |
| 47  | Z     | 203  | 3PE  | C1-O11-P-O12   |
| 47  | Z     | 203  | 3PE  | C1-O11-P-O14   |
| 47  | Z     | 203  | 3PE  | C11-O13-P-O11  |
| 47  | Z     | 203  | 3PE  | C11-O13-P-O12  |
| 47  | b     | 103  | 3PE  | C1-O11-P-O14   |
| 47  | b     | 103  | 3PE  | C11-O13-P-O12  |
| 47  | b     | 103  | 3PE  | C11-O13-P-O14  |
| 47  | b     | 103  | 3PE  | O22-C21-O21-C2 |
| 47  | b     | 103  | 3PE  | C22-C21-O21-C2 |
| 47  | f     | 101  | 3PE  | C1-O11-P-O12   |
| 47  | f     | 101  | 3PE  | C1-O11-P-O14   |
| 47  | f     | 101  | 3PE  | O11-C1-C2-O21  |
| 47  | f     | 101  | 3PE  | O22-C21-O21-C2 |
| 47  | f     | 101  | 3PE  | C22-C21-O21-C2 |
| 47  | j     | 101  | 3PE  | C1-O11-P-O12   |
| 47  | j     | 101  | 3PE  | C1-O11-P-O14   |
| 47  | j     | 101  | 3PE  | C11-O13-P-O12  |
| 47  | m     | 101  | 3PE  | C1-O11-P-O12   |
| 47  | m     | 101  | 3PE  | C1-O11-P-O13   |
| 47  | m     | 101  | 3PE  | C1-O11-P-O14   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | m     | 101 | 3PE  | C11-O13-P-O14   |
| 47  | m     | 101 | 3PE  | C22-C21-O21-C2  |
| 47  | m     | 102 | 3PE  | C11-O13-P-O12   |
| 48  | O     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | P     | 503 | CDL  | OA6-CA4-CA6-OA8 |
| 48  | P     | 503 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | P     | 503 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | P     | 503 | CDL  | C51-CB5-OB6-CB4 |
| 48  | Z     | 202 | CDL  | CA3-OA5-PA1-OA2 |
| 48  | Z     | 202 | CDL  | CA3-OA5-PA1-OA4 |
| 48  | Z     | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 48  | Z     | 202 | CDL  | CB3-OB5-PB2-OB2 |
| 48  | Z     | 202 | CDL  | CB3-OB5-PB2-OB3 |
| 48  | Z     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | b     | 102 | CDL  | CA3-OA5-PA1-OA3 |
| 48  | b     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 48  | c     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 48  | c     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 48  | c     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 48  | c     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 48  | c     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 48  | c     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 49  | P     | 501 | NDP  | PA-O3-PN-O5D    |
| 51  | T     | 201 | EHZ  | C5-C6-C7-C8     |
| 51  | T     | 201 | EHZ  | C15-C16-C17-C18 |
| 51  | T     | 201 | EHZ  | C15-C16-C17-C19 |
| 51  | T     | 201 | EHZ  | C15-C16-C17-C20 |
| 51  | T     | 201 | EHZ  | O5-C16-C17-C18  |
| 51  | T     | 201 | EHZ  | O5-C16-C17-C19  |
| 51  | T     | 201 | EHZ  | O5-C16-C17-C20  |
| 51  | T     | 201 | EHZ  | O2-C9-S1-C10    |
| 51  | T     | 201 | EHZ  | C8-C9-S1-C10    |
| 51  | U     | 201 | EHZ  | C6-C7-C8-C9     |
| 51  | U     | 201 | EHZ  | S1-C10-C11-N1   |
| 51  | U     | 201 | EHZ  | C16-C17-C20-O6  |
| 51  | U     | 201 | EHZ  | C18-C17-C20-O6  |
| 51  | U     | 201 | EHZ  | C19-C17-C20-O6  |
| 51  | U     | 201 | EHZ  | O2-C9-S1-C10    |
| 51  | U     | 201 | EHZ  | C8-C9-S1-C10    |
| 43  | a     | 201 | PLC  | C1'-C'-O2-C2    |
| 48  | Z     | 202 | CDL  | C11-CA5-OA6-CA4 |
| 43  | a     | 201 | PLC  | O'-C'-O2-C2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | m     | 101 | 3PE  | O22-C21-O21-C2  |
| 47  | L     | 703 | 3PE  | O32-C31-O31-C3  |
| 47  | m     | 101 | 3PE  | O32-C31-O31-C3  |
| 48  | c     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 48  | Z     | 202 | CDL  | OA7-CA5-OA6-CA4 |
| 47  | m     | 101 | 3PE  | C32-C31-O31-C3  |
| 47  | L     | 712 | 3PE  | O32-C31-O31-C3  |
| 47  | N     | 601 | 3PE  | O32-C31-O31-C3  |
| 47  | b     | 103 | 3PE  | O32-C31-O31-C3  |
| 47  | j     | 101 | 3PE  | O32-C31-O31-C3  |
| 48  | b     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 43  | Y     | 301 | PLC  | O'-C'-O2-C2     |
| 43  | q     | 202 | PLC  | O'-C'-O2-C2     |
| 47  | H     | 402 | 3PE  | O22-C21-O21-C2  |
| 47  | L     | 706 | 3PE  | O22-C21-O21-C2  |
| 47  | L     | 707 | 3PE  | O22-C21-O21-C2  |
| 47  | L     | 709 | 3PE  | O22-C21-O21-C2  |
| 47  | L     | 711 | 3PE  | O22-C21-O21-C2  |
| 47  | N     | 601 | 3PE  | O22-C21-O21-C2  |
| 48  | O     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 48  | b     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 48  | c     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 43  | L     | 705 | PLC  | OB-CB-O3-C3     |
| 47  | N     | 601 | 3PE  | C32-C31-O31-C3  |
| 48  | b     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 43  | Y     | 303 | PLC  | C1'-C'-O2-C2    |
| 47  | L     | 709 | 3PE  | C22-C21-O21-C2  |
| 47  | L     | 712 | 3PE  | C22-C21-O21-C2  |
| 48  | O     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 48  | O     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 48  | Z     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 47  | L     | 708 | 3PE  | O32-C31-O31-C3  |
| 43  | L     | 702 | PLC  | C1B-CB-O3-C3    |
| 43  | L     | 705 | PLC  | C1B-CB-O3-C3    |
| 47  | L     | 708 | 3PE  | C32-C31-O31-C3  |
| 47  | L     | 712 | 3PE  | C32-C31-O31-C3  |
| 47  | O     | 203 | 3PE  | C32-C31-O31-C3  |
| 47  | Z     | 203 | 3PE  | C32-C31-O31-C3  |
| 47  | b     | 103 | 3PE  | C32-C31-O31-C3  |
| 47  | j     | 101 | 3PE  | C32-C31-O31-C3  |
| 48  | O     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 43  | D     | 501 | PLC  | O'-C'-O2-C2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | L     | 702 | PLC  | OB-CB-O3-C3     |
| 47  | Z     | 203 | 3PE  | O32-C31-O31-C3  |
| 47  | f     | 101 | 3PE  | O32-C31-O31-C3  |
| 48  | O     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 48  | c     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 48  | b     | 102 | CDL  | O1-C1-CB2-OB2   |
| 47  | f     | 101 | 3PE  | C32-C31-O31-C3  |
| 48  | c     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 47  | O     | 203 | 3PE  | O32-C31-O31-C3  |
| 43  | B     | 302 | PLC  | C1'-C'-O2-C2    |
| 43  | h     | 201 | PLC  | C1'-C'-O2-C2    |
| 47  | L     | 703 | 3PE  | C22-C21-O21-C2  |
| 47  | O     | 202 | 3PE  | C22-C21-O21-C2  |
| 47  | Z     | 203 | 3PE  | C22-C21-O21-C2  |
| 48  | c     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 48  | c     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 49  | P     | 501 | NDP  | O4B-C4B-C5B-O5B |
| 49  | P     | 501 | NDP  | C3B-C4B-C5B-O5B |
| 47  | L     | 709 | 3PE  | C32-C31-O31-C3  |
| 48  | b     | 102 | CDL  | CA2-C1-CB2-OB2  |
| 43  | B     | 302 | PLC  | O'-C'-O2-C2     |
| 43  | h     | 201 | PLC  | O'-C'-O2-C2     |
| 47  | L     | 703 | 3PE  | O22-C21-O21-C2  |
| 47  | O     | 202 | 3PE  | O22-C21-O21-C2  |
| 47  | Z     | 203 | 3PE  | O22-C21-O21-C2  |
| 48  | c     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 43  | P     | 502 | PLC  | C1B-CB-O3-C3    |
| 43  | Y     | 303 | PLC  | C1B-CB-O3-C3    |
| 49  | P     | 501 | NDP  | O4D-C1D-N1N-C6N |
| 47  | Z     | 203 | 3PE  | C21-C22-C23-C24 |
| 48  | c     | 201 | CDL  | CA7-C31-C32-C33 |
| 47  | L     | 703 | 3PE  | O11-C1-C2-O21   |
| 47  | L     | 707 | 3PE  | O11-C1-C2-O21   |
| 43  | d     | 101 | PLC  | C'-C1'-C2'-C3'  |
| 43  | d     | 102 | PLC  | C'-C1'-C2'-C3'  |
| 47  | L     | 712 | 3PE  | O21-C2-C3-O31   |
| 43  | Y     | 303 | PLC  | OB-CB-O3-C3     |
| 47  | L     | 708 | 3PE  | C22-C21-O21-C2  |
| 47  | L     | 706 | 3PE  | C31-C32-C33-C34 |
| 47  | L     | 711 | 3PE  | C21-C22-C23-C24 |
| 43  | Z     | 201 | PLC  | C1B-CB-O3-C3    |
| 43  | q     | 201 | PLC  | CB-C1B-C2B-C3B  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | L     | 711  | 3PE  | C31-C32-C33-C34 |
| 43  | M     | 1002 | PLC  | C'-C1'-C2'-C3'  |
| 43  | Y     | 303  | PLC  | C'-C1'-C2'-C3'  |
| 43  | q     | 201  | PLC  | C'-C1'-C2'-C3'  |
| 47  | f     | 101  | 3PE  | C31-C32-C33-C34 |
| 48  | O     | 201  | CDL  | CA5-C11-C12-C13 |
| 48  | c     | 201  | CDL  | CA5-C11-C12-C13 |
| 43  | Z     | 201  | PLC  | C5B-C6B-C7B-C8B |
| 51  | T     | 201  | EHZ  | C5-C6-C7-O1     |
| 47  | L     | 709  | 3PE  | C2-C3-O31-C31   |
| 43  | h     | 201  | PLC  | C6B-C7B-C8B-C9B |
| 48  | O     | 201  | CDL  | CA7-C31-C32-C33 |
| 43  | q     | 201  | PLC  | C1B-CB-O3-C3    |
| 43  | P     | 502  | PLC  | OB-CB-O3-C3     |
| 47  | L     | 707  | 3PE  | C32-C31-O31-C3  |
| 49  | P     | 501  | NDP  | C3B-C2B-O2B-P2B |
| 47  | L     | 709  | 3PE  | O32-C31-O31-C3  |
| 48  | P     | 503  | CDL  | CA5-C11-C12-C13 |
| 43  | q     | 201  | PLC  | C1'-C'-O2-C2    |
| 43  | B     | 302  | PLC  | C1-O3P-P-O4P    |
| 43  | H     | 401  | PLC  | C4-O4P-P-O3P    |
| 43  | M     | 1001 | PLC  | C1-O3P-P-O4P    |
| 43  | M     | 1002 | PLC  | C1-O3P-P-O4P    |
| 43  | Y     | 303  | PLC  | C1-O3P-P-O4P    |
| 43  | b     | 101  | PLC  | C1-O3P-P-O4P    |
| 43  | b     | 101  | PLC  | C4-O4P-P-O3P    |
| 43  | d     | 101  | PLC  | C1-O3P-P-O4P    |
| 43  | d     | 101  | PLC  | C4-O4P-P-O3P    |
| 43  | g     | 301  | PLC  | C4-O4P-P-O3P    |
| 43  | q     | 201  | PLC  | C4-O4P-P-O3P    |
| 47  | H     | 402  | 3PE  | C1-O11-P-O13    |
| 47  | L     | 701  | 3PE  | C11-O13-P-O11   |
| 47  | L     | 706  | 3PE  | C1-O11-P-O13    |
| 47  | L     | 707  | 3PE  | C11-O13-P-O11   |
| 47  | L     | 709  | 3PE  | C11-O13-P-O11   |
| 47  | L     | 712  | 3PE  | C11-O13-P-O11   |
| 47  | M     | 1003 | 3PE  | C11-O13-P-O11   |
| 47  | O     | 202  | 3PE  | C11-O13-P-O11   |
| 47  | O     | 203  | 3PE  | C1-O11-P-O13    |
| 47  | O     | 203  | 3PE  | C11-O13-P-O11   |
| 47  | Z     | 203  | 3PE  | C1-O11-P-O13    |
| 47  | b     | 103  | 3PE  | C11-O13-P-O11   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | f     | 101 | 3PE  | C1-O11-P-O13    |
| 47  | j     | 101 | 3PE  | C1-O11-P-O13    |
| 47  | j     | 101 | 3PE  | C11-O13-P-O11   |
| 47  | m     | 102 | 3PE  | C11-O13-P-O11   |
| 48  | P     | 503 | CDL  | CB3-OB5-PB2-OB2 |
| 48  | Z     | 202 | CDL  | CB2-OB2-PB2-OB5 |
| 48  | b     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 48  | b     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 48  | c     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 43  | Y     | 303 | PLC  | CB-C1B-C2B-C3B  |
| 43  | q     | 201 | PLC  | O'-C'-O2-C2     |
| 47  | L     | 708 | 3PE  | O22-C21-O21-C2  |
| 48  | O     | 201 | CDL  | C76-C77-C78-C79 |
| 43  | Z     | 201 | PLC  | OB-CB-O3-C3     |
| 47  | Y     | 302 | 3PE  | C33-C34-C35-C36 |
| 43  | L     | 702 | PLC  | C2B-C3B-C4B-C5B |
| 43  | q     | 202 | PLC  | C7'-C8'-C9'-CA' |
| 47  | L     | 708 | 3PE  | C39-C3A-C3B-C3C |
| 47  | L     | 710 | 3PE  | C35-C36-C37-C38 |
| 43  | d     | 102 | PLC  | C1'-C2'-C3'-C4' |
| 43  | h     | 201 | PLC  | C4'-C5'-C6'-C7' |
| 43  | q     | 201 | PLC  | C2B-C3B-C4B-C5B |
| 47  | L     | 708 | 3PE  | C3D-C3E-C3F-C3G |
| 48  | O     | 201 | CDL  | C81-C82-C83-C84 |
| 47  | L     | 708 | 3PE  | C37-C38-C39-C3A |
| 48  | c     | 201 | CDL  | C56-C57-C58-C59 |
| 43  | q     | 201 | PLC  | OB-CB-O3-C3     |
| 47  | L     | 707 | 3PE  | C37-C38-C39-C3A |
| 47  | L     | 709 | 3PE  | C37-C38-C39-C3A |
| 47  | Z     | 203 | 3PE  | C28-C29-C2A-C2B |
| 43  | q     | 202 | PLC  | C1'-C2'-C3'-C4' |
| 43  | q     | 202 | PLC  | C3'-C4'-C5'-C6' |
| 47  | m     | 102 | 3PE  | C27-C28-C29-C2A |
| 43  | q     | 202 | PLC  | CB-C1B-C2B-C3B  |
| 47  | L     | 703 | 3PE  | C21-C22-C23-C24 |
| 43  | d     | 101 | PLC  | C6B-C7B-C8B-C9B |
| 47  | L     | 709 | 3PE  | C33-C34-C35-C36 |
| 47  | L     | 710 | 3PE  | C28-C29-C2A-C2B |
| 47  | L     | 712 | 3PE  | C38-C39-C3A-C3B |
| 47  | O     | 202 | 3PE  | C27-C28-C29-C2A |
| 47  | N     | 601 | 3PE  | C29-C2A-C2B-C2C |
| 48  | O     | 201 | CDL  | CB7-C71-C72-C73 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | L     | 706 | 3PE  | C33-C34-C35-C36 |
| 47  | L     | 707 | 3PE  | C35-C36-C37-C38 |
| 47  | L     | 712 | 3PE  | C36-C37-C38-C39 |
| 47  | f     | 101 | 3PE  | C37-C38-C39-C3A |
| 48  | O     | 201 | CDL  | C78-C79-C80-C81 |
| 48  | c     | 201 | CDL  | C12-C13-C14-C15 |
| 47  | L     | 711 | 3PE  | C37-C38-C39-C3A |
| 43  | B     | 302 | PLC  | C1B-C2B-C3B-C4B |
| 47  | L     | 709 | 3PE  | C35-C36-C37-C38 |
| 47  | f     | 101 | 3PE  | C2B-C2C-C2D-C2E |
| 48  | O     | 201 | CDL  | C80-C81-C82-C83 |
| 48  | Z     | 202 | CDL  | CB5-C51-C52-C53 |
| 47  | H     | 402 | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 707 | 3PE  | C39-C3A-C3B-C3C |
| 47  | L     | 708 | 3PE  | C29-C2A-C2B-C2C |
| 47  | L     | 710 | 3PE  | C26-C27-C28-C29 |
| 47  | f     | 101 | 3PE  | C3A-C3B-C3C-C3D |
| 43  | L     | 702 | PLC  | C1'-C2'-C3'-C4' |
| 43  | L     | 705 | PLC  | C7'-C8'-C9'-CA' |
| 47  | Y     | 302 | 3PE  | C35-C36-C37-C38 |
| 47  | L     | 708 | 3PE  | O13-C11-C12-N   |
| 43  | D     | 501 | PLC  | C4'-C5'-C6'-C7' |
| 43  | Z     | 201 | PLC  | C2'-C3'-C4'-C5' |
| 48  | c     | 201 | CDL  | C51-C52-C53-C54 |
| 43  | L     | 702 | PLC  | C4'-C5'-C6'-C7' |
| 47  | L     | 709 | 3PE  | C32-C33-C34-C35 |
| 47  | L     | 707 | 3PE  | C32-C33-C34-C35 |
| 47  | L     | 707 | 3PE  | C3E-C3F-C3G-C3H |
| 47  | L     | 707 | 3PE  | C2E-C2F-C2G-C2H |
| 48  | O     | 201 | CDL  | C77-C78-C79-C80 |
| 43  | Y     | 301 | PLC  | C4B-C5B-C6B-C7B |
| 47  | L     | 708 | 3PE  | C3E-C3F-C3G-C3H |
| 47  | L     | 708 | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 711 | 3PE  | C2B-C2C-C2D-C2E |
| 43  | L     | 704 | PLC  | C1-C2-C3-O3     |
| 48  | b     | 102 | CDL  | CB5-C51-C52-C53 |
| 43  | L     | 704 | PLC  | C1'-C'-O2-C2    |
| 47  | b     | 103 | 3PE  | C38-C39-C3A-C3B |
| 43  | L     | 702 | PLC  | C3'-C4'-C5'-C6' |
| 47  | L     | 707 | 3PE  | C2B-C2C-C2D-C2E |
| 48  | O     | 201 | CDL  | C15-C16-C17-C18 |
| 47  | L     | 707 | 3PE  | O32-C31-O31-C3  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | B     | 302  | PLC  | C'-C1'-C2'-C3'  |
| 48  | O     | 201  | CDL  | O1-C1-CA2-OA2   |
| 48  | b     | 102  | CDL  | O1-C1-CA2-OA2   |
| 43  | D     | 501  | PLC  | C6B-C7B-C8B-C9B |
| 47  | O     | 203  | 3PE  | C27-C28-C29-C2A |
| 47  | b     | 103  | 3PE  | C35-C36-C37-C38 |
| 47  | L     | 707  | 3PE  | C33-C34-C35-C36 |
| 47  | L     | 712  | 3PE  | C3B-C3C-C3D-C3E |
| 48  | O     | 201  | CDL  | C14-C15-C16-C17 |
| 43  | L     | 704  | PLC  | O'-C'-O2-C2     |
| 43  | q     | 201  | PLC  | C1B-C2B-C3B-C4B |
| 47  | O     | 202  | 3PE  | C26-C27-C28-C29 |
| 43  | g     | 301  | PLC  | C4-C5-N-C8      |
| 47  | L     | 708  | 3PE  | C21-C22-C23-C24 |
| 47  | Y     | 302  | 3PE  | C31-C32-C33-C34 |
| 43  | h     | 201  | PLC  | C1B-CB-O3-C3    |
| 47  | M     | 1003 | 3PE  | C31-C32-C33-C34 |
| 47  | L     | 708  | 3PE  | C33-C34-C35-C36 |
| 47  | N     | 601  | 3PE  | C2D-C2E-C2F-C2G |
| 47  | L     | 712  | 3PE  | C23-C24-C25-C26 |
| 47  | L     | 709  | 3PE  | C31-C32-C33-C34 |
| 47  | L     | 712  | 3PE  | C21-C22-C23-C24 |
| 48  | O     | 201  | CDL  | C33-C34-C35-C36 |
| 48  | P     | 503  | CDL  | C71-CB7-OB8-CB6 |
| 43  | M     | 1001 | PLC  | C'-C1'-C2'-C3'  |
| 47  | L     | 707  | 3PE  | C31-C32-C33-C34 |
| 47  | O     | 203  | 3PE  | C31-C32-C33-C34 |
| 47  | M     | 1003 | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 712  | 3PE  | C2C-C2D-C2E-C2F |
| 43  | h     | 201  | PLC  | OB-CB-O3-C3     |
| 43  | M     | 1001 | PLC  | C1B-C2B-C3B-C4B |
| 47  | b     | 103  | 3PE  | C31-C32-C33-C34 |
| 43  | L     | 702  | PLC  | C1'-C'-O2-C2    |
| 43  | L     | 705  | PLC  | C1'-C'-O2-C2    |
| 43  | d     | 102  | PLC  | C1'-C'-O2-C2    |
| 47  | O     | 203  | 3PE  | C22-C21-O21-C2  |
| 43  | P     | 502  | PLC  | O3P-C1-C2-O2    |
| 43  | q     | 201  | PLC  | O3P-C1-C2-O2    |
| 43  | d     | 102  | PLC  | C3'-C4'-C5'-C6' |
| 43  | d     | 102  | PLC  | C6'-C7'-C8'-C9' |
| 43  | L     | 702  | PLC  | O'-C'-O2-C2     |
| 43  | L     | 705  | PLC  | O'-C'-O2-C2     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | O     | 203  | 3PE  | O22-C21-O21-C2  |
| 43  | L     | 705  | PLC  | C2'-C3'-C4'-C5' |
| 48  | O     | 201  | CDL  | OB6-CB4-CB6-OB8 |
| 48  | c     | 201  | CDL  | OB6-CB4-CB6-OB8 |
| 47  | L     | 710  | 3PE  | C39-C3A-C3B-C3C |
| 47  | L     | 712  | 3PE  | C39-C3A-C3B-C3C |
| 48  | O     | 201  | CDL  | C52-C53-C54-C55 |
| 49  | P     | 501  | NDP  | O4D-C4D-C5D-O5D |
| 47  | L     | 711  | 3PE  | C33-C34-C35-C36 |
| 51  | U     | 201  | EHZ  | C1-C2-C3-C4     |
| 43  | d     | 102  | PLC  | O'-C'-O2-C2     |
| 43  | M     | 1002 | PLC  | C4-O4P-P-O3P    |
| 43  | d     | 102  | PLC  | C1-O3P-P-O4P    |
| 47  | L     | 703  | 3PE  | C1-O11-P-O13    |
| 47  | L     | 707  | 3PE  | C1-O11-P-O13    |
| 47  | L     | 712  | 3PE  | C1-O11-P-O13    |
| 47  | m     | 102  | 3PE  | C1-O11-P-O13    |
| 48  | b     | 102  | CDL  | CA3-OA5-PA1-OA2 |
| 47  | L     | 709  | 3PE  | C26-C27-C28-C29 |
| 47  | L     | 707  | 3PE  | C21-C22-C23-C24 |
| 47  | L     | 703  | 3PE  | O11-C1-C2-C3    |
| 47  | L     | 707  | 3PE  | O11-C1-C2-C3    |
| 47  | M     | 1003 | 3PE  | O11-C1-C2-C3    |
| 47  | O     | 202  | 3PE  | O11-C1-C2-C3    |
| 47  | f     | 101  | 3PE  | O11-C1-C2-C3    |
| 43  | P     | 502  | PLC  | C1'-C2'-C3'-C4' |
| 47  | L     | 703  | 3PE  | C39-C3A-C3B-C3C |
| 47  | f     | 101  | 3PE  | C34-C35-C36-C37 |
| 48  | O     | 201  | CDL  | CB2-C1-CA2-OA2  |
| 48  | b     | 102  | CDL  | CB2-C1-CA2-OA2  |
| 43  | q     | 201  | PLC  | C3B-C4B-C5B-C6B |
| 47  | L     | 712  | 3PE  | C25-C26-C27-C28 |
| 47  | m     | 101  | 3PE  | C33-C34-C35-C36 |
| 51  | T     | 201  | EHZ  | C1-C2-C3-C4     |
| 47  | L     | 703  | 3PE  | C31-C32-C33-C34 |
| 43  | Z     | 201  | PLC  | C1'-C2'-C3'-C4' |
| 47  | L     | 710  | 3PE  | C2C-C2D-C2E-C2F |
| 47  | b     | 103  | 3PE  | C3B-C3C-C3D-C3E |
| 51  | U     | 201  | EHZ  | C2-C3-C4-C5     |
| 43  | D     | 501  | PLC  | C1-C2-C3-O3     |
| 43  | L     | 705  | PLC  | C6B-C7B-C8B-C9B |
| 43  | M     | 1001 | PLC  | C7B-C8B-C9B-CAA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | P     | 502  | PLC  | C1-C2-C3-O3     |
| 43  | Z     | 201  | PLC  | C1-C2-C3-O3     |
| 47  | L     | 701  | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 706  | 3PE  | C1-C2-C3-O31    |
| 47  | L     | 710  | 3PE  | C1-C2-C3-O31    |
| 48  | O     | 201  | CDL  | CB3-CB4-CB6-OB8 |
| 48  | P     | 503  | CDL  | CA3-CA4-CA6-OA8 |
| 48  | b     | 102  | CDL  | CA3-CA4-CA6-OA8 |
| 48  | b     | 102  | CDL  | CB3-CB4-CB6-OB8 |
| 48  | c     | 201  | CDL  | CA3-CA4-CA6-OA8 |
| 43  | b     | 101  | PLC  | C'-C1'-C2'-C3'  |
| 47  | L     | 711  | 3PE  | C2E-C2F-C2G-C2H |
| 51  | T     | 201  | EHZ  | C3-C4-C5-C6     |
| 51  | U     | 201  | EHZ  | C2-C1-C21-C22   |
| 43  | L     | 704  | PLC  | C4B-C5B-C6B-C7B |
| 48  | O     | 201  | CDL  | C36-C37-C38-C39 |
| 47  | L     | 710  | 3PE  | C3F-C3G-C3H-C3I |
| 48  | Z     | 202  | CDL  | C74-C75-C76-C77 |
| 48  | b     | 102  | CDL  | C31-C32-C33-C34 |
| 47  | L     | 708  | 3PE  | C35-C36-C37-C38 |
| 47  | f     | 101  | 3PE  | C36-C37-C38-C39 |
| 47  | f     | 101  | 3PE  | C21-C22-C23-C24 |
| 47  | M     | 1003 | 3PE  | C29-C2A-C2B-C2C |
| 48  | O     | 201  | CDL  | C53-C54-C55-C56 |
| 47  | b     | 103  | 3PE  | C37-C38-C39-C3A |
| 48  | Z     | 202  | CDL  | C71-CB7-OB8-CB6 |
| 48  | O     | 201  | CDL  | C75-C76-C77-C78 |
| 47  | L     | 709  | 3PE  | C3-C2-O21-C21   |
| 47  | O     | 202  | 3PE  | C3-C2-O21-C21   |
| 47  | m     | 101  | 3PE  | C1-C2-O21-C21   |
| 48  | O     | 201  | CDL  | CA3-CA4-OA6-CA5 |
| 48  | Z     | 202  | CDL  | CA6-CA4-OA6-CA5 |
| 43  | M     | 1002 | PLC  | C6B-C7B-C8B-C9B |
| 43  | Y     | 303  | PLC  | C7'-C8'-C9'-CA' |
| 48  | P     | 503  | CDL  | OA5-CA3-CA4-OA6 |
| 48  | b     | 102  | CDL  | OB5-CB3-CB4-OB6 |
| 43  | d     | 102  | PLC  | C5B-C6B-C7B-C8B |
| 43  | g     | 301  | PLC  | C3'-C4'-C5'-C6' |
| 43  | d     | 102  | PLC  | C7B-C8B-C9B-CAA |
| 47  | L     | 710  | 3PE  | C36-C37-C38-C39 |
| 47  | O     | 202  | 3PE  | C23-C24-C25-C26 |
| 47  | O     | 202  | 3PE  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | N     | 601  | 3PE  | C2F-C2G-C2H-C2I |
| 43  | M     | 1002 | PLC  | O2-C2-C3-O3     |
| 43  | d     | 101  | PLC  | C5B-C6B-C7B-C8B |
| 43  | L     | 704  | PLC  | C1B-C2B-C3B-C4B |
| 43  | b     | 101  | PLC  | C1'-C2'-C3'-C4' |
| 47  | L     | 709  | 3PE  | C39-C3A-C3B-C3C |
| 47  | b     | 103  | 3PE  | C39-C3A-C3B-C3C |
| 47  | f     | 101  | 3PE  | C3C-C3D-C3E-C3F |
| 47  | O     | 203  | 3PE  | C33-C34-C35-C36 |
| 47  | Z     | 203  | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 707  | 3PE  | C3A-C3B-C3C-C3D |
| 48  | O     | 201  | CDL  | C83-C84-C85-C86 |
| 48  | Z     | 202  | CDL  | C51-C52-C53-C54 |
| 47  | O     | 203  | 3PE  | C21-C22-C23-C24 |
| 47  | L     | 703  | 3PE  | C23-C24-C25-C26 |
| 47  | L     | 711  | 3PE  | C2C-C2D-C2E-C2F |
| 49  | P     | 501  | NDP  | C3D-C4D-C5D-O5D |
| 43  | A     | 201  | PLC  | O3P-C1-C2-C3    |
| 43  | M     | 1001 | PLC  | O3P-C1-C2-C3    |
| 43  | P     | 502  | PLC  | O3P-C1-C2-C3    |
| 43  | Y     | 303  | PLC  | O3P-C1-C2-C3    |
| 43  | h     | 201  | PLC  | O3P-C1-C2-C3    |
| 43  | q     | 201  | PLC  | O3P-C1-C2-C3    |
| 47  | L     | 711  | 3PE  | O11-C1-C2-C3    |
| 47  | b     | 103  | 3PE  | O11-C1-C2-C3    |
| 48  | P     | 503  | CDL  | OA5-CA3-CA4-CA6 |
| 48  | b     | 102  | CDL  | OA5-CA3-CA4-CA6 |
| 47  | j     | 101  | 3PE  | O13-C11-C12-N   |
| 43  | L     | 704  | PLC  | C2B-C3B-C4B-C5B |
| 43  | h     | 201  | PLC  | C5'-C6'-C7'-C8' |
| 47  | L     | 706  | 3PE  | C23-C24-C25-C26 |
| 47  | L     | 711  | 3PE  | C35-C36-C37-C38 |
| 43  | d     | 102  | PLC  | CB-C1B-C2B-C3B  |
| 43  | h     | 201  | PLC  | C'-C1'-C2'-C3'  |
| 47  | H     | 402  | 3PE  | C2-C1-O11-P     |
| 48  | Z     | 202  | CDL  | C1-CA2-OA2-PA1  |
| 47  | L     | 706  | 3PE  | C38-C39-C3A-C3B |
| 47  | L     | 710  | 3PE  | C33-C34-C35-C36 |
| 47  | H     | 402  | 3PE  | C23-C24-C25-C26 |
| 48  | P     | 503  | CDL  | C31-CA7-OA8-CA6 |
| 47  | L     | 709  | 3PE  | C22-C23-C24-C25 |
| 48  | Z     | 202  | CDL  | C31-C32-C33-C34 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | Y     | 301  | PLC  | C1-C2-C3-O3     |
| 43  | d     | 101  | PLC  | C1-C2-C3-O3     |
| 47  | H     | 402  | 3PE  | C1-C2-C3-O31    |
| 47  | L     | 703  | 3PE  | C1-C2-C3-O31    |
| 47  | L     | 707  | 3PE  | C1-C2-C3-O31    |
| 47  | L     | 711  | 3PE  | C1-C2-C3-O31    |
| 47  | L     | 712  | 3PE  | C1-C2-C3-O31    |
| 47  | N     | 601  | 3PE  | C1-C2-C3-O31    |
| 47  | b     | 103  | 3PE  | C1-C2-C3-O31    |
| 48  | c     | 201  | CDL  | CB3-CB4-CB6-OB8 |
| 48  | O     | 201  | CDL  | C32-C33-C34-C35 |
| 47  | L     | 707  | 3PE  | C2A-C2B-C2C-C2D |
| 47  | Z     | 203  | 3PE  | C34-C35-C36-C37 |
| 47  | Z     | 203  | 3PE  | C27-C28-C29-C2A |
| 43  | M     | 1002 | PLC  | C2'-C3'-C4'-C5' |
| 43  | D     | 501  | PLC  | C7B-C8B-C9B-CAA |
| 48  | Z     | 202  | CDL  | OB9-CB7-OB8-CB6 |
| 43  | q     | 201  | PLC  | C7B-C8B-C9B-CAA |
| 48  | c     | 201  | CDL  | C11-C12-C13-C14 |
| 47  | b     | 103  | 3PE  | C1-O11-P-O13    |
| 47  | m     | 101  | 3PE  | C11-O13-P-O11   |
| 47  | m     | 102  | 3PE  | C21-C22-C23-C24 |
| 43  | h     | 201  | PLC  | C3'-C4'-C5'-C6' |
| 43  | A     | 201  | PLC  | O3P-C1-C2-O2    |
| 43  | B     | 302  | PLC  | O3P-C1-C2-O2    |
| 43  | Z     | 201  | PLC  | O3P-C1-C2-O2    |
| 47  | L     | 711  | 3PE  | O11-C1-C2-O21   |
| 47  | M     | 1003 | 3PE  | O11-C1-C2-O21   |
| 47  | O     | 202  | 3PE  | O11-C1-C2-O21   |
| 48  | Z     | 202  | CDL  | OA5-CA3-CA4-OA6 |
| 48  | c     | 201  | CDL  | OA5-CA3-CA4-OA6 |
| 48  | P     | 503  | CDL  | CA7-C31-C32-C33 |
| 47  | b     | 103  | 3PE  | C3F-C3G-C3H-C3I |
| 47  | f     | 101  | 3PE  | C3D-C3E-C3F-C3G |
| 51  | T     | 201  | EHZ  | C21-C1-C2-C3    |
| 47  | L     | 701  | 3PE  | O21-C2-C3-O31   |
| 48  | b     | 102  | CDL  | OB6-CB4-CB6-OB8 |
| 48  | c     | 201  | CDL  | OA6-CA4-CA6-OA8 |
| 43  | M     | 1001 | PLC  | C1B-CB-O3-C3    |
| 47  | L     | 709  | 3PE  | C34-C35-C36-C37 |
| 47  | Z     | 203  | 3PE  | C23-C24-C25-C26 |
| 47  | O     | 202  | 3PE  | C22-C23-C24-C25 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | Y     | 303  | PLC  | C5'-C6'-C7'-C8' |
| 43  | h     | 201  | PLC  | C1B-C2B-C3B-C4B |
| 47  | Z     | 203  | 3PE  | C32-C33-C34-C35 |
| 47  | L     | 711  | 3PE  | C22-C23-C24-C25 |
| 47  | M     | 1003 | 3PE  | C2-C1-O11-P     |
| 48  | O     | 201  | CDL  | C1-CA2-OA2-PA1  |
| 47  | L     | 703  | 3PE  | C36-C37-C38-C39 |
| 47  | N     | 601  | 3PE  | C2A-C2B-C2C-C2D |
| 43  | L     | 705  | PLC  | C'-C1'-C2'-C3'  |
| 48  | Z     | 202  | CDL  | CA7-C31-C32-C33 |
| 48  | P     | 503  | CDL  | OB9-CB7-OB8-CB6 |
| 43  | M     | 1001 | PLC  | C2B-C3B-C4B-C5B |
| 43  | d     | 102  | PLC  | C7'-C8'-C9'-CA' |
| 47  | L     | 712  | 3PE  | C2A-C2B-C2C-C2D |
| 49  | P     | 501  | NDP  | PN-O3-PA-O5B    |
| 48  | O     | 201  | CDL  | C51-C52-C53-C54 |
| 43  | B     | 302  | PLC  | O3P-C1-C2-C3    |
| 43  | g     | 301  | PLC  | O3P-C1-C2-C3    |
| 43  | d     | 101  | PLC  | C2B-C3B-C4B-C5B |
| 47  | L     | 708  | 3PE  | C3B-C3C-C3D-C3E |
| 47  | L     | 701  | 3PE  | C23-C24-C25-C26 |
| 47  | b     | 103  | 3PE  | C32-C33-C34-C35 |
| 47  | f     | 101  | 3PE  | C39-C3A-C3B-C3C |
| 48  | O     | 201  | CDL  | C74-C75-C76-C77 |
| 51  | T     | 201  | EHZ  | C18-C17-C20-O6  |
| 43  | L     | 705  | PLC  | C1-C2-O2-C'     |
| 43  | Y     | 303  | PLC  | C3-C2-O2-C'     |
| 48  | c     | 201  | CDL  | CA6-CA4-OA6-CA5 |
| 47  | N     | 601  | 3PE  | C27-C28-C29-C2A |
| 43  | M     | 1002 | PLC  | C1B-CB-O3-C3    |
| 48  | P     | 503  | CDL  | C11-C12-C13-C14 |
| 43  | B     | 302  | PLC  | C2-C1-O3P-P     |
| 43  | L     | 702  | PLC  | C2-C1-O3P-P     |
| 43  | L     | 705  | PLC  | C2-C1-O3P-P     |
| 43  | M     | 1002 | PLC  | C1-C2-C3-O3     |
| 48  | P     | 503  | CDL  | CB3-CB4-CB6-OB8 |
| 43  | M     | 1001 | PLC  | OB-CB-O3-C3     |
| 43  | L     | 702  | PLC  | O3P-C1-C2-O2    |
| 43  | L     | 704  | PLC  | O3P-C1-C2-O2    |
| 43  | Y     | 301  | PLC  | O3P-C1-C2-O2    |
| 43  | q     | 202  | PLC  | O3P-C1-C2-O2    |
| 47  | Z     | 203  | 3PE  | O11-C1-C2-O21   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | b     | 103  | 3PE  | O11-C1-C2-O21   |
| 48  | O     | 201  | CDL  | OA5-CA3-CA4-OA6 |
| 48  | b     | 102  | CDL  | OA5-CA3-CA4-OA6 |
| 43  | g     | 301  | PLC  | C4B-C5B-C6B-C7B |
| 48  | c     | 201  | CDL  | C54-C55-C56-C57 |
| 49  | P     | 501  | NDP  | C1B-C2B-O2B-P2B |
| 51  | T     | 201  | EHZ  | O1-C7-C8-C9     |
| 51  | U     | 201  | EHZ  | O1-C7-C8-C9     |
| 48  | P     | 503  | CDL  | OA9-CA7-OA8-CA6 |
| 43  | L     | 704  | PLC  | O2-C2-C3-O3     |
| 47  | L     | 706  | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 707  | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 710  | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 711  | 3PE  | O21-C2-C3-O31   |
| 47  | N     | 601  | 3PE  | O21-C2-C3-O31   |
| 47  | b     | 103  | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 703  | 3PE  | C32-C33-C34-C35 |
| 47  | f     | 101  | 3PE  | C3B-C3C-C3D-C3E |
| 47  | N     | 601  | 3PE  | C25-C26-C27-C28 |
| 47  | f     | 101  | 3PE  | C26-C27-C28-C29 |
| 43  | d     | 102  | PLC  | C4'-C5'-C6'-C7' |
| 47  | L     | 710  | 3PE  | C37-C38-C39-C3A |
| 47  | H     | 402  | 3PE  | C25-C26-C27-C28 |
| 47  | O     | 203  | 3PE  | C25-C26-C27-C28 |
| 43  | P     | 502  | PLC  | C4-O4P-P-O3P    |
| 47  | N     | 601  | 3PE  | C1-O11-P-O13    |
| 48  | O     | 201  | CDL  | CA2-OA2-PA1-OA5 |
| 48  | O     | 201  | CDL  | CB2-OB2-PB2-OB5 |
| 47  | L     | 711  | 3PE  | C24-C25-C26-C27 |
| 43  | L     | 704  | PLC  | C2-C1-O3P-P     |
| 47  | L     | 706  | 3PE  | C2-C1-O11-P     |
| 47  | O     | 202  | 3PE  | C2-C1-O11-P     |
| 48  | c     | 201  | CDL  | C1-CB2-OB2-PB2  |
| 43  | M     | 1002 | PLC  | OB-CB-O3-C3     |
| 43  | A     | 201  | PLC  | C4-O4P-P-O1P    |
| 43  | B     | 302  | PLC  | C1-O3P-P-O1P    |
| 43  | D     | 501  | PLC  | C4-C5-N-C6      |
| 43  | H     | 401  | PLC  | C1-O3P-P-O2P    |
| 43  | M     | 1001 | PLC  | C1-O3P-P-O1P    |
| 43  | M     | 1002 | PLC  | C1-O3P-P-O1P    |
| 43  | M     | 1002 | PLC  | C4-O4P-P-O2P    |
| 43  | Y     | 303  | PLC  | C1-O3P-P-O2P    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | Z     | 201  | PLC  | C4-C5-N-C8      |
| 43  | b     | 101  | PLC  | C4-O4P-P-O2P    |
| 43  | d     | 101  | PLC  | C1-O3P-P-O1P    |
| 43  | d     | 102  | PLC  | C1-O3P-P-O2P    |
| 43  | g     | 301  | PLC  | C4-C5-N-C6      |
| 43  | g     | 301  | PLC  | C4-O4P-P-O1P    |
| 43  | q     | 201  | PLC  | C1-O3P-P-O2P    |
| 43  | q     | 201  | PLC  | C4-O4P-P-O1P    |
| 43  | q     | 201  | PLC  | C4-O4P-P-O2P    |
| 47  | L     | 701  | 3PE  | C11-O13-P-O14   |
| 47  | L     | 703  | 3PE  | C1-O11-P-O14    |
| 47  | L     | 707  | 3PE  | C1-O11-P-O12    |
| 47  | L     | 707  | 3PE  | C1-O11-P-O14    |
| 47  | L     | 710  | 3PE  | C1-O11-P-O12    |
| 47  | M     | 1003 | 3PE  | C11-O13-P-O12   |
| 47  | M     | 1003 | 3PE  | C11-O13-P-O14   |
| 47  | O     | 202  | 3PE  | C11-O13-P-O14   |
| 47  | Y     | 302  | 3PE  | C1-O11-P-O12    |
| 47  | Z     | 203  | 3PE  | C11-O13-P-O14   |
| 47  | j     | 101  | 3PE  | C11-O13-P-O14   |
| 47  | m     | 101  | 3PE  | C11-O13-P-O12   |
| 47  | m     | 102  | 3PE  | C11-O13-P-O14   |
| 48  | O     | 201  | CDL  | CA2-OA2-PA1-OA3 |
| 48  | O     | 201  | CDL  | CA3-OA5-PA1-OA3 |
| 48  | O     | 201  | CDL  | CB2-OB2-PB2-OB3 |
| 48  | O     | 201  | CDL  | CB2-OB2-PB2-OB4 |
| 48  | P     | 503  | CDL  | CB3-OB5-PB2-OB4 |
| 48  | Z     | 202  | CDL  | CA3-OA5-PA1-OA3 |
| 48  | Z     | 202  | CDL  | CB2-OB2-PB2-OB4 |
| 48  | b     | 102  | CDL  | CA3-OA5-PA1-OA4 |
| 48  | b     | 102  | CDL  | CB2-OB2-PB2-OB4 |
| 48  | b     | 102  | CDL  | CB3-OB5-PB2-OB3 |
| 48  | b     | 102  | CDL  | CB3-OB5-PB2-OB4 |
| 48  | c     | 201  | CDL  | CA3-OA5-PA1-OA4 |
| 48  | c     | 201  | CDL  | CB2-OB2-PB2-OB4 |
| 51  | T     | 201  | EHZ  | C6-C7-C8-C9     |
| 43  | D     | 501  | PLC  | O3P-C1-C2-C3    |
| 43  | L     | 702  | PLC  | O3P-C1-C2-C3    |
| 43  | Y     | 301  | PLC  | O3P-C1-C2-C3    |
| 43  | Z     | 201  | PLC  | O3P-C1-C2-C3    |
| 47  | L     | 706  | 3PE  | O11-C1-C2-C3    |
| 47  | O     | 203  | 3PE  | O11-C1-C2-C3    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 48  | O     | 201  | CDL  | OA5-CA3-CA4-CA6 |
| 48  | Z     | 202  | CDL  | OA5-CA3-CA4-CA6 |
| 48  | c     | 201  | CDL  | OA5-CA3-CA4-CA6 |
| 47  | O     | 202  | 3PE  | O13-C11-C12-N   |
| 47  | L     | 711  | 3PE  | C3A-C3B-C3C-C3D |
| 43  | g     | 301  | PLC  | C5-C4-O4P-P     |
| 47  | L     | 712  | 3PE  | C12-C11-O13-P   |
| 47  | b     | 103  | 3PE  | C12-C11-O13-P   |
| 47  | j     | 101  | 3PE  | C12-C11-O13-P   |
| 47  | L     | 707  | 3PE  | C38-C39-C3A-C3B |
| 47  | M     | 1003 | 3PE  | C21-C22-C23-C24 |
| 43  | D     | 501  | PLC  | O3P-C1-C2-O2    |
| 43  | g     | 301  | PLC  | O3P-C1-C2-O2    |
| 47  | L     | 706  | 3PE  | O11-C1-C2-O21   |
| 47  | O     | 203  | 3PE  | O11-C1-C2-O21   |
| 47  | m     | 102  | 3PE  | O11-C1-C2-O21   |
| 47  | L     | 708  | 3PE  | C34-C35-C36-C37 |
| 43  | a     | 201  | PLC  | C1B-CB-O3-C3    |
| 48  | c     | 201  | CDL  | CB5-C51-C52-C53 |
| 43  | M     | 1002 | PLC  | C1B-C2B-C3B-C4B |
| 48  | b     | 102  | CDL  | C55-C56-C57-C58 |
| 43  | b     | 101  | PLC  | C4-C5-N-C7      |
| 43  | q     | 201  | PLC  | C4-C5-N-C6      |
| 43  | H     | 401  | PLC  | O4P-C4-C5-N     |
| 43  | L     | 704  | PLC  | O4P-C4-C5-N     |
| 43  | d     | 101  | PLC  | O4P-C4-C5-N     |
| 43  | g     | 301  | PLC  | O4P-C4-C5-N     |
| 51  | T     | 201  | EHZ  | C2-C1-C21-C22   |
| 43  | D     | 501  | PLC  | O2-C2-C3-O3     |
| 43  | Y     | 301  | PLC  | O2-C2-C3-O3     |
| 43  | d     | 101  | PLC  | O2-C2-C3-O3     |
| 47  | H     | 402  | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 703  | 3PE  | O21-C2-C3-O31   |
| 48  | b     | 102  | CDL  | OA6-CA4-CA6-OA8 |
| 43  | d     | 102  | PLC  | C5'-C6'-C7'-C8' |
| 47  | N     | 601  | 3PE  | C2B-C2C-C2D-C2E |
| 47  | j     | 101  | 3PE  | C2-C1-O11-P     |
| 48  | b     | 102  | CDL  | C51-CB5-OB6-CB4 |
| 43  | A     | 201  | PLC  | C4B-C5B-C6B-C7B |
| 43  | Y     | 303  | PLC  | C1B-C2B-C3B-C4B |
| 47  | M     | 1003 | 3PE  | C33-C34-C35-C36 |
| 51  | U     | 201  | EHZ  | C21-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 43  | Y     | 303  | PLC  | C4-C5-N-C7      |
| 43  | g     | 301  | PLC  | C4-C5-N-C7      |
| 47  | L     | 710  | 3PE  | C3E-C3F-C3G-C3H |
| 47  | Y     | 302  | 3PE  | C36-C37-C38-C39 |
| 51  | T     | 201  | EHZ  | C19-C17-C20-O6  |
| 43  | h     | 201  | PLC  | C2B-C3B-C4B-C5B |
| 43  | d     | 102  | PLC  | C8'-C9'-CA'-CB' |
| 43  | q     | 202  | PLC  | C1B-C2B-C3B-C4B |
| 48  | Z     | 202  | CDL  | CB7-C71-C72-C73 |
| 47  | b     | 103  | 3PE  | C3A-C3B-C3C-C3D |
| 47  | L     | 708  | 3PE  | C3-C2-O21-C21   |
| 48  | b     | 102  | CDL  | OB5-CB3-CB4-CB6 |
| 48  | b     | 102  | CDL  | OB7-CB5-OB6-CB4 |
| 43  | L     | 705  | PLC  | C1'-C2'-C3'-C4' |
| 47  | j     | 101  | 3PE  | C31-C32-C33-C34 |
| 43  | L     | 705  | PLC  | C3B-C4B-C5B-C6B |
| 43  | M     | 1001 | PLC  | O3P-C1-C2-O2    |
| 47  | L     | 710  | 3PE  | O11-C1-C2-O21   |
| 47  | L     | 710  | 3PE  | C3D-C3E-C3F-C3G |
| 43  | b     | 101  | PLC  | C4-C5-N-C8      |
| 43  | D     | 501  | PLC  | C1-O3P-P-O4P    |
| 43  | Z     | 201  | PLC  | C4-O4P-P-O3P    |
| 43  | a     | 201  | PLC  | C4-O4P-P-O3P    |
| 43  | q     | 202  | PLC  | C4-O4P-P-O3P    |
| 47  | L     | 710  | 3PE  | C1-O11-P-O13    |
| 47  | M     | 1003 | 3PE  | C1-O11-P-O13    |
| 47  | O     | 202  | 3PE  | C1-O11-P-O13    |
| 47  | Y     | 302  | 3PE  | C11-O13-P-O11   |
| 47  | L     | 701  | 3PE  | C1-C2-C3-O31    |
| 43  | Y     | 303  | PLC  | C4-C5-N-C8      |
| 49  | P     | 501  | NDP  | PN-O3-PA-O1A    |
| 47  | N     | 601  | 3PE  | C33-C34-C35-C36 |
| 51  | T     | 201  | EHZ  | C22-C23-C24-C25 |
| 43  | L     | 704  | PLC  | CB-C1B-C2B-C3B  |
| 47  | f     | 101  | 3PE  | C29-C2A-C2B-C2C |
| 47  | L     | 707  | 3PE  | C25-C26-C27-C28 |
| 43  | g     | 301  | PLC  | C7'-C8'-C9'-CA' |
| 48  | b     | 102  | CDL  | C57-C58-C59-C60 |
| 47  | b     | 103  | 3PE  | C23-C24-C25-C26 |
| 43  | L     | 705  | PLC  | C5B-C6B-C7B-C8B |
| 47  | L     | 711  | 3PE  | C2D-C2E-C2F-C2G |
| 47  | N     | 601  | 3PE  | C2E-C2F-C2G-C2H |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 51  | T     | 201  | EHZ  | C4-C5-C6-C7     |
| 47  | L     | 706  | 3PE  | O13-C11-C12-N   |
| 48  | O     | 201  | CDL  | C72-C73-C74-C75 |
| 43  | M     | 1001 | PLC  | C4'-C5'-C6'-C7' |
| 47  | L     | 711  | 3PE  | C39-C3A-C3B-C3C |
| 47  | L     | 703  | 3PE  | C24-C25-C26-C27 |
| 43  | q     | 202  | PLC  | C2B-C3B-C4B-C5B |
| 47  | M     | 1003 | 3PE  | O21-C2-C3-O31   |
| 47  | L     | 701  | 3PE  | C33-C34-C35-C36 |
| 51  | T     | 201  | EHZ  | S1-C10-C11-N1   |
| 47  | L     | 712  | 3PE  | C2B-C2C-C2D-C2E |
| 47  | L     | 712  | 3PE  | C33-C34-C35-C36 |
| 43  | L     | 704  | PLC  | C2B-C1B-CB-O3   |
| 43  | L     | 705  | PLC  | C6'-C7'-C8'-C9' |
| 47  | L     | 711  | 3PE  | C25-C26-C27-C28 |
| 47  | b     | 103  | 3PE  | C36-C37-C38-C39 |
| 47  | L     | 712  | 3PE  | C26-C27-C28-C29 |
| 48  | b     | 102  | CDL  | C16-C17-C18-C19 |
| 48  | Z     | 202  | CDL  | CB3-CB4-OB6-CB5 |
| 48  | Z     | 202  | CDL  | CB6-CB4-OB6-CB5 |
| 48  | P     | 503  | CDL  | C12-C13-C14-C15 |
| 43  | D     | 501  | PLC  | C4-C5-N-C7      |
| 43  | M     | 1001 | PLC  | C4-C5-N-C8      |
| 43  | Z     | 201  | PLC  | C4-C5-N-C7      |
| 43  | q     | 201  | PLC  | C4-C5-N-C7      |
| 43  | Z     | 201  | PLC  | C7B-C8B-C9B-CAA |
| 47  | L     | 706  | 3PE  | C22-C23-C24-C25 |
| 47  | L     | 711  | 3PE  | C38-C39-C3A-C3B |
| 47  | H     | 402  | 3PE  | C21-C22-C23-C24 |
| 43  | q     | 202  | PLC  | O3P-C1-C2-C3    |
| 47  | L     | 710  | 3PE  | O11-C1-C2-C3    |
| 47  | L     | 712  | 3PE  | C37-C38-C39-C3A |
| 47  | L     | 710  | 3PE  | C3C-C3D-C3E-C3F |
| 43  | b     | 101  | PLC  | C5'-C6'-C7'-C8' |
| 43  | M     | 1001 | PLC  | C4-C5-N-C6      |
| 43  | M     | 1001 | PLC  | C4-C5-N-C7      |
| 47  | L     | 701  | 3PE  | O22-C21-O21-C2  |
| 51  | T     | 201  | EHZ  | C11-C10-S1-C9   |
| 51  | U     | 201  | EHZ  | C11-C10-S1-C9   |
| 48  | Z     | 202  | CDL  | C73-C74-C75-C76 |
| 43  | A     | 201  | PLC  | C2-C1-O3P-P     |
| 47  | b     | 103  | 3PE  | C2-C1-O11-P     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | L     | 703  | 3PE  | C25-C26-C27-C28 |
| 47  | L     | 709  | 3PE  | C3A-C3B-C3C-C3D |
| 47  | L     | 707  | 3PE  | C2F-C2G-C2H-C2I |
| 47  | L     | 711  | 3PE  | C27-C28-C29-C2A |
| 47  | L     | 707  | 3PE  | C23-C24-C25-C26 |
| 47  | O     | 202  | 3PE  | C31-C32-C33-C34 |
| 43  | D     | 501  | PLC  | C4-C5-N-C8      |
| 43  | L     | 702  | PLC  | C4-C5-N-C7      |
| 43  | D     | 501  | PLC  | C2'-C3'-C4'-C5' |
| 43  | M     | 1002 | PLC  | C3B-C4B-C5B-C6B |
| 43  | L     | 704  | PLC  | O3P-C1-C2-C3    |
| 47  | m     | 102  | 3PE  | O11-C1-C2-C3    |
| 51  | U     | 201  | EHZ  | C21-C1-C2-C3    |
| 43  | B     | 302  | PLC  | O2-C2-C3-O3     |
| 47  | Y     | 302  | 3PE  | O31-C31-C32-C33 |
| 47  | m     | 102  | 3PE  | O21-C21-C22-C23 |
| 43  | M     | 1002 | PLC  | C5B-C6B-C7B-C8B |
| 47  | L     | 712  | 3PE  | C2E-C2F-C2G-C2H |
| 43  | b     | 101  | PLC  | C6'-C7'-C8'-C9' |
| 48  | b     | 102  | CDL  | CA2-OA2-PA1-OA5 |
| 43  | P     | 502  | PLC  | C2B-C3B-C4B-C5B |
| 43  | Z     | 201  | PLC  | C4-C5-N-C6      |
| 43  | q     | 201  | PLC  | C4-C5-N-C8      |
| 43  | L     | 705  | PLC  | C2-C3-O3-CB     |
| 43  | L     | 702  | PLC  | C2'-C3'-C4'-C5' |
| 47  | H     | 402  | 3PE  | O31-C31-C32-C33 |
| 47  | L     | 703  | 3PE  | C33-C34-C35-C36 |
| 48  | c     | 201  | CDL  | C14-C15-C16-C17 |
| 47  | L     | 701  | 3PE  | O21-C21-C22-C23 |
| 47  | L     | 707  | 3PE  | O31-C31-C32-C33 |
| 47  | N     | 601  | 3PE  | O31-C31-C32-C33 |
| 43  | d     | 101  | PLC  | C4B-C5B-C6B-C7B |
| 47  | f     | 101  | 3PE  | C35-C36-C37-C38 |
| 47  | b     | 103  | 3PE  | C33-C34-C35-C36 |
| 43  | d     | 102  | PLC  | C2B-C1B-CB-O3   |
| 47  | L     | 710  | 3PE  | O31-C31-C32-C33 |
| 47  | O     | 202  | 3PE  | O31-C31-C32-C33 |
| 47  | O     | 203  | 3PE  | O21-C21-C22-C23 |
| 43  | g     | 301  | PLC  | C3B-C4B-C5B-C6B |
| 47  | L     | 711  | 3PE  | O31-C31-C32-C33 |
| 47  | Z     | 203  | 3PE  | O21-C21-C22-C23 |
| 48  | O     | 201  | CDL  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | Z     | 203 | 3PE  | O11-C1-C2-C3    |
| 48  | O     | 201 | CDL  | C13-C14-C15-C16 |
| 48  | O     | 201 | CDL  | C32-C31-CA7-OA8 |
| 47  | H     | 402 | 3PE  | C27-C28-C29-C2A |
| 43  | b     | 101 | PLC  | C4-C5-N-C6      |
| 49  | P     | 501 | NDP  | C5D-O5D-PN-O3   |
| 47  | L     | 701 | 3PE  | C22-C21-O21-C2  |
| 51  | U     | 201 | EHZ  | C1-C21-C22-C23  |
| 47  | m     | 102 | 3PE  | C2-C1-O11-P     |
| 43  | L     | 704 | PLC  | C3B-C4B-C5B-C6B |
| 47  | m     | 101 | 3PE  | O31-C31-C32-C33 |
| 47  | L     | 712 | 3PE  | C22-C23-C24-C25 |
| 43  | H     | 401 | PLC  | C4-C5-N-C8      |
| 43  | L     | 702 | PLC  | C4-C5-N-C6      |
| 47  | N     | 601 | 3PE  | O32-C31-C32-C33 |
| 47  | L     | 709 | 3PE  | C3E-C3F-C3G-C3H |
| 47  | m     | 102 | 3PE  | C35-C36-C37-C38 |
| 48  | c     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 47  | L     | 701 | 3PE  | O22-C21-C22-C23 |
| 47  | L     | 707 | 3PE  | O32-C31-C32-C33 |
| 47  | m     | 102 | 3PE  | O22-C21-C22-C23 |
| 43  | d     | 102 | PLC  | C2B-C1B-CB-OB   |
| 47  | L     | 711 | 3PE  | O32-C31-C32-C33 |
| 47  | Z     | 203 | 3PE  | C29-C2A-C2B-C2C |
| 43  | g     | 301 | PLC  | C4'-C5'-C6'-C7' |
| 43  | a     | 201 | PLC  | OB-CB-O3-C3     |
| 47  | L     | 710 | 3PE  | O32-C31-C32-C33 |
| 43  | D     | 501 | PLC  | C1-O3P-P-O1P    |
| 43  | Y     | 303 | PLC  | C4-C5-N-C6      |
| 43  | a     | 201 | PLC  | C4-O4P-P-O1P    |
| 43  | q     | 202 | PLC  | C4-O4P-P-O1P    |
| 48  | O     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 48  | P     | 503 | CDL  | CA2-OA2-PA1-OA3 |
| 47  | H     | 402 | 3PE  | O13-C11-C12-N   |
| 47  | L     | 707 | 3PE  | O13-C11-C12-N   |
| 47  | f     | 101 | 3PE  | O13-C11-C12-N   |
| 47  | O     | 203 | 3PE  | O22-C21-C22-C23 |
| 47  | m     | 101 | 3PE  | O32-C31-C32-C33 |
| 48  | c     | 201 | CDL  | C33-C34-C35-C36 |
| 43  | h     | 201 | PLC  | C6'-C7'-C8'-C9' |
| 43  | L     | 702 | PLC  | C3B-C4B-C5B-C6B |
| 43  | B     | 302 | PLC  | CB-C1B-C2B-C3B  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 47  | O     | 203  | 3PE  | C32-C33-C34-C35 |
| 43  | B     | 302  | PLC  | C5-C4-O4P-P     |
| 43  | D     | 501  | PLC  | C5-C4-O4P-P     |
| 43  | L     | 702  | PLC  | C5-C4-O4P-P     |
| 43  | b     | 101  | PLC  | C5-C4-O4P-P     |
| 43  | d     | 102  | PLC  | C5-C4-O4P-P     |
| 43  | h     | 201  | PLC  | C5-C4-O4P-P     |
| 47  | L     | 701  | 3PE  | C12-C11-O13-P   |
| 47  | L     | 708  | 3PE  | C12-C11-O13-P   |
| 47  | L     | 709  | 3PE  | C12-C11-O13-P   |
| 47  | L     | 710  | 3PE  | C12-C11-O13-P   |
| 47  | M     | 1003 | 3PE  | C12-C11-O13-P   |
| 47  | O     | 203  | 3PE  | C12-C11-O13-P   |
| 47  | Y     | 302  | 3PE  | C12-C11-O13-P   |
| 47  | Z     | 203  | 3PE  | C12-C11-O13-P   |
| 47  | f     | 101  | 3PE  | C12-C11-O13-P   |
| 47  | m     | 101  | 3PE  | C12-C11-O13-P   |
| 47  | O     | 202  | 3PE  | O32-C31-C32-C33 |
| 43  | L     | 705  | PLC  | C2B-C1B-CB-O3   |
| 43  | P     | 502  | PLC  | O2-C'-C1'-C2'   |
| 47  | b     | 103  | 3PE  | O21-C21-C22-C23 |
| 43  | L     | 705  | PLC  | C8'-C9'-CA'-CB' |
| 43  | L     | 702  | PLC  | O2-C'-C1'-C2'   |
| 48  | P     | 503  | CDL  | C32-C31-CA7-OA8 |
| 43  | H     | 401  | PLC  | C2-C1-O3P-P     |
| 47  | L     | 701  | 3PE  | C21-C22-C23-C24 |
| 43  | L     | 705  | PLC  | C2B-C1B-CB-OB   |
| 48  | P     | 503  | CDL  | C32-C31-CA7-OA9 |
| 48  | O     | 201  | CDL  | C32-C31-CA7-OA9 |
| 47  | f     | 101  | 3PE  | O21-C21-C22-C23 |
| 47  | b     | 103  | 3PE  | O22-C21-C22-C23 |
| 47  | L     | 712  | 3PE  | C3C-C3D-C3E-C3F |
| 43  | P     | 502  | PLC  | O'-C'-C1'-C2'   |

There are no ring outliers.

46 monomers are involved in 112 short contacts:

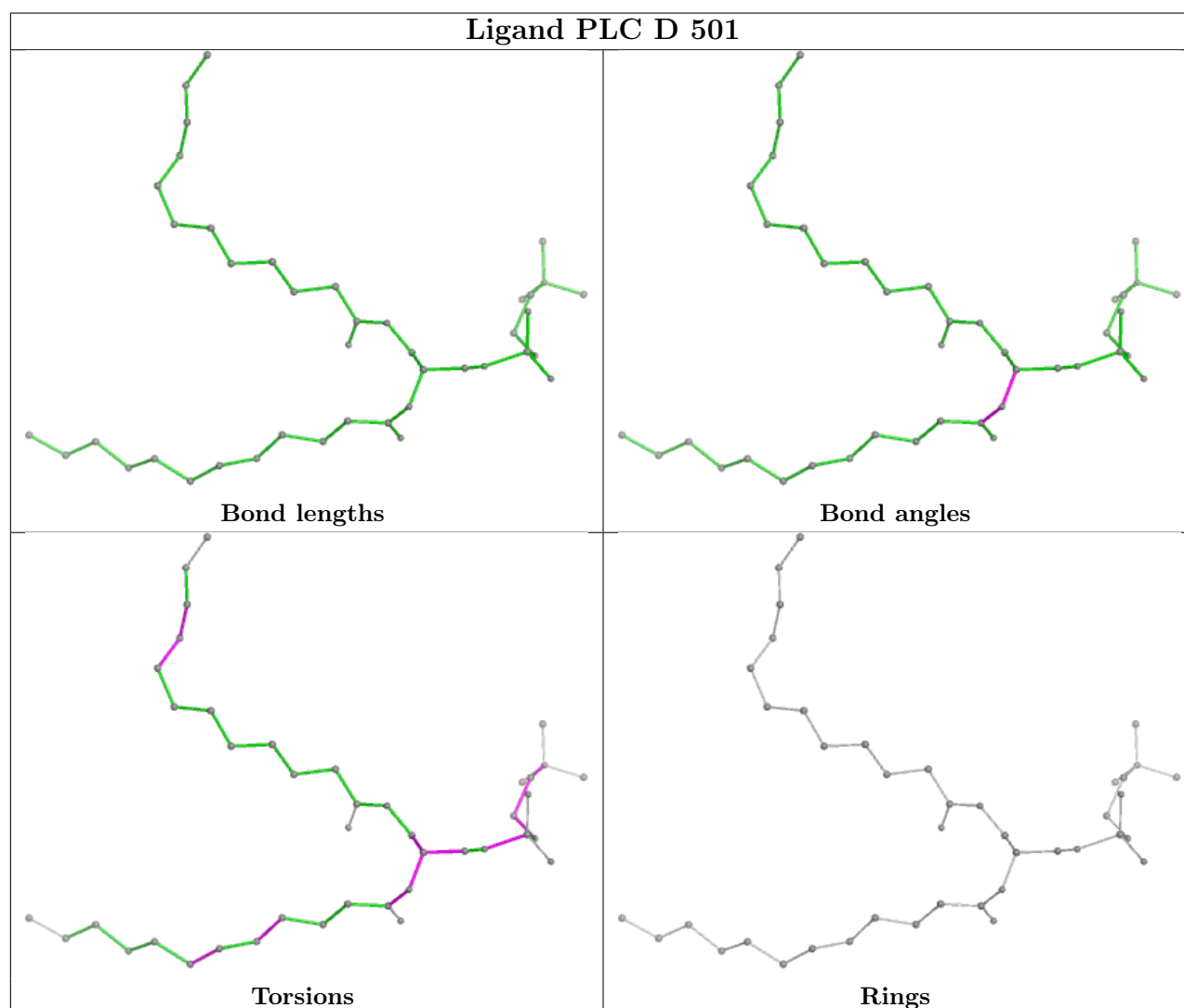
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 43  | D     | 501 | PLC  | 2       | 0            |
| 47  | L     | 707 | 3PE  | 8       | 0            |
| 47  | j     | 101 | 3PE  | 1       | 0            |
| 48  | b     | 102 | CDL  | 3       | 0            |

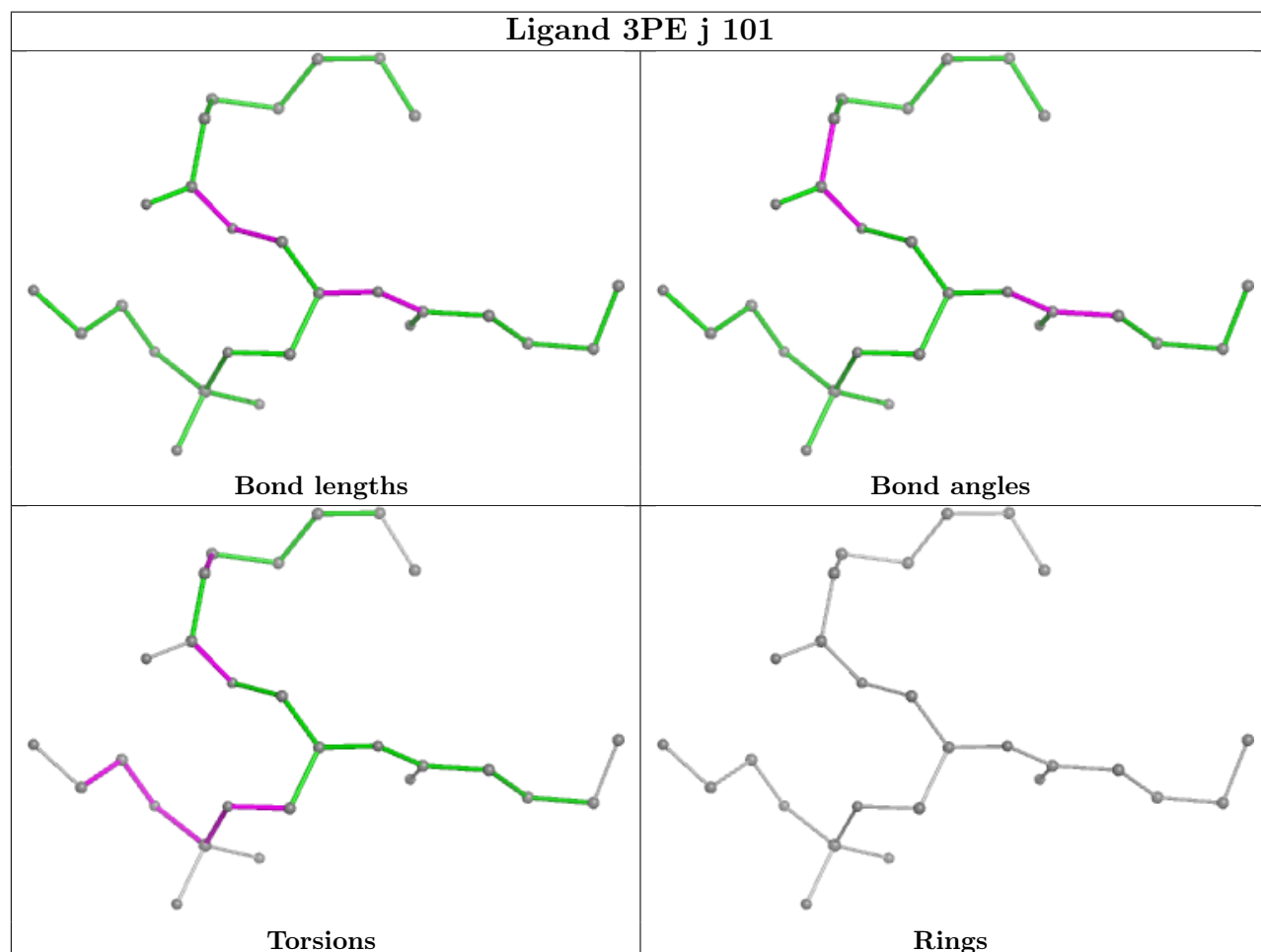
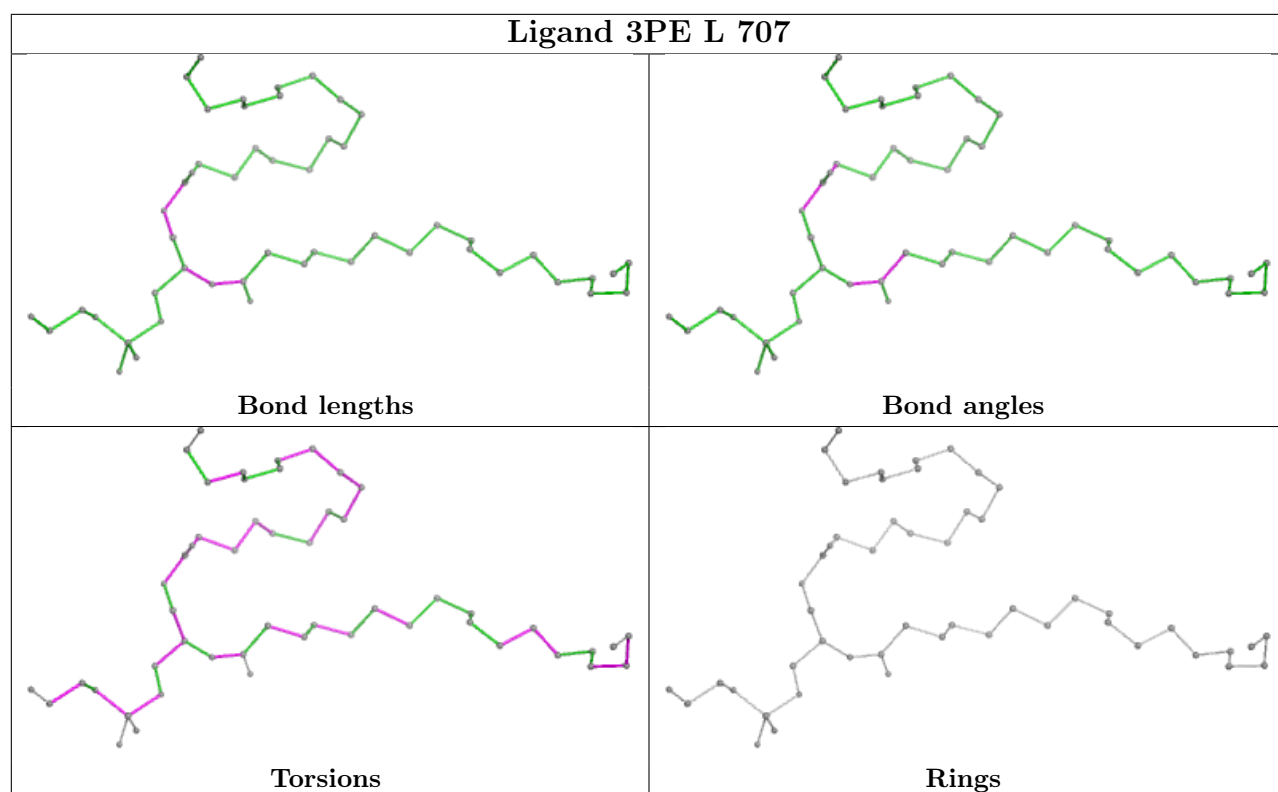
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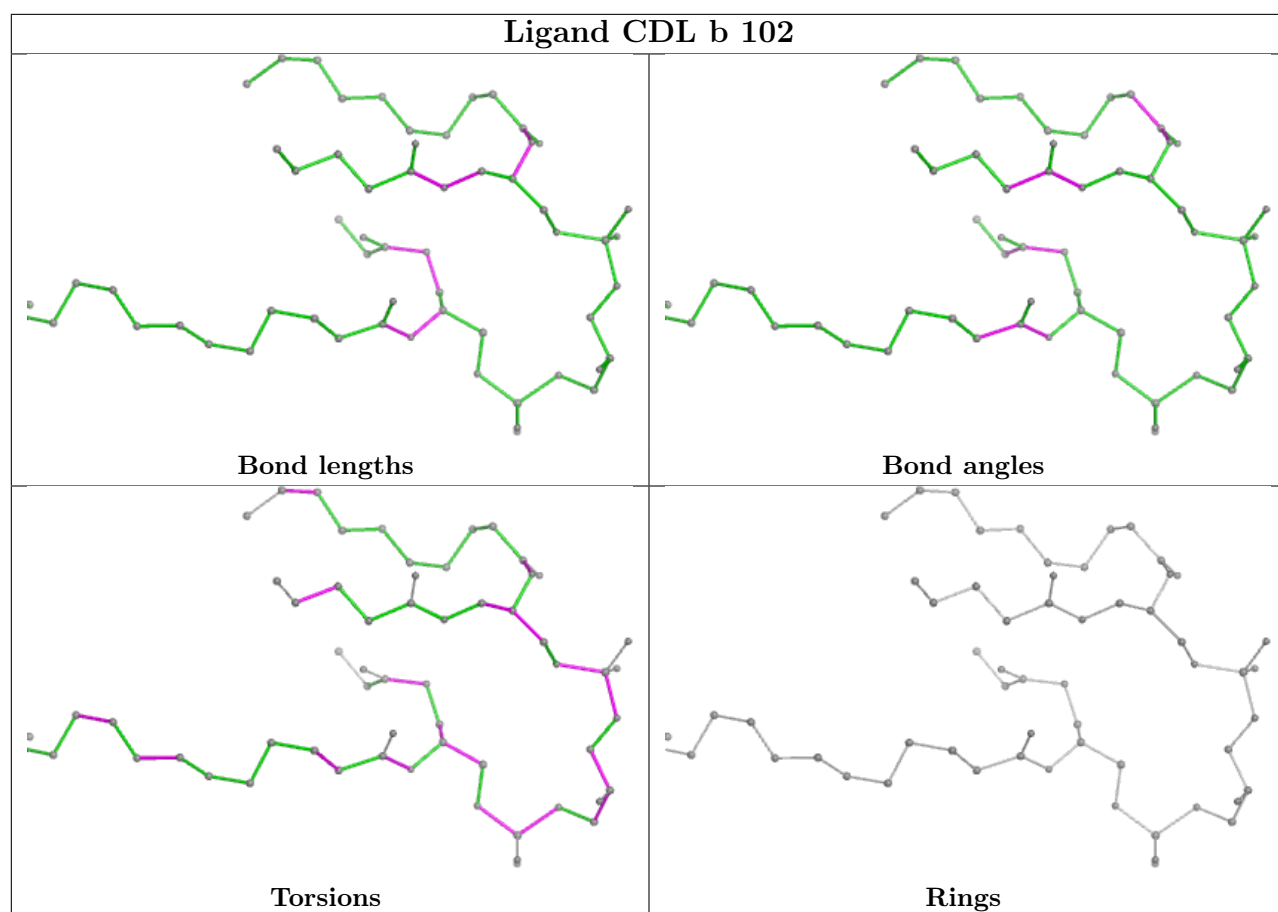
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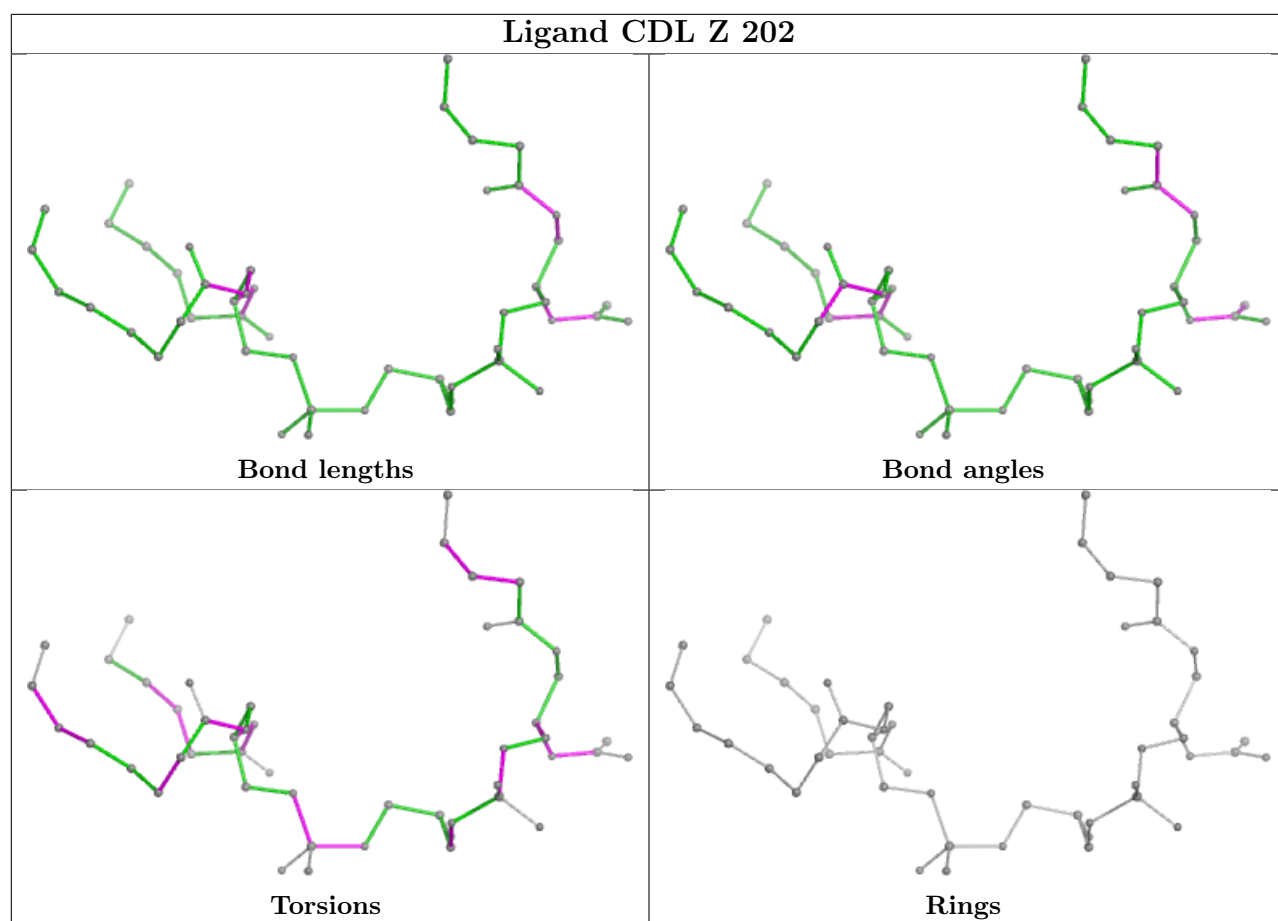
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 48  | c     | 201  | CDL  | 3       | 0            |
| 47  | Z     | 203  | 3PE  | 3       | 0            |
| 47  | m     | 102  | 3PE  | 2       | 0            |
| 43  | q     | 202  | PLC  | 3       | 0            |
| 47  | f     | 101  | 3PE  | 6       | 0            |
| 47  | m     | 101  | 3PE  | 1       | 0            |
| 47  | L     | 711  | 3PE  | 8       | 0            |
| 47  | N     | 601  | 3PE  | 1       | 0            |
| 44  | I     | 302  | SF4  | 2       | 0            |
| 47  | L     | 703  | 3PE  | 6       | 0            |
| 43  | L     | 702  | PLC  | 3       | 0            |
| 43  | d     | 102  | PLC  | 2       | 0            |
| 43  | h     | 201  | PLC  | 2       | 0            |
| 43  | d     | 101  | PLC  | 2       | 0            |
| 43  | Y     | 301  | PLC  | 1       | 0            |
| 44  | I     | 301  | SF4  | 2       | 0            |
| 47  | L     | 708  | 3PE  | 4       | 0            |
| 47  | L     | 710  | 3PE  | 2       | 0            |
| 47  | L     | 712  | 3PE  | 6       | 0            |
| 43  | P     | 502  | PLC  | 4       | 0            |
| 47  | Y     | 302  | 3PE  | 2       | 0            |
| 47  | L     | 709  | 3PE  | 1       | 0            |
| 51  | U     | 201  | EHZ  | 1       | 0            |
| 43  | a     | 201  | PLC  | 2       | 0            |
| 43  | L     | 705  | PLC  | 6       | 0            |
| 48  | O     | 201  | CDL  | 4       | 0            |
| 43  | M     | 1002 | PLC  | 1       | 0            |
| 43  | b     | 101  | PLC  | 1       | 0            |
| 43  | H     | 401  | PLC  | 1       | 0            |
| 43  | M     | 1001 | PLC  | 4       | 0            |
| 43  | q     | 201  | PLC  | 1       | 0            |
| 48  | P     | 503  | CDL  | 1       | 0            |
| 43  | A     | 201  | PLC  | 2       | 0            |
| 47  | M     | 1003 | 3PE  | 1       | 0            |
| 44  | G     | 801  | SF4  | 1       | 0            |
| 47  | L     | 706  | 3PE  | 1       | 0            |
| 47  | O     | 202  | 3PE  | 1       | 0            |
| 43  | g     | 301  | PLC  | 3       | 0            |
| 47  | b     | 103  | 3PE  | 1       | 0            |
| 47  | O     | 203  | 3PE  | 1       | 0            |
| 47  | L     | 701  | 3PE  | 2       | 0            |
| 43  | Y     | 303  | PLC  | 4       | 0            |

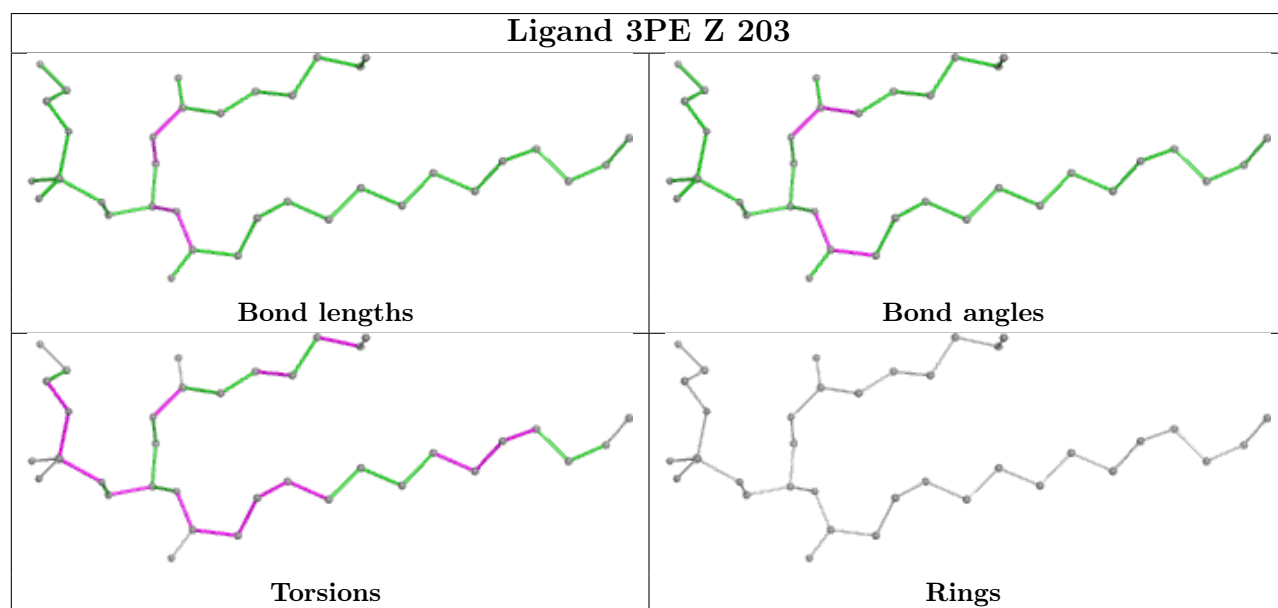
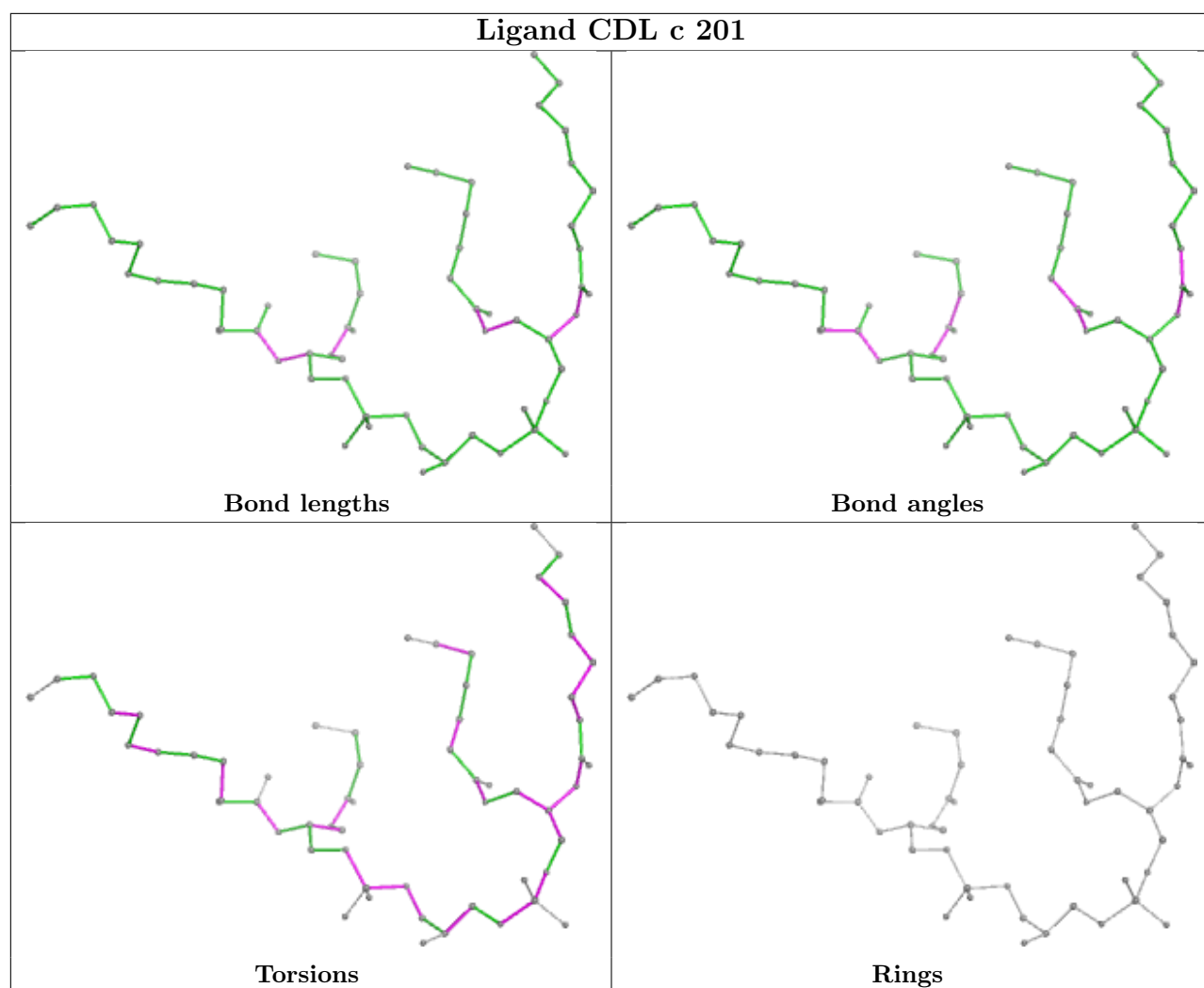
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



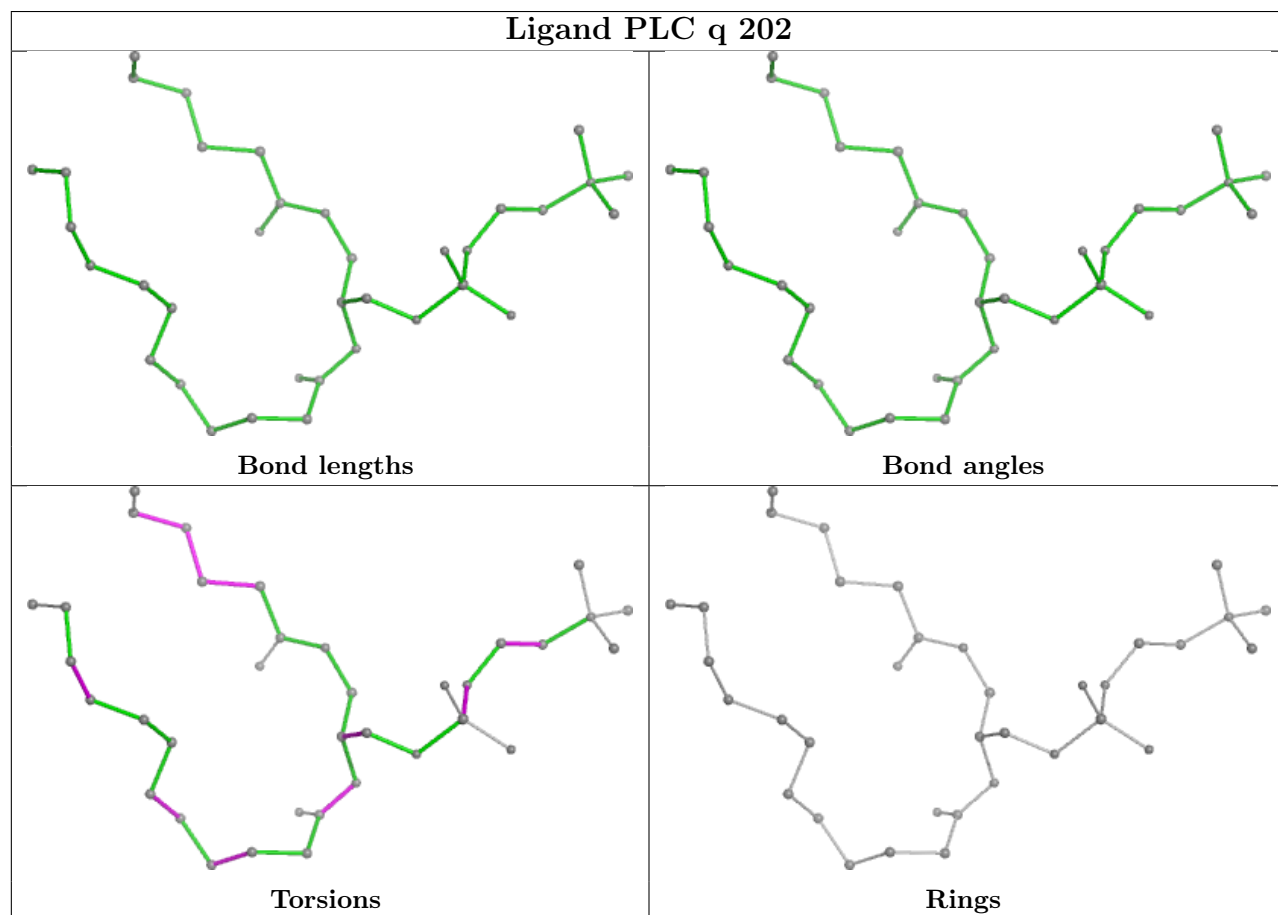
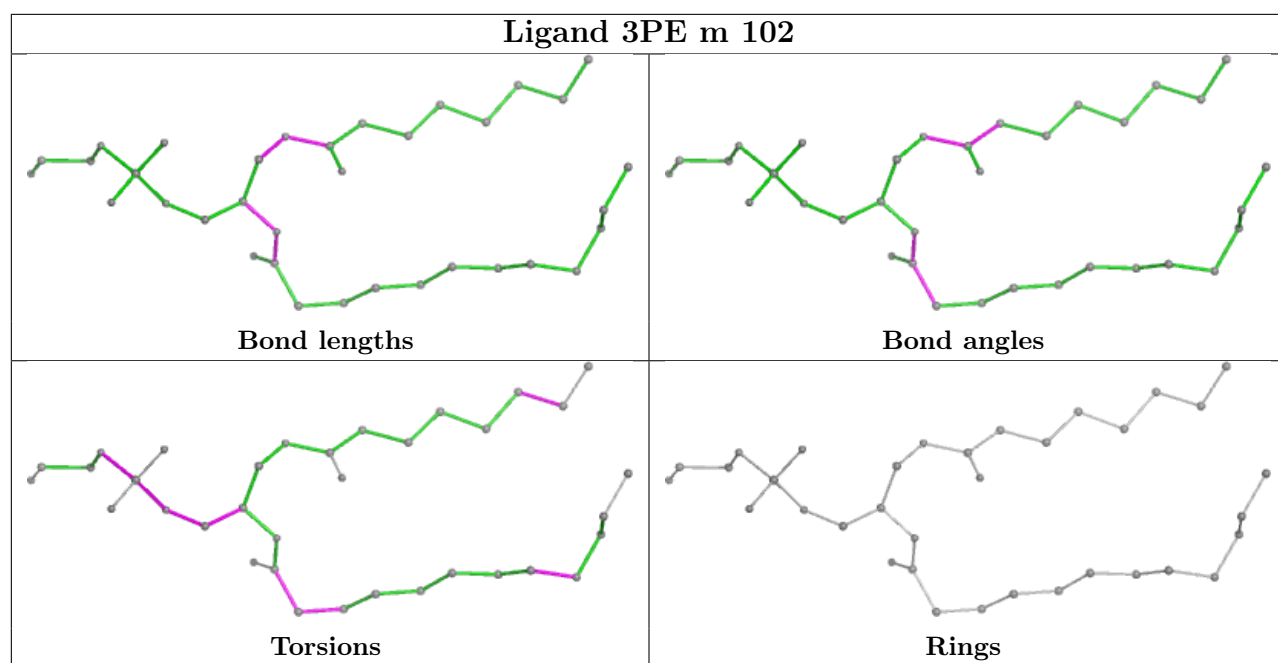


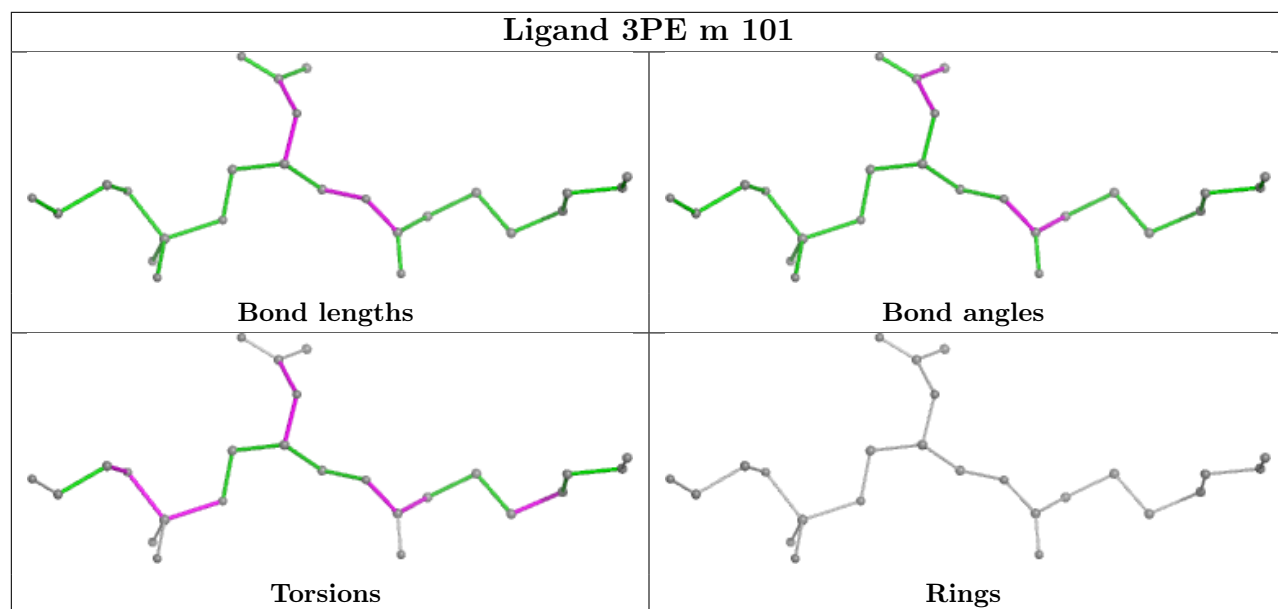
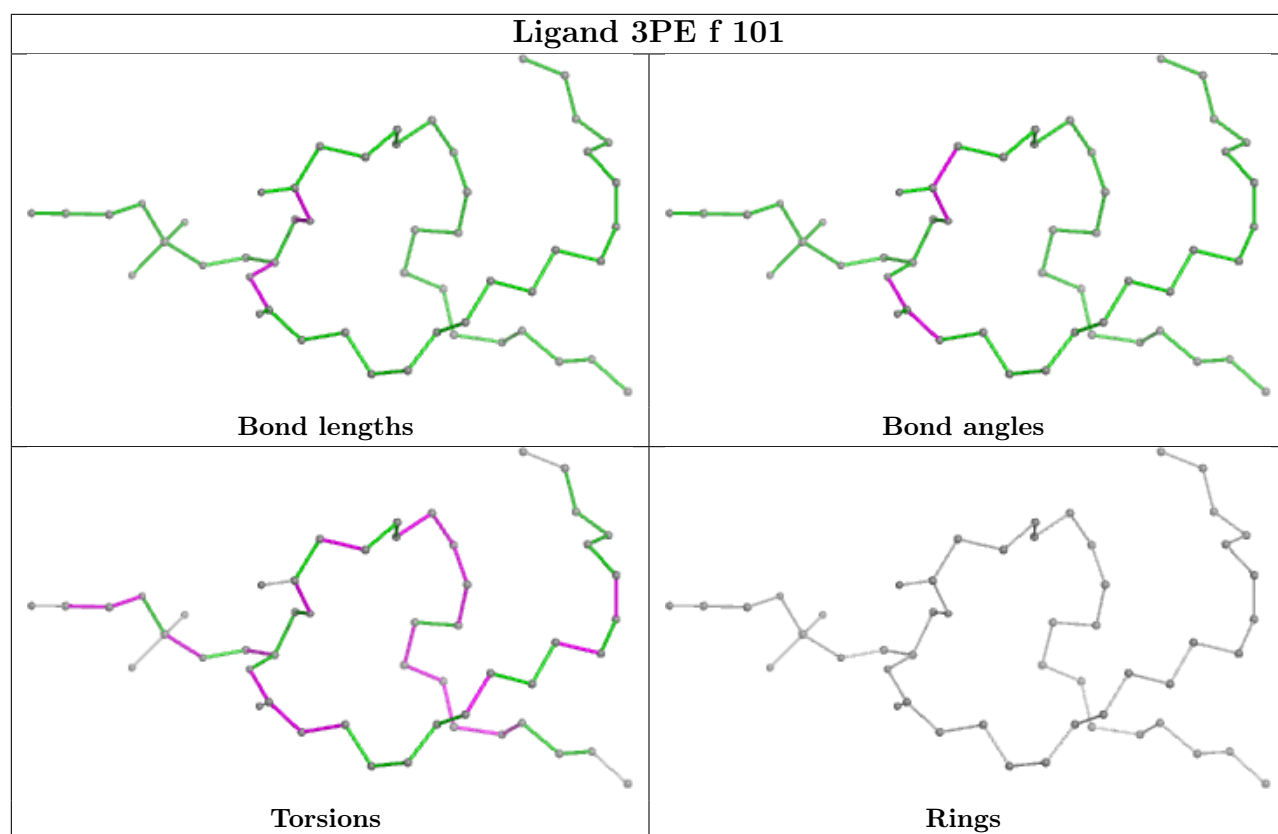




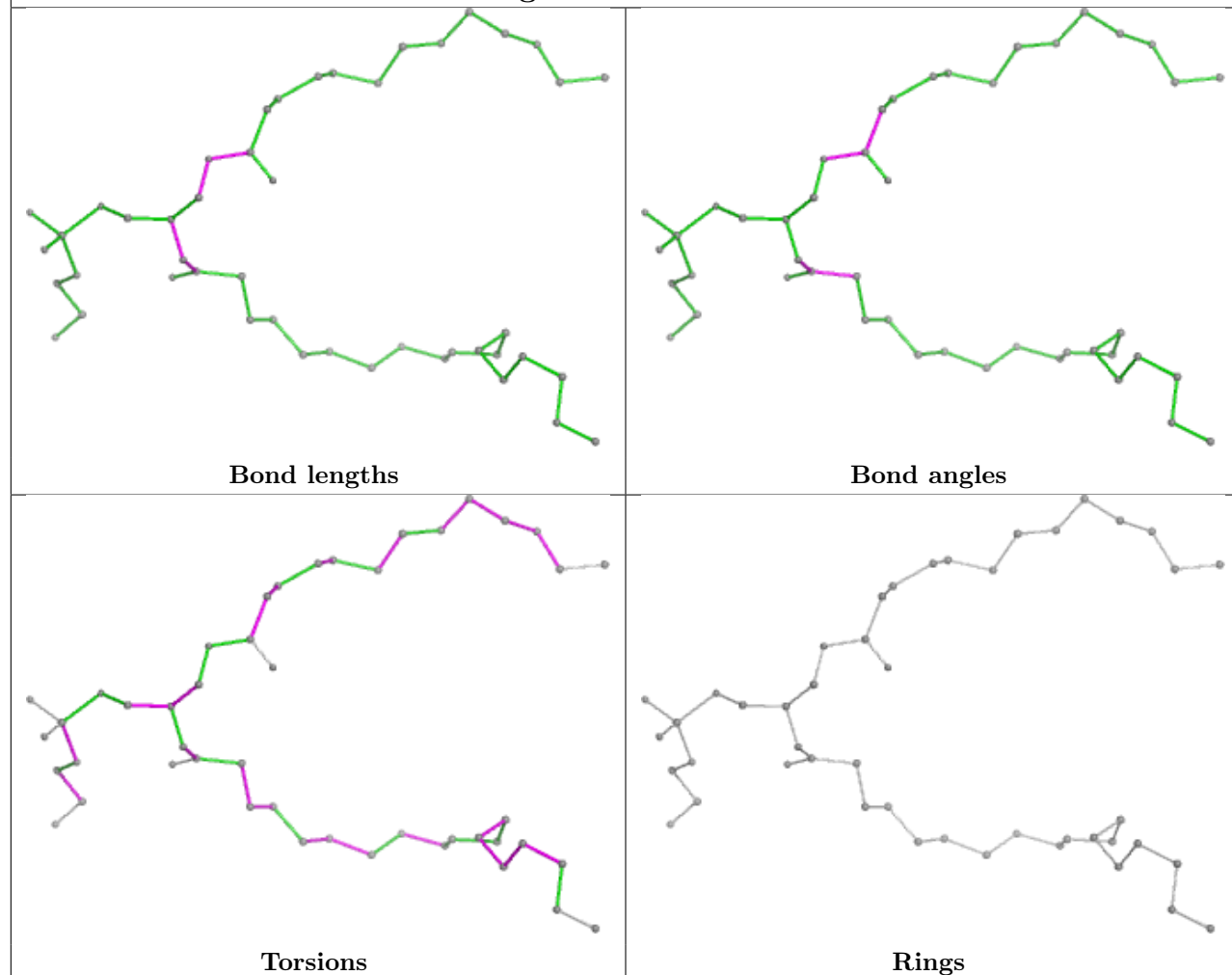




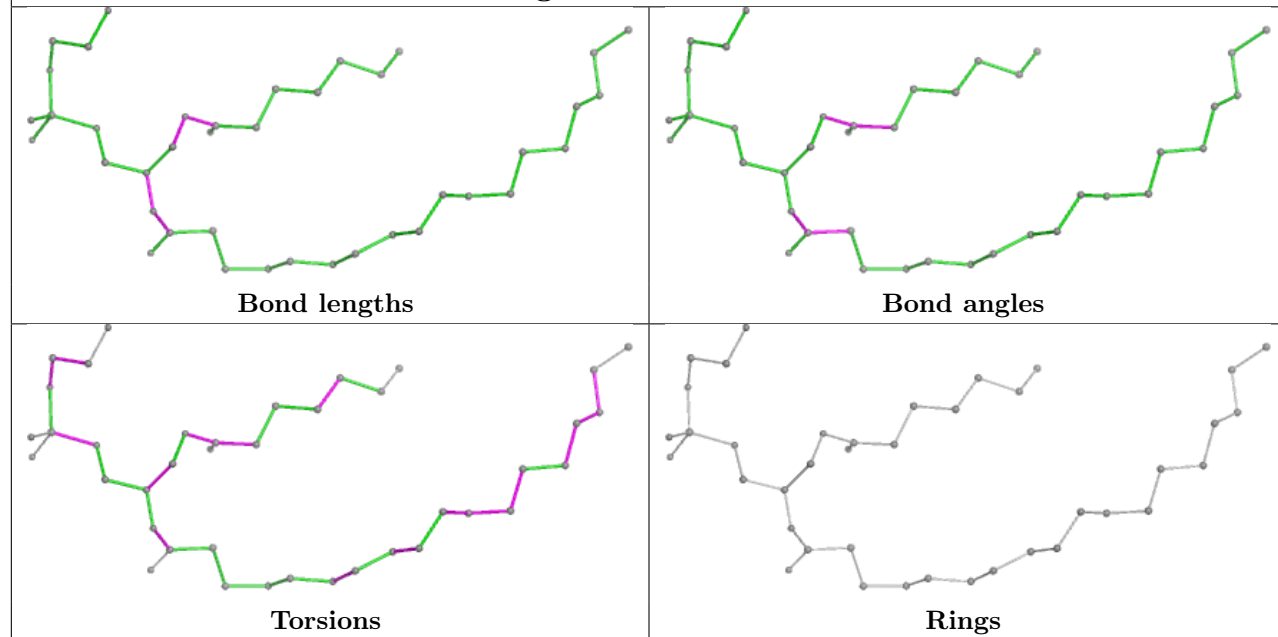


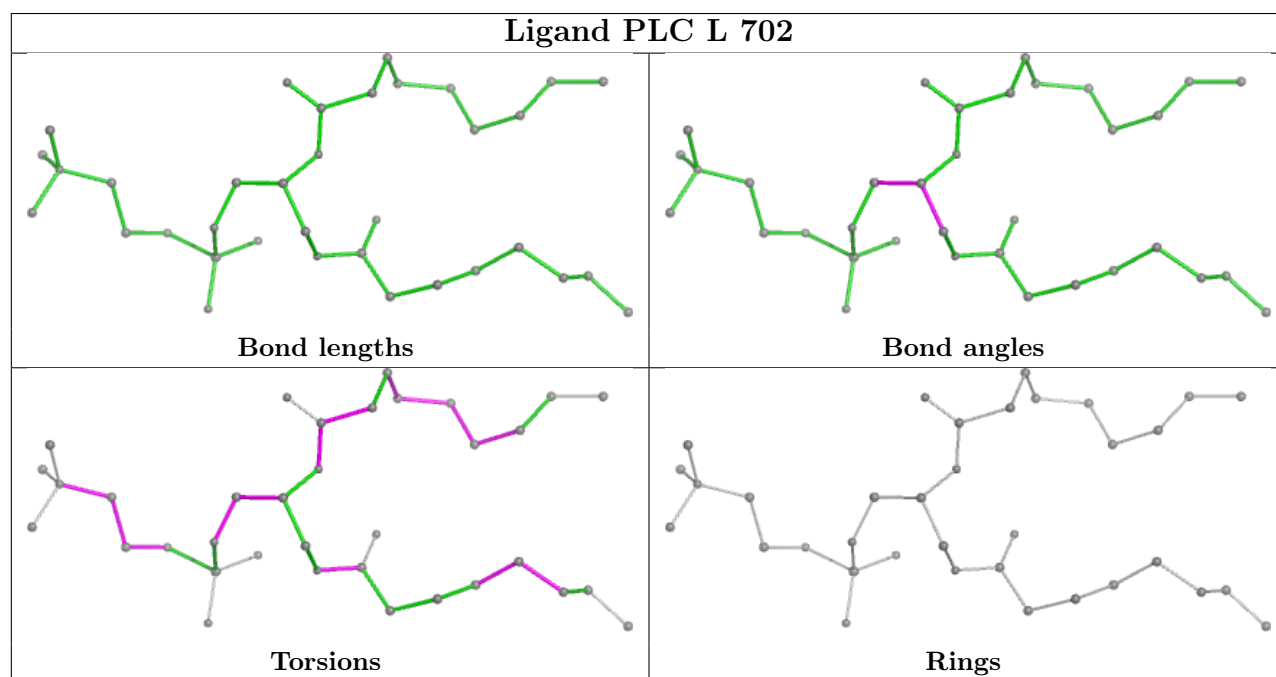
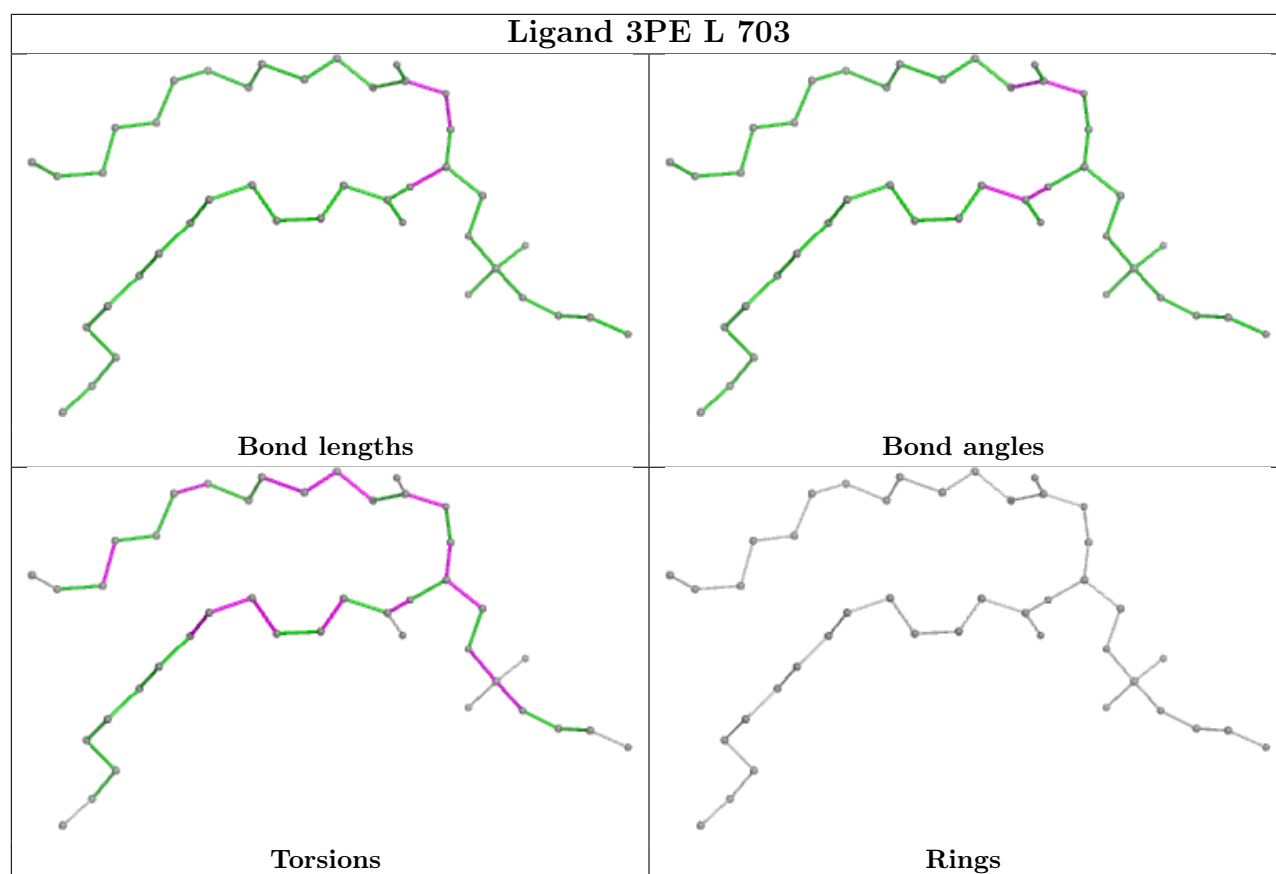


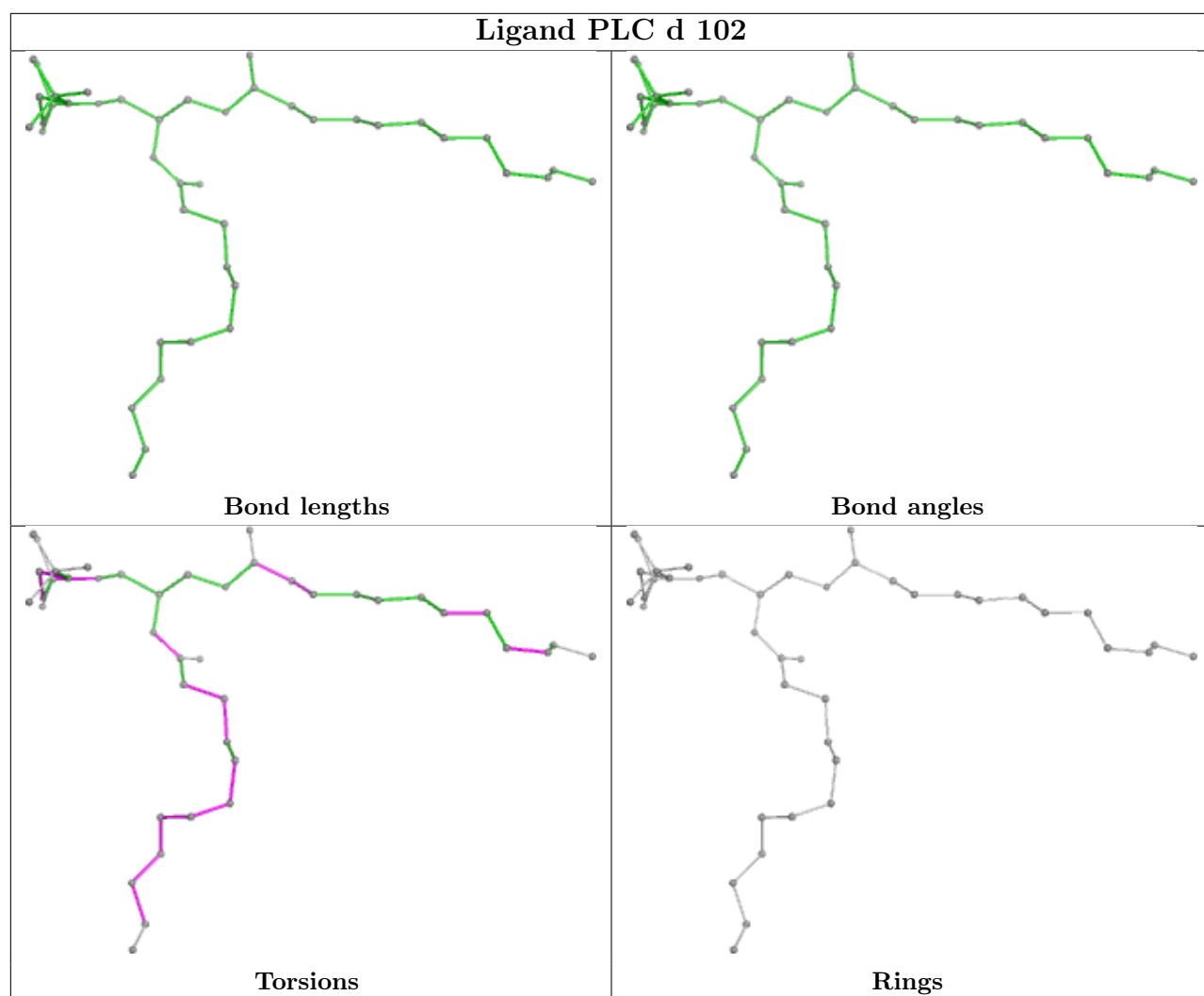
## Ligand 3PE L 711

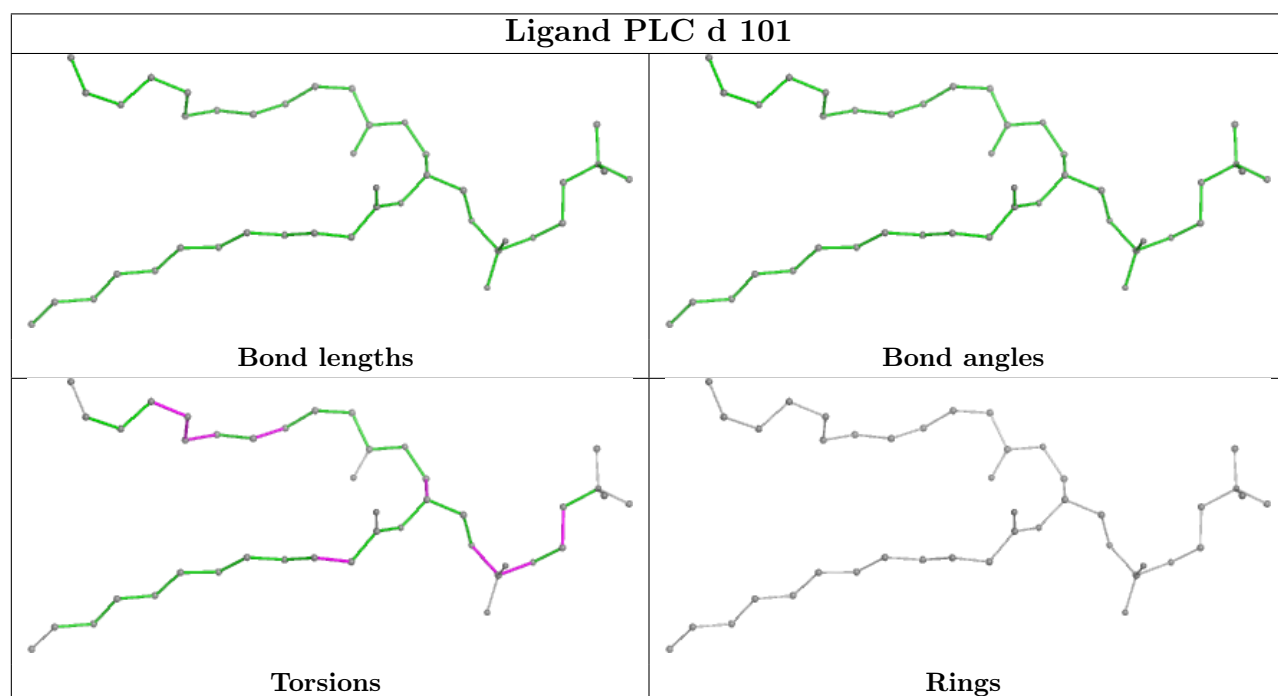
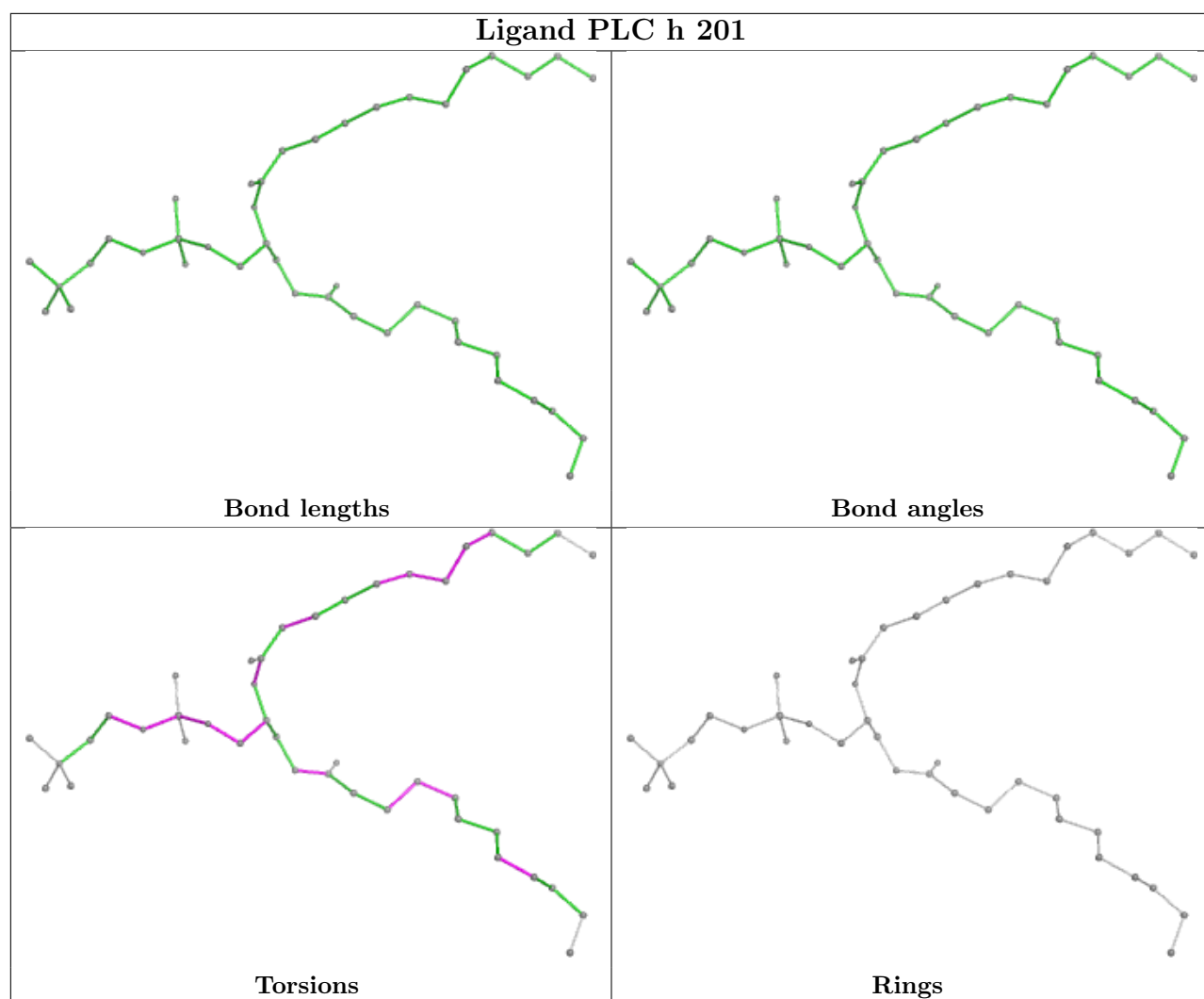


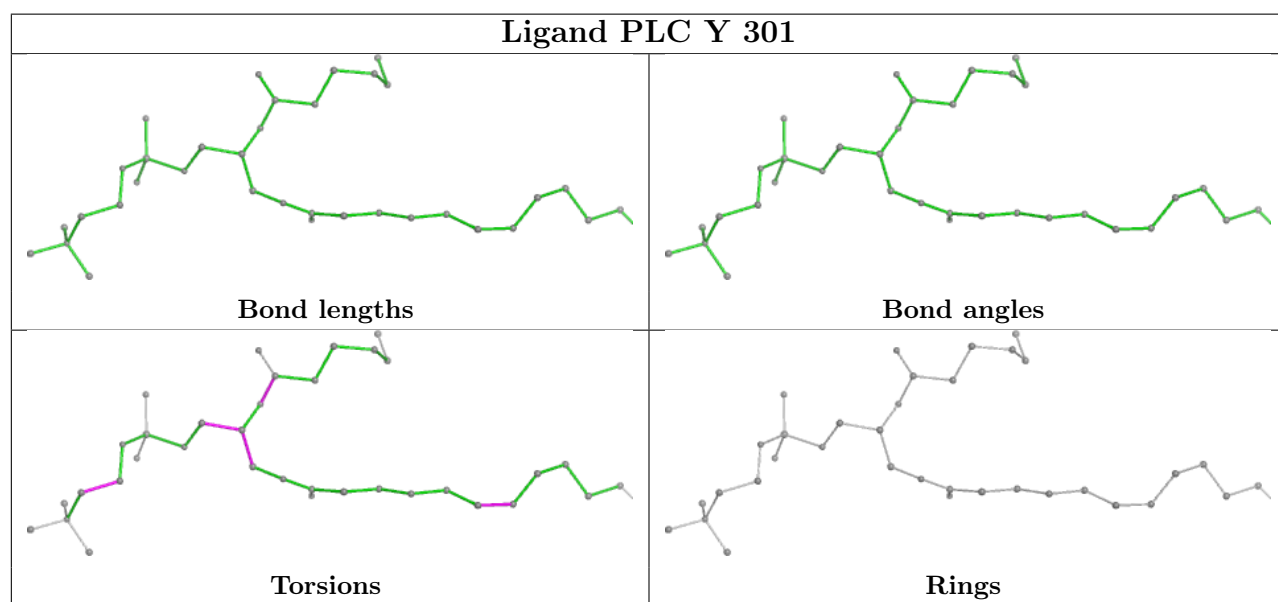
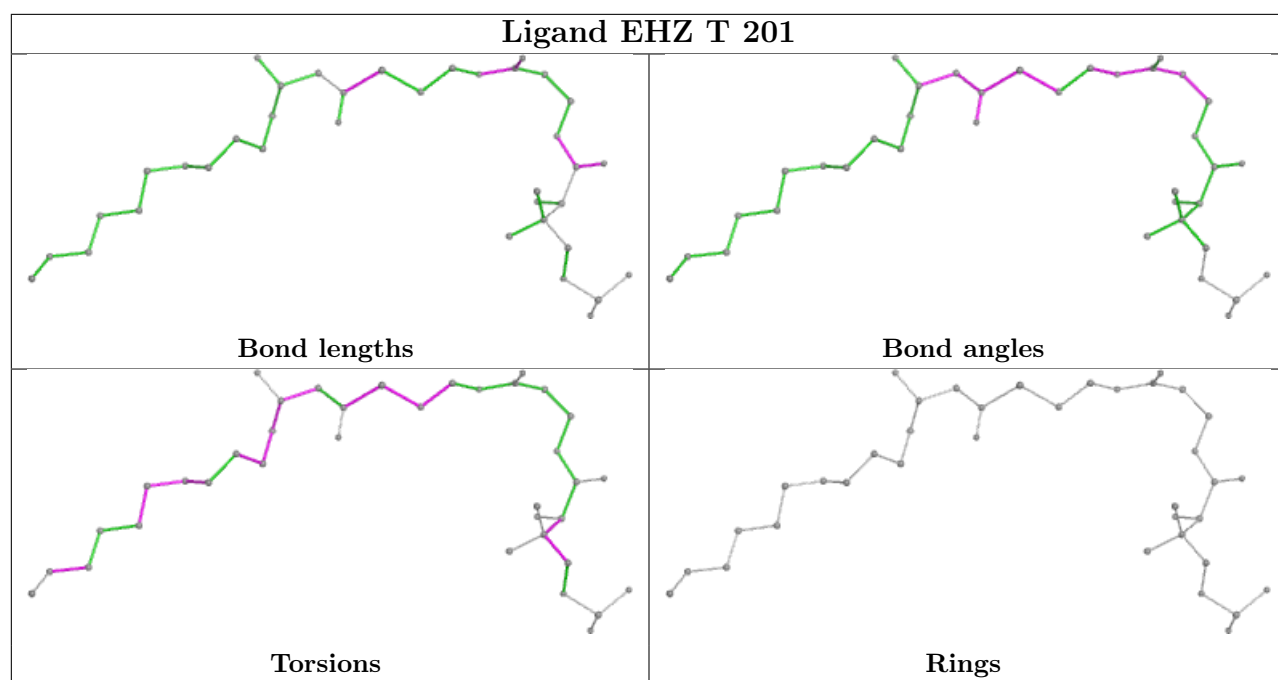
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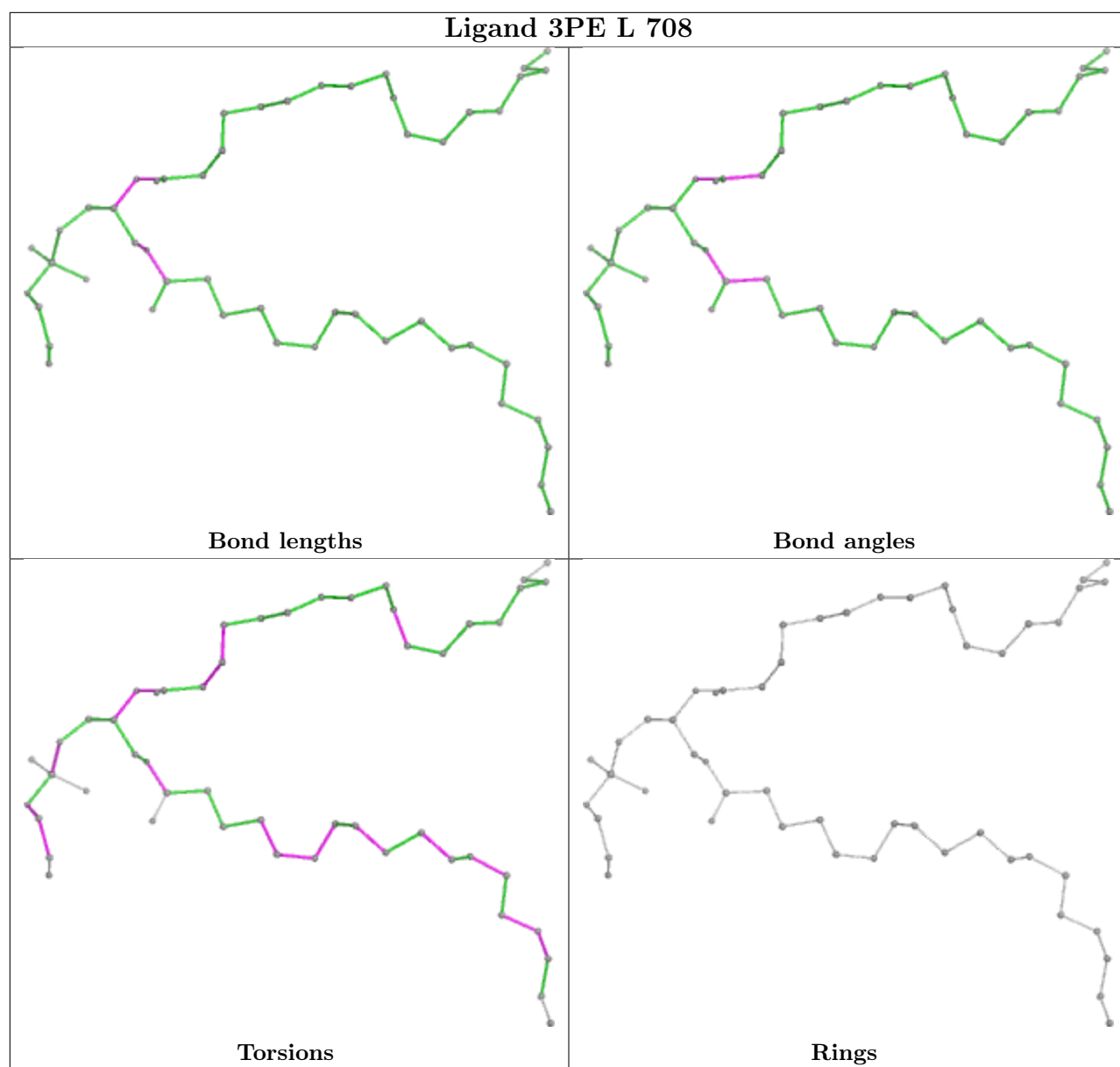




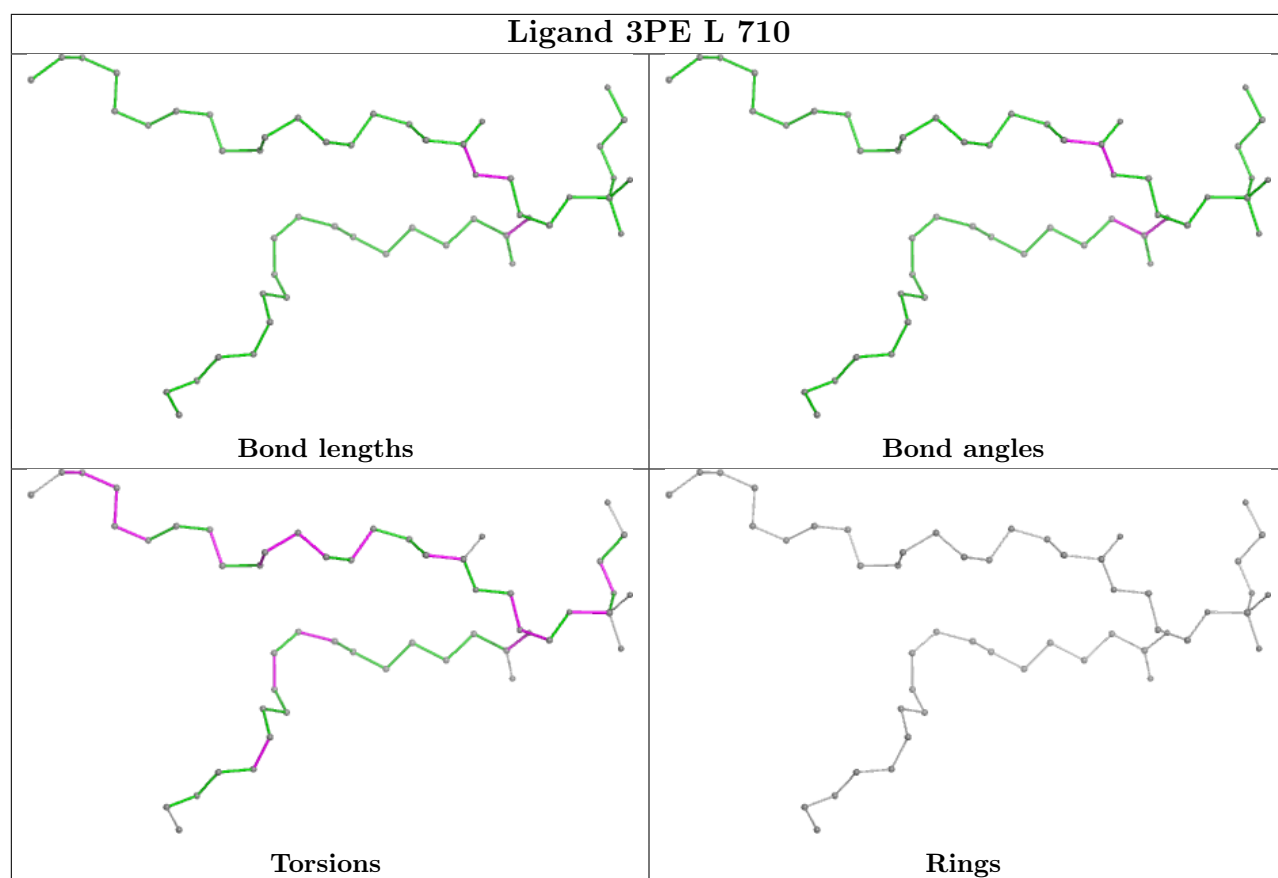


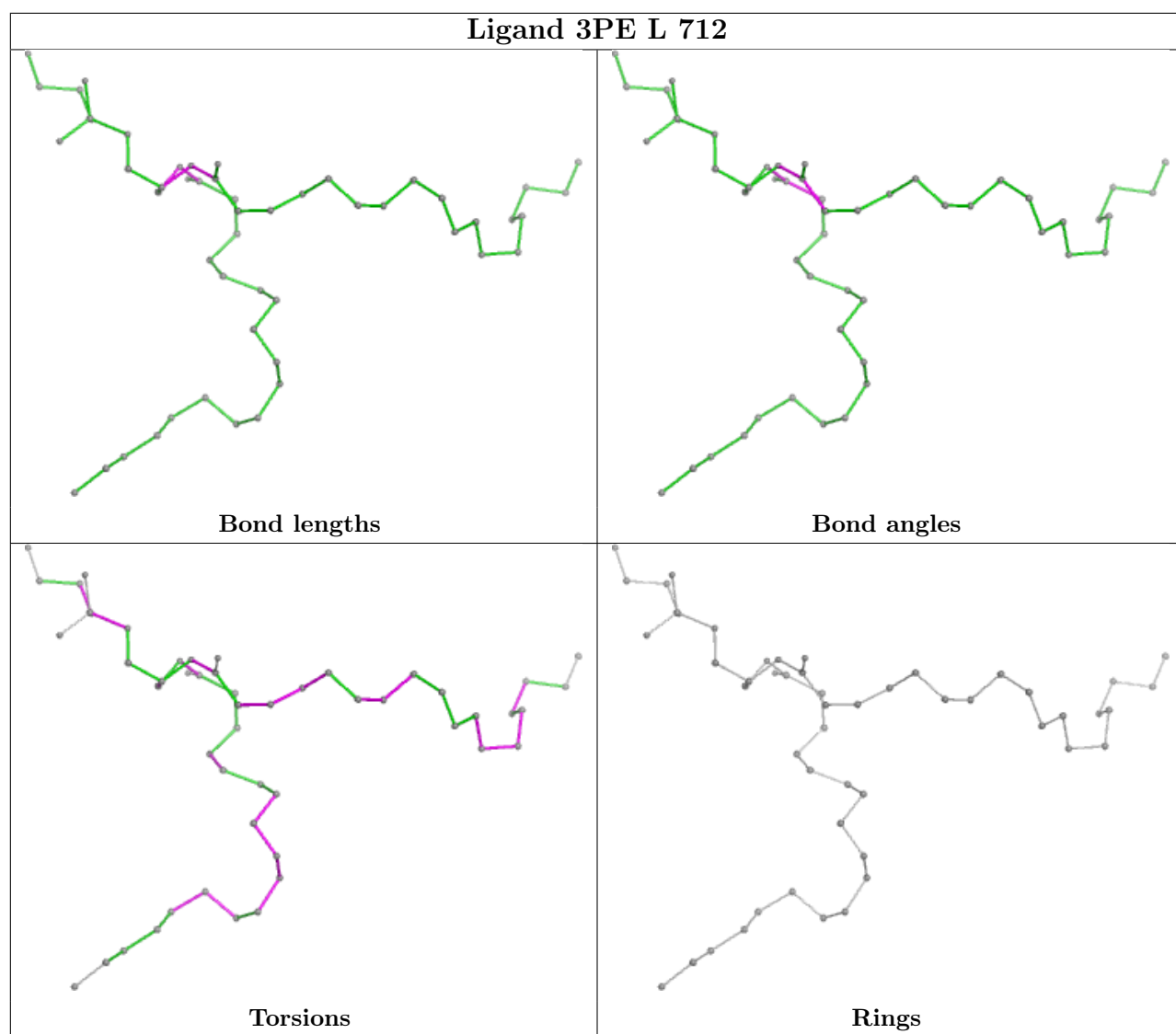


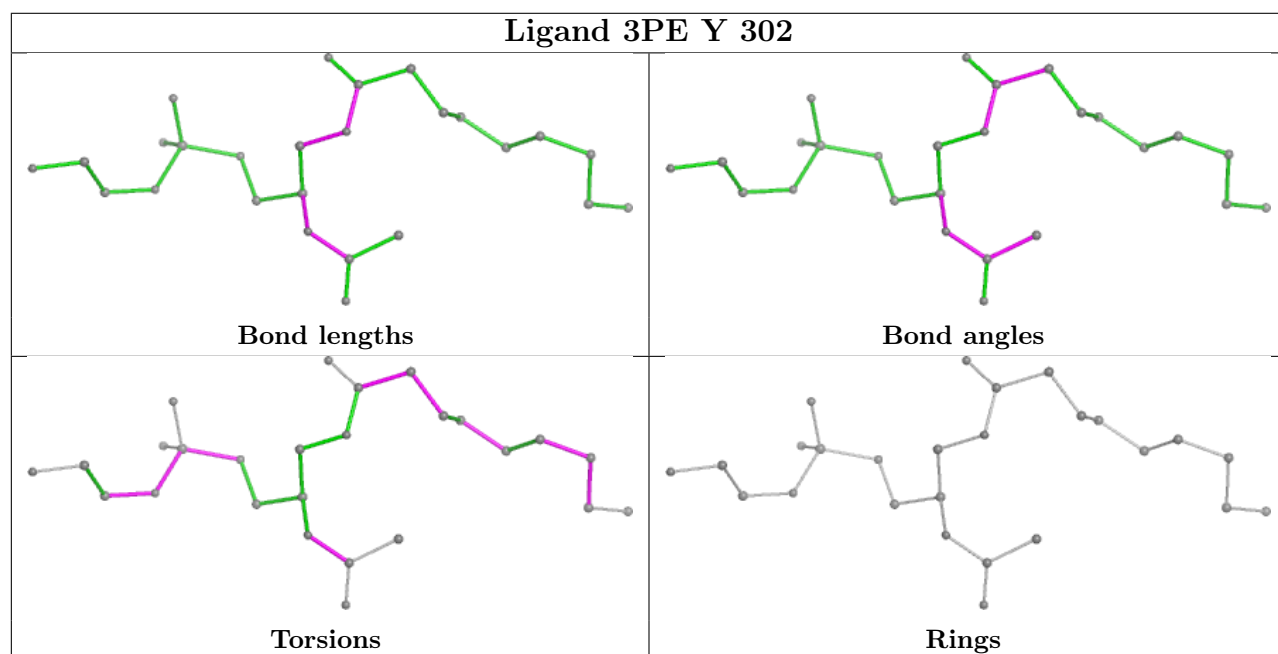
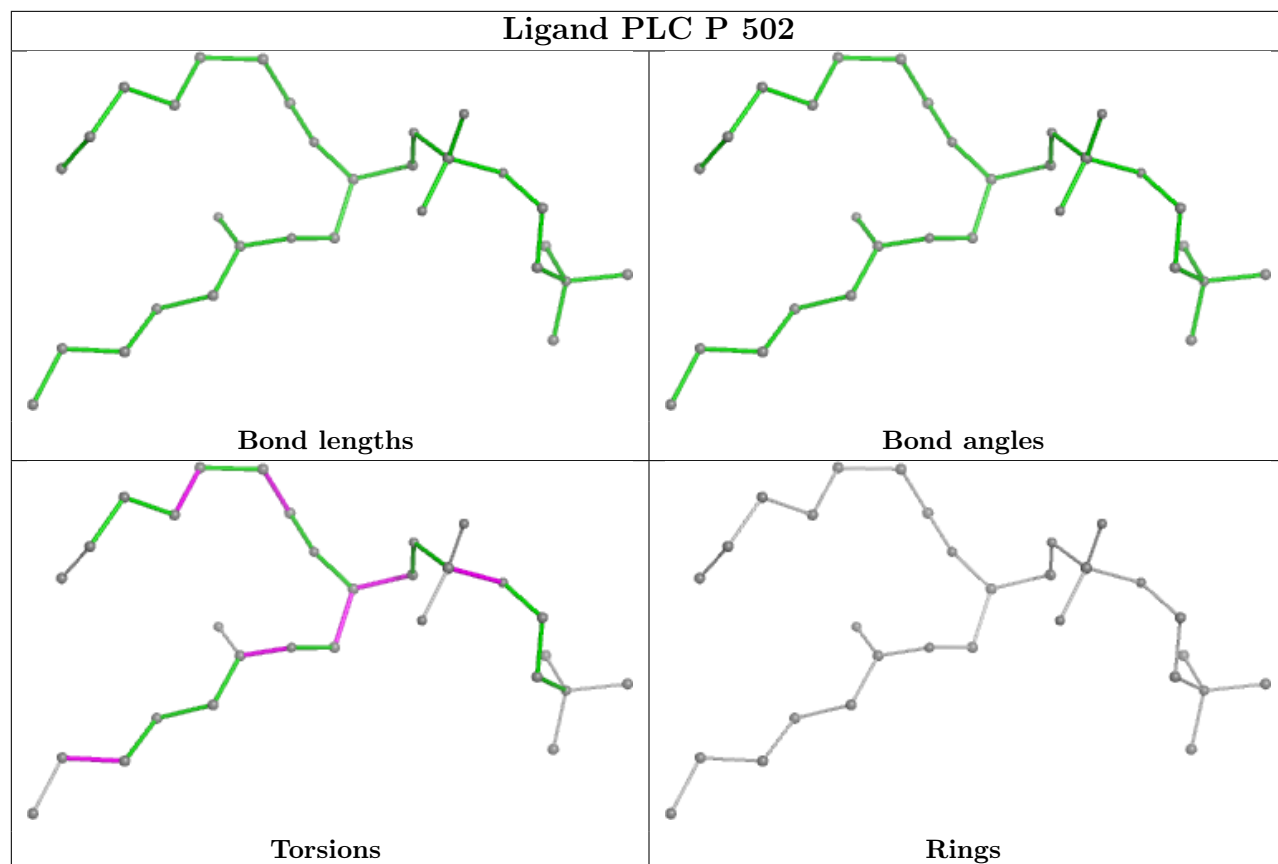


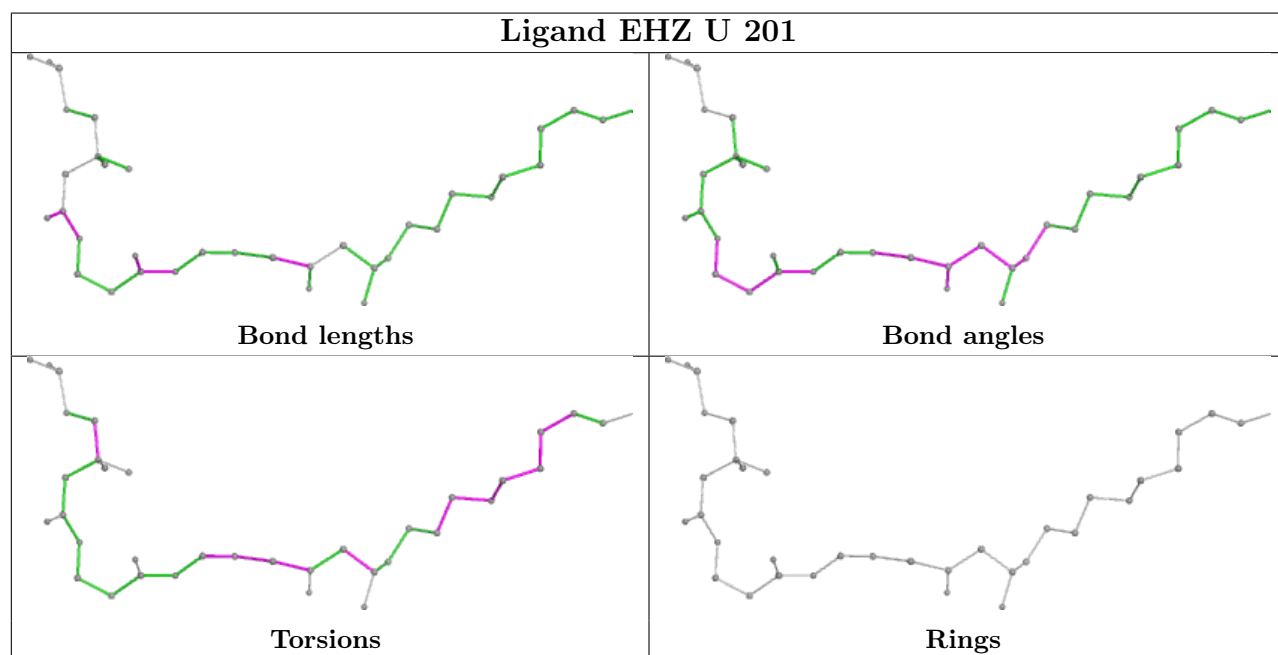
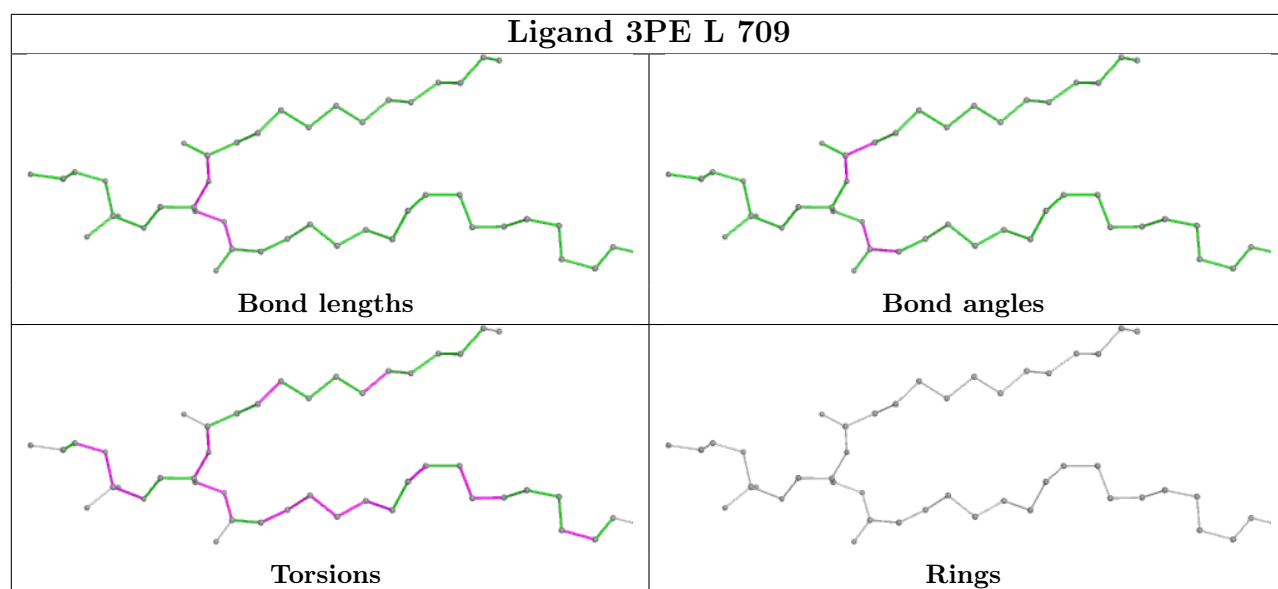


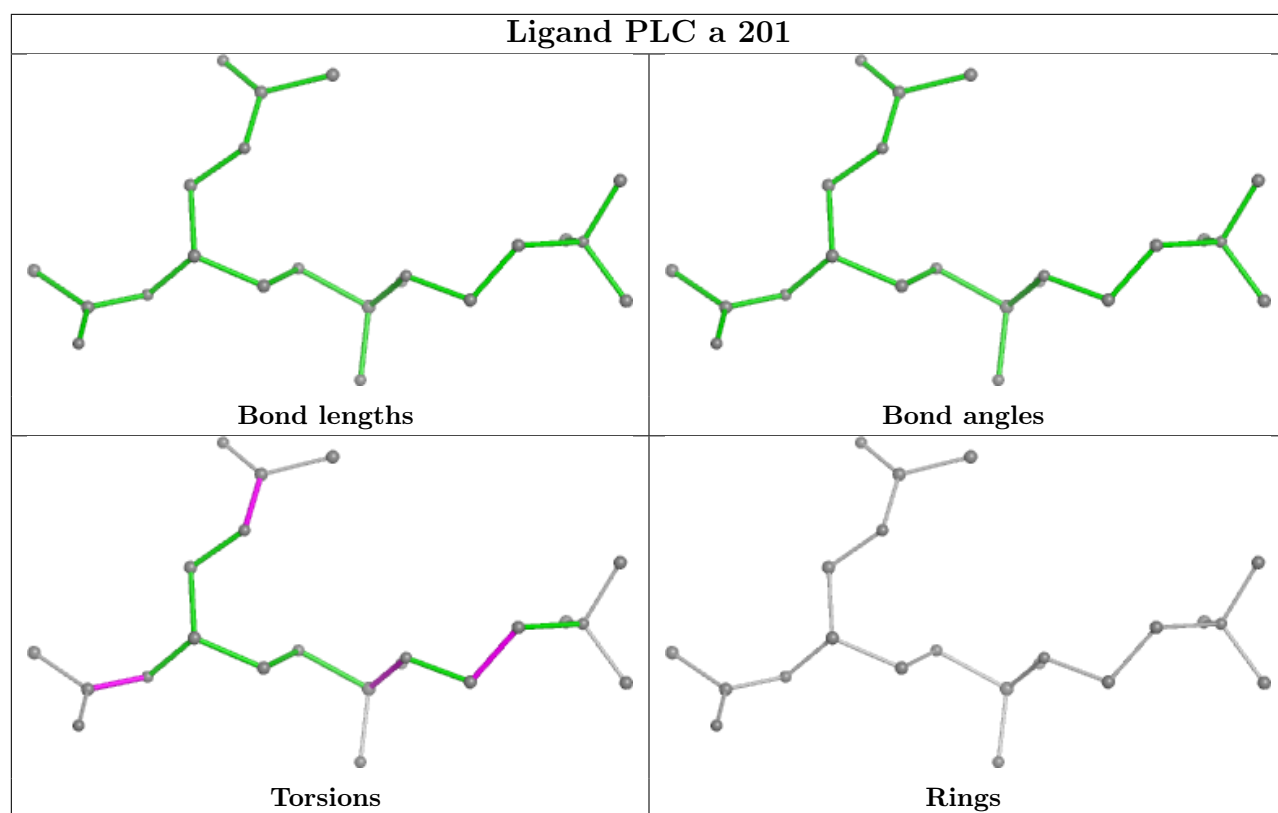


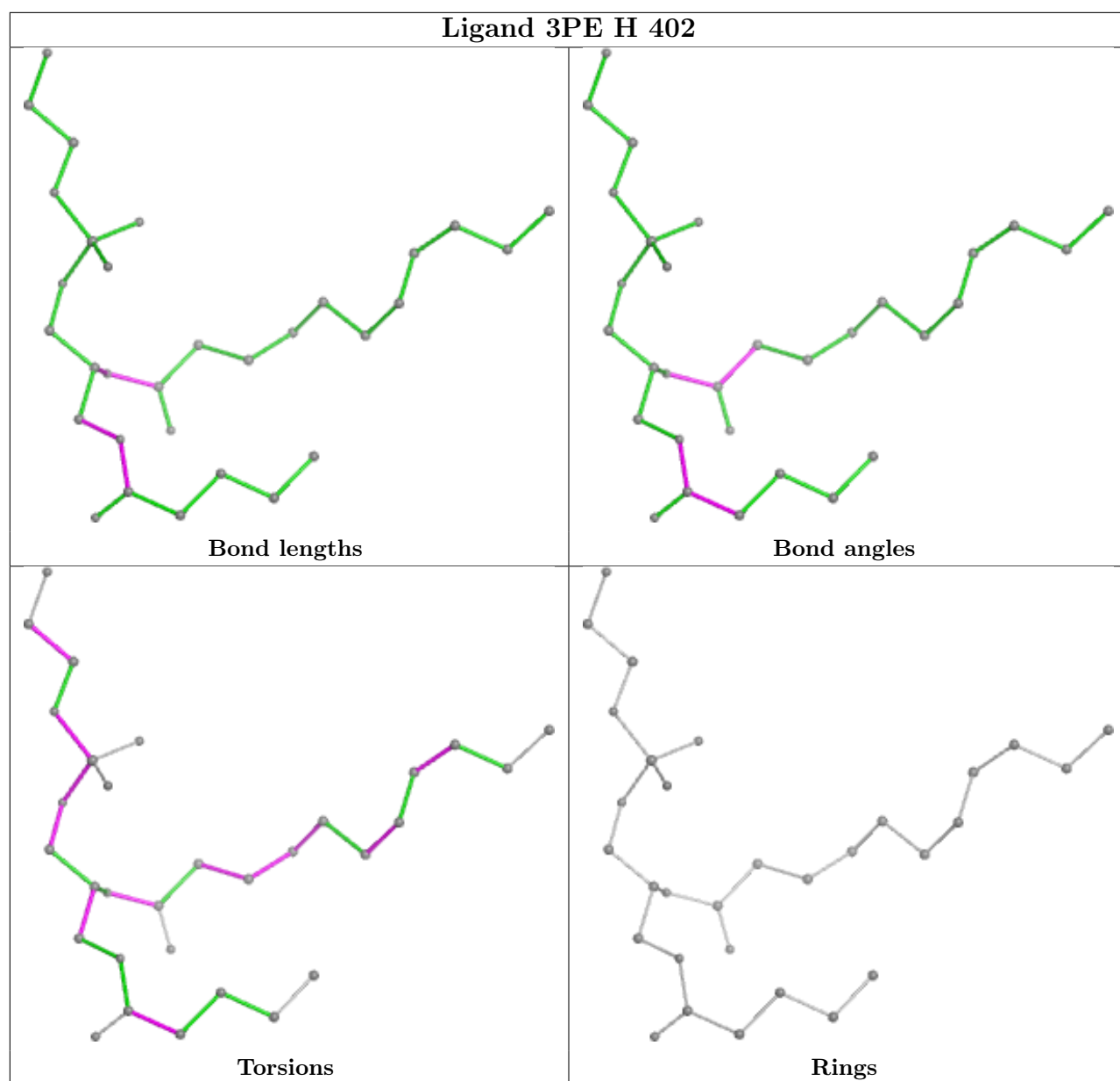


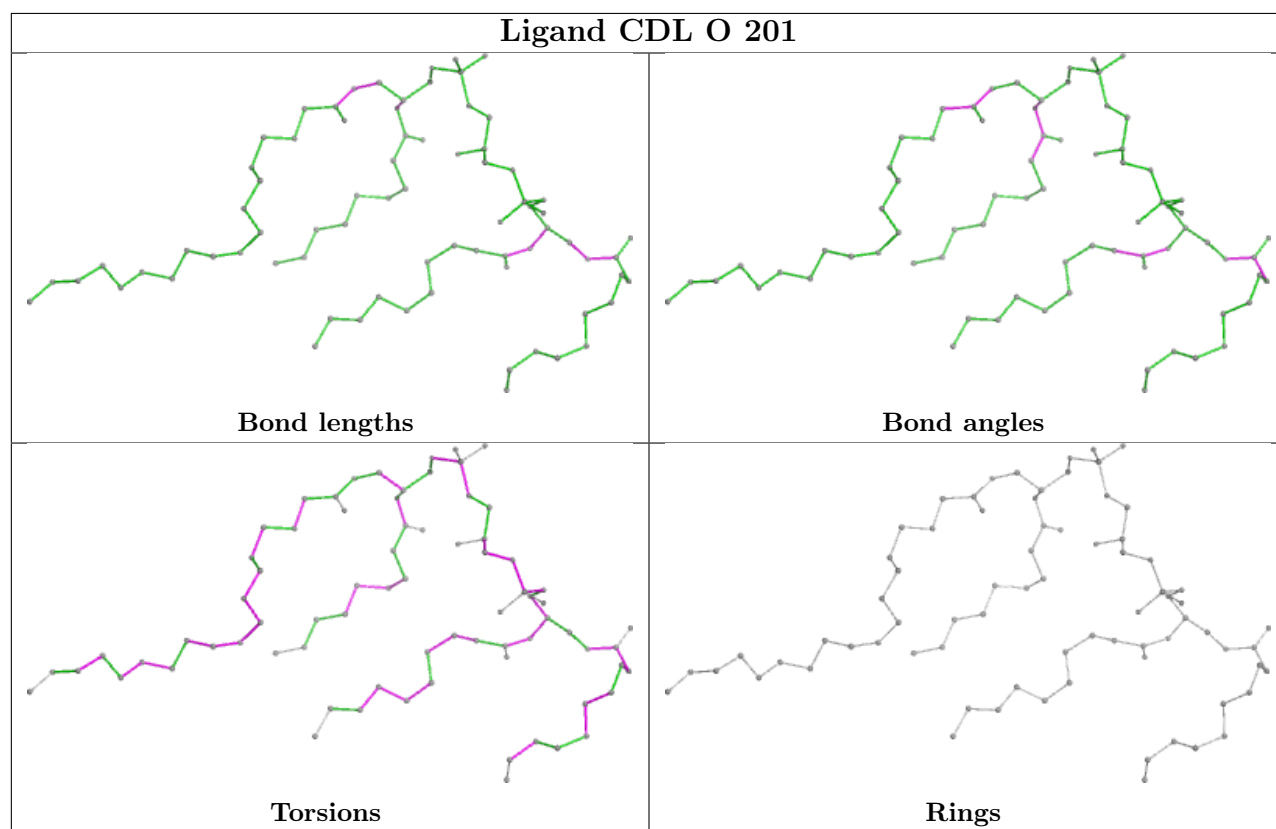
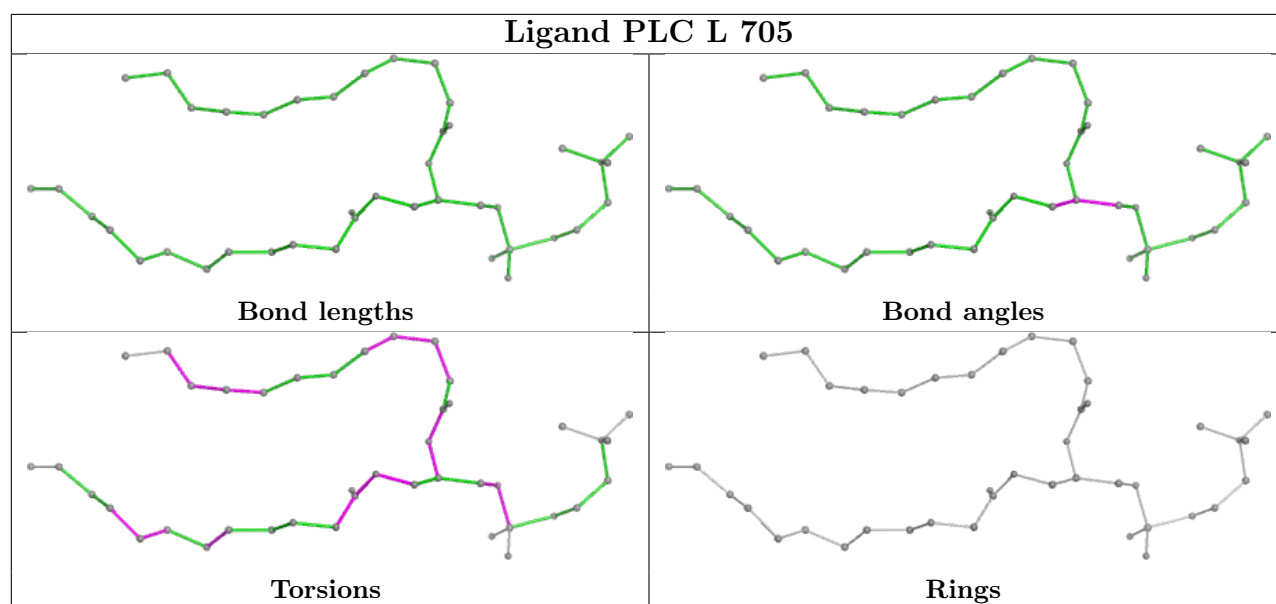


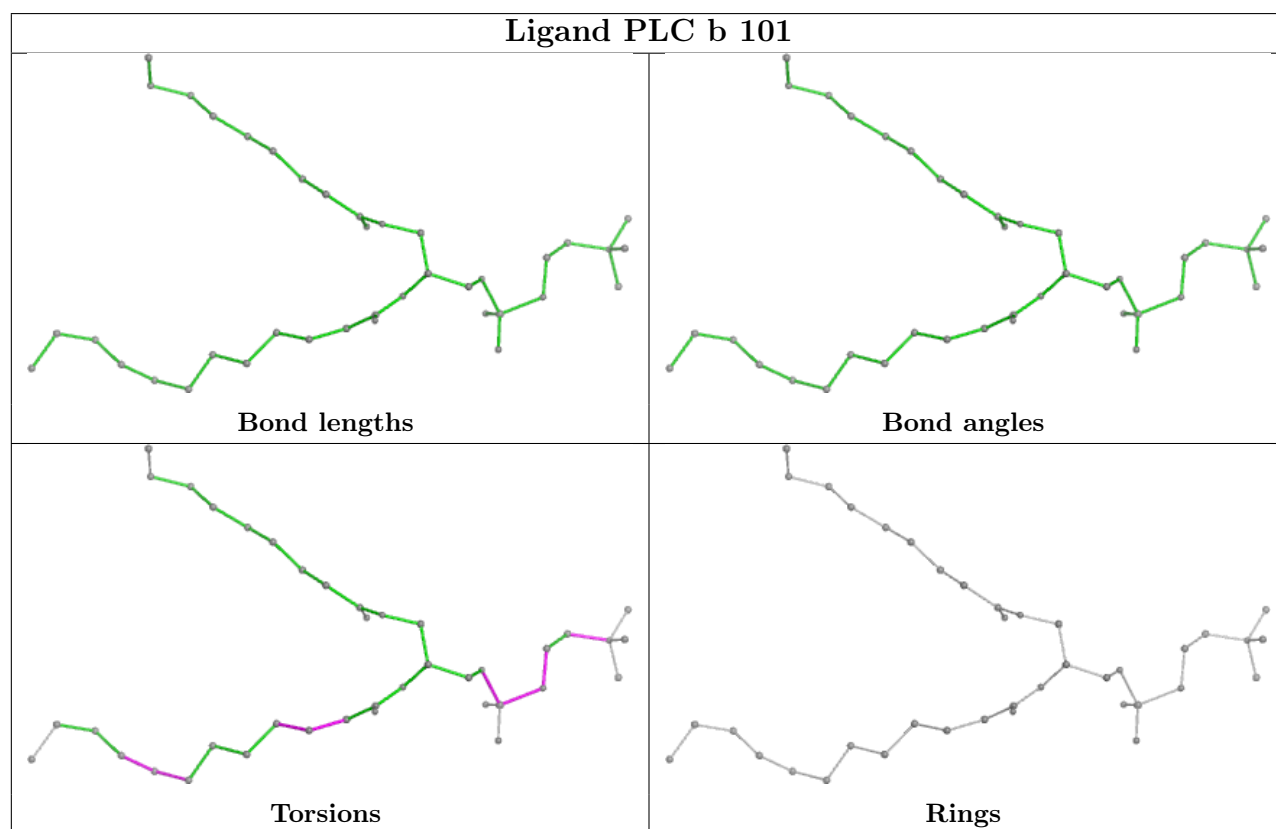
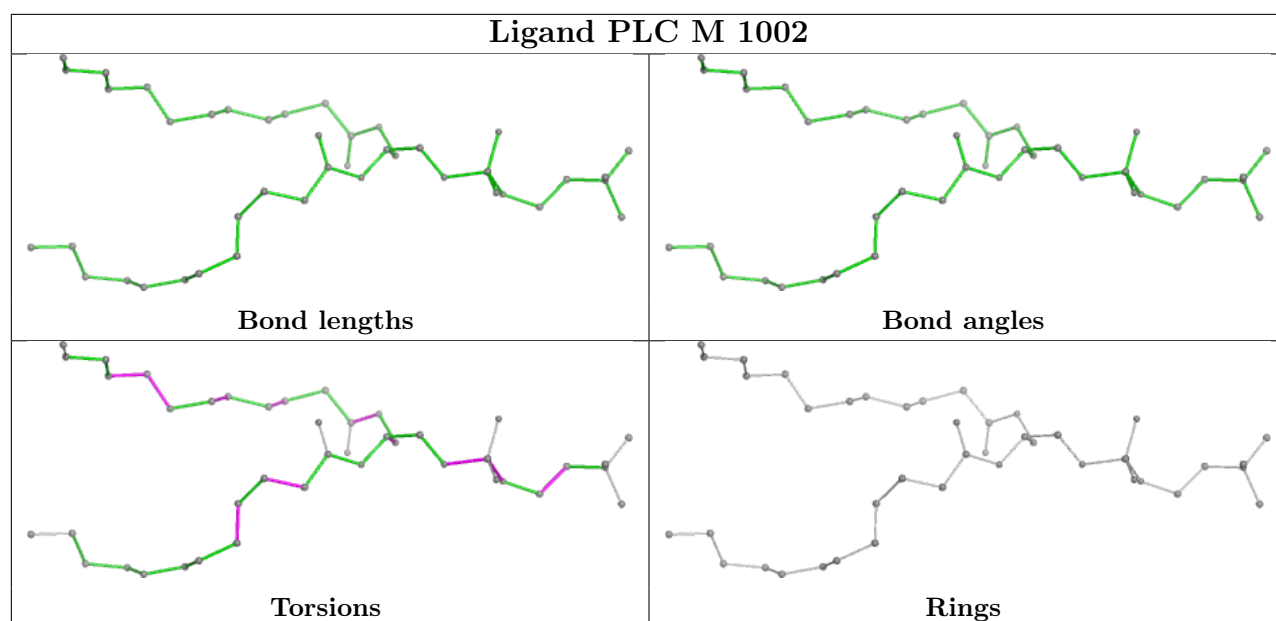




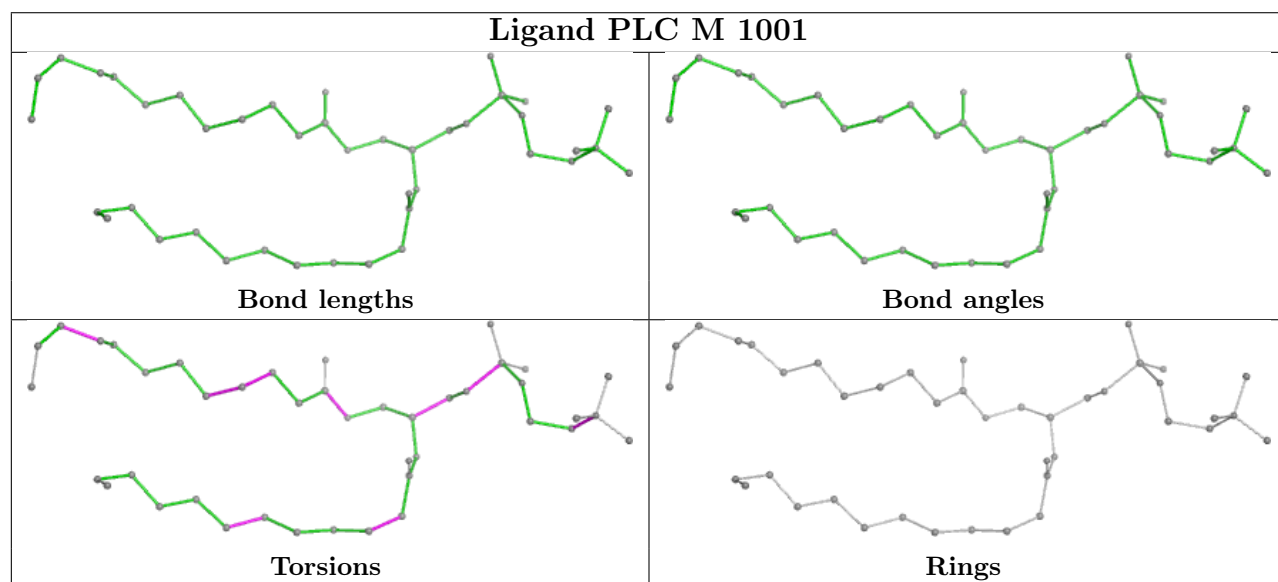
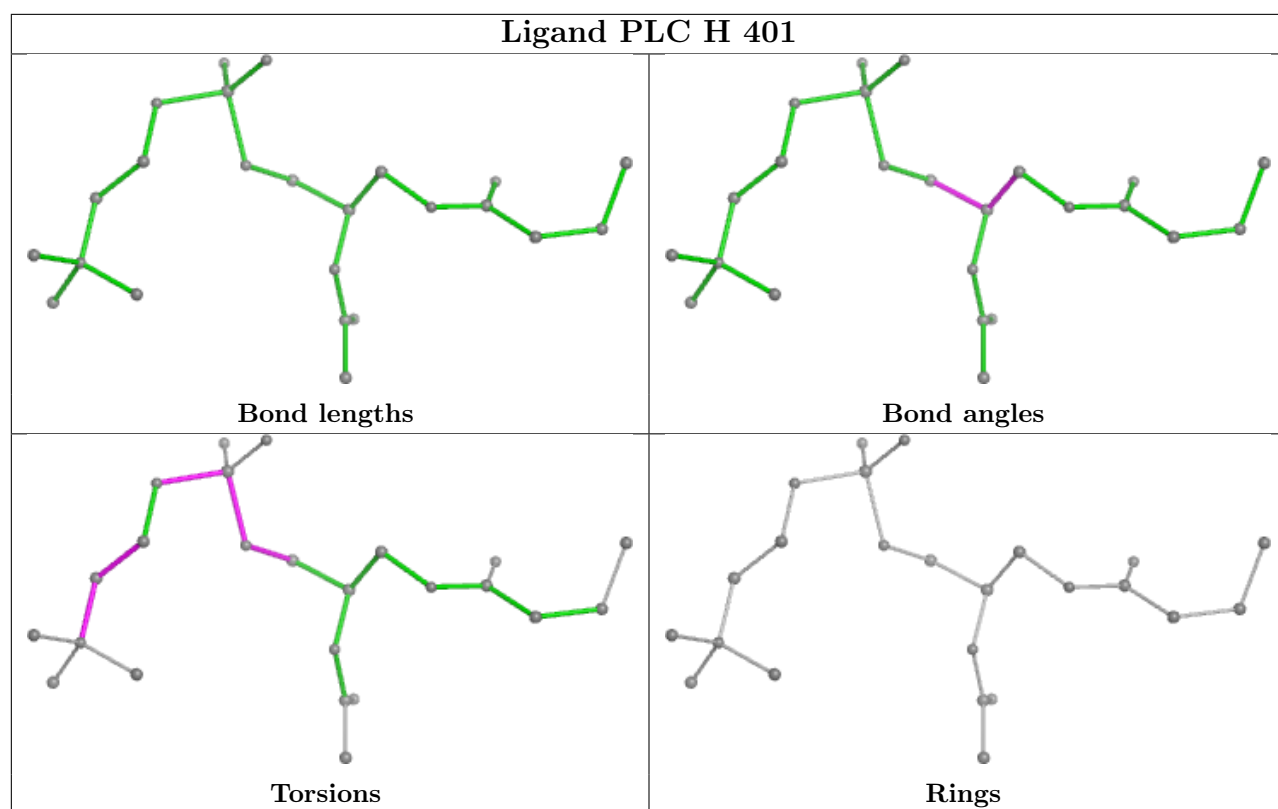


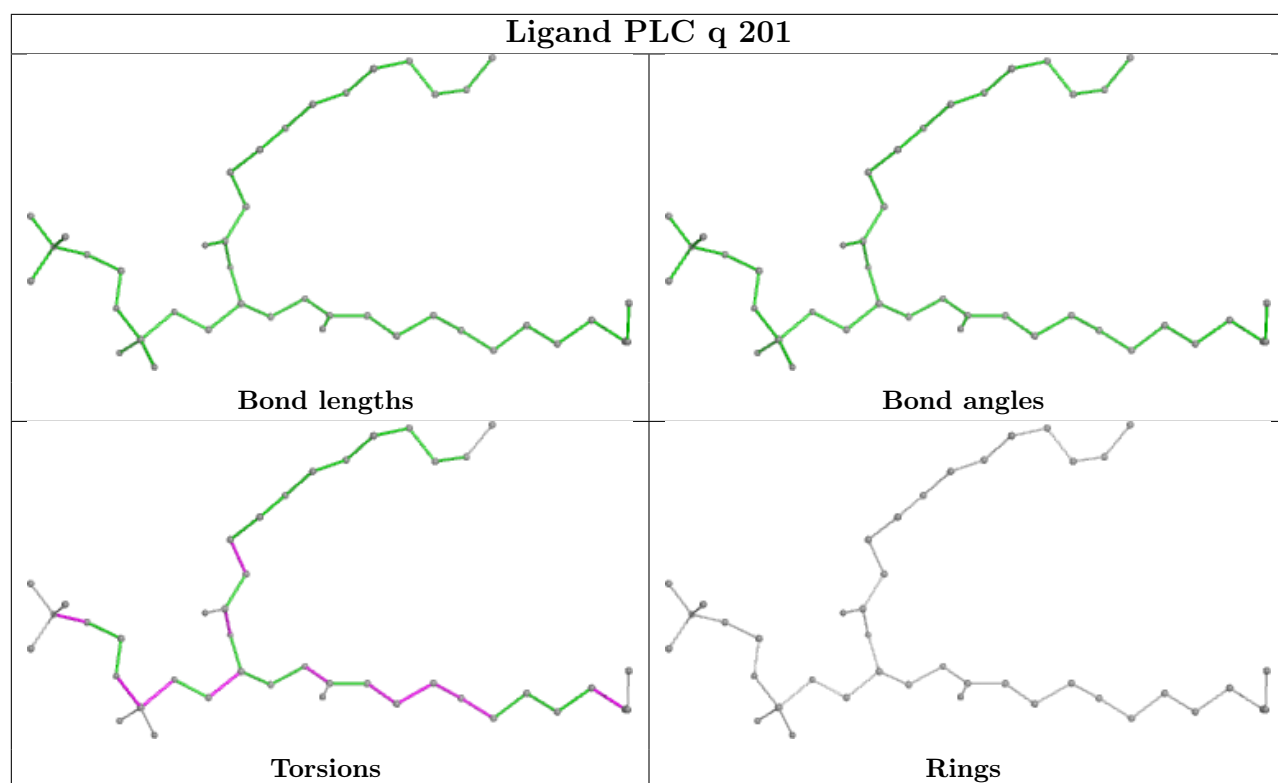


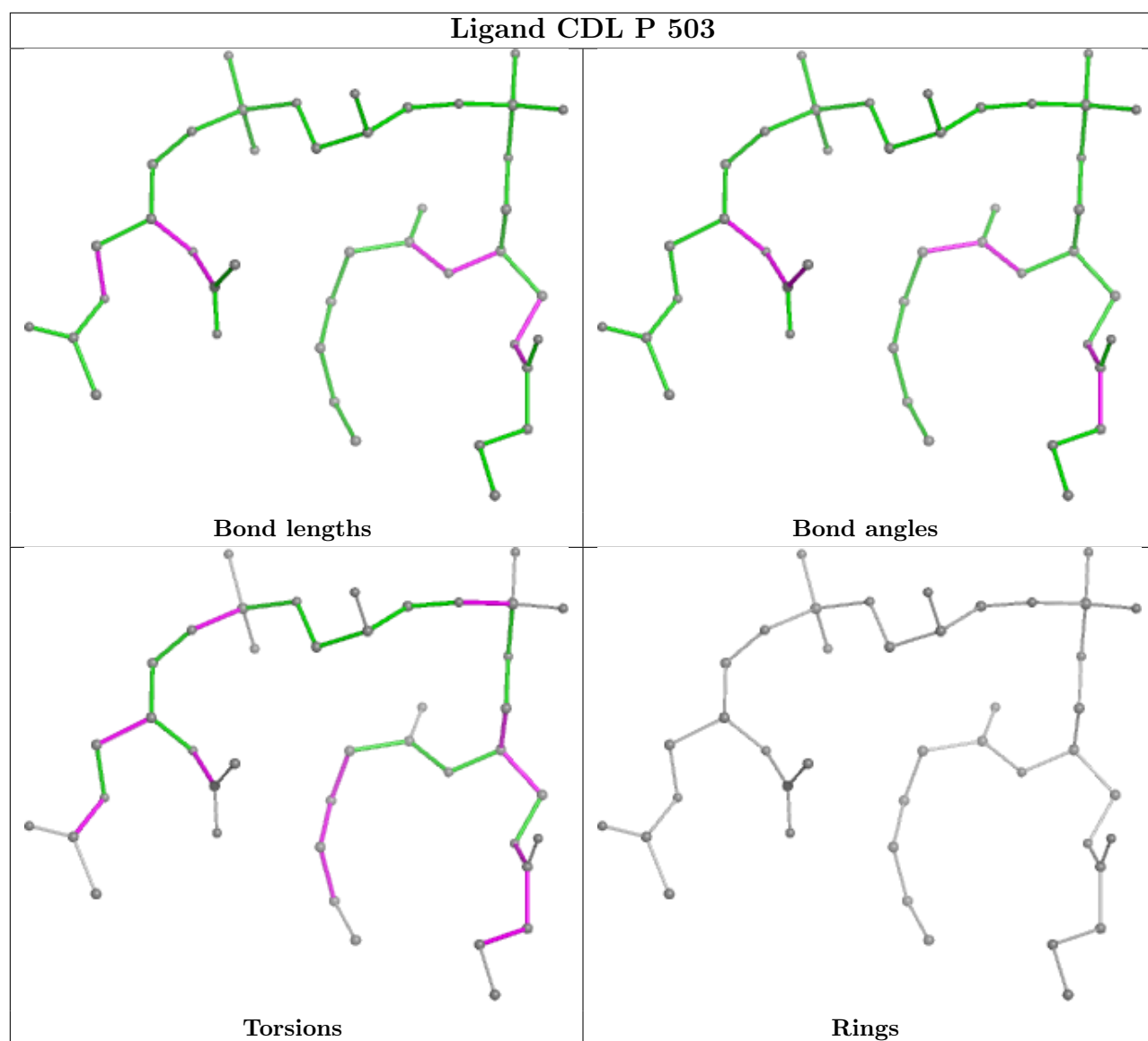


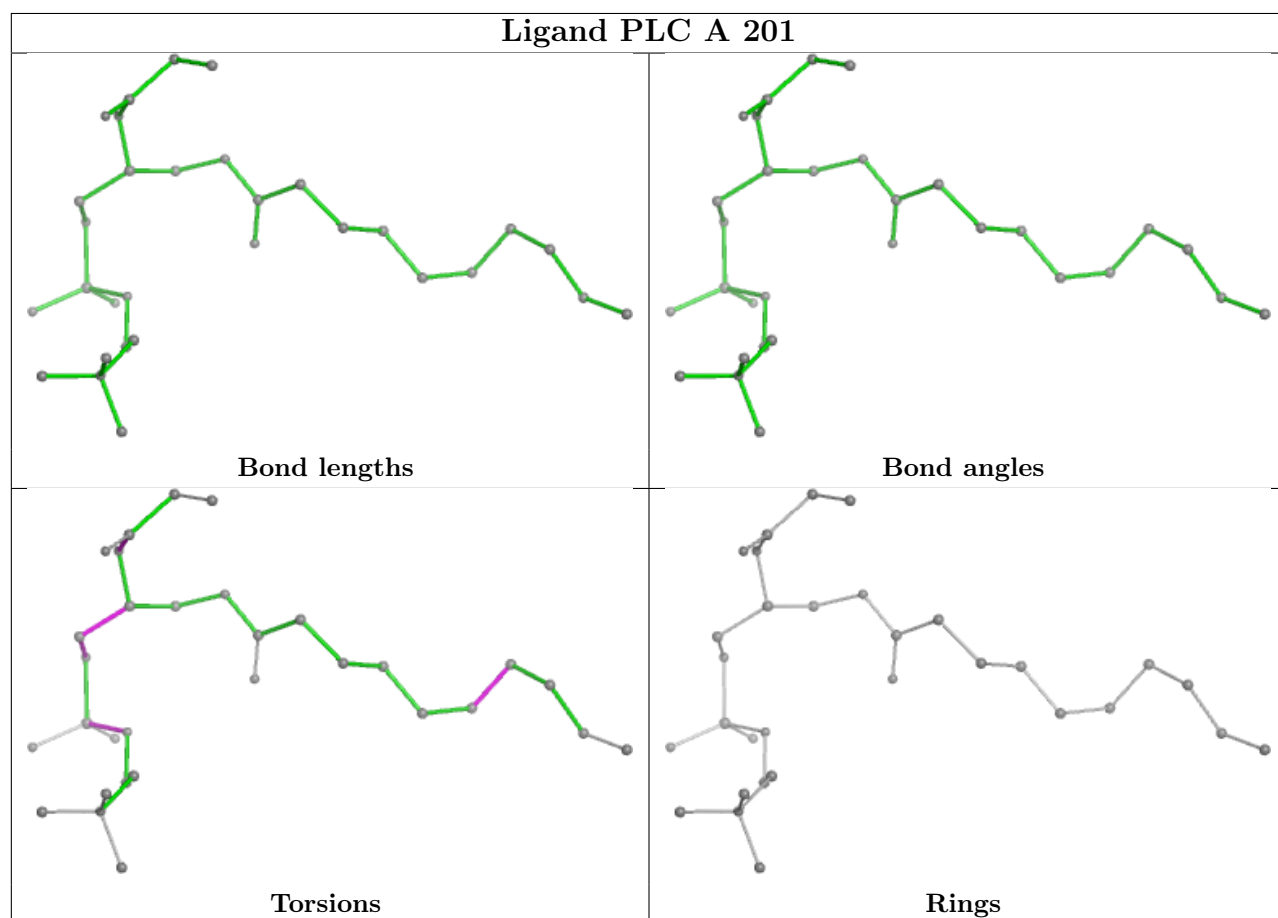
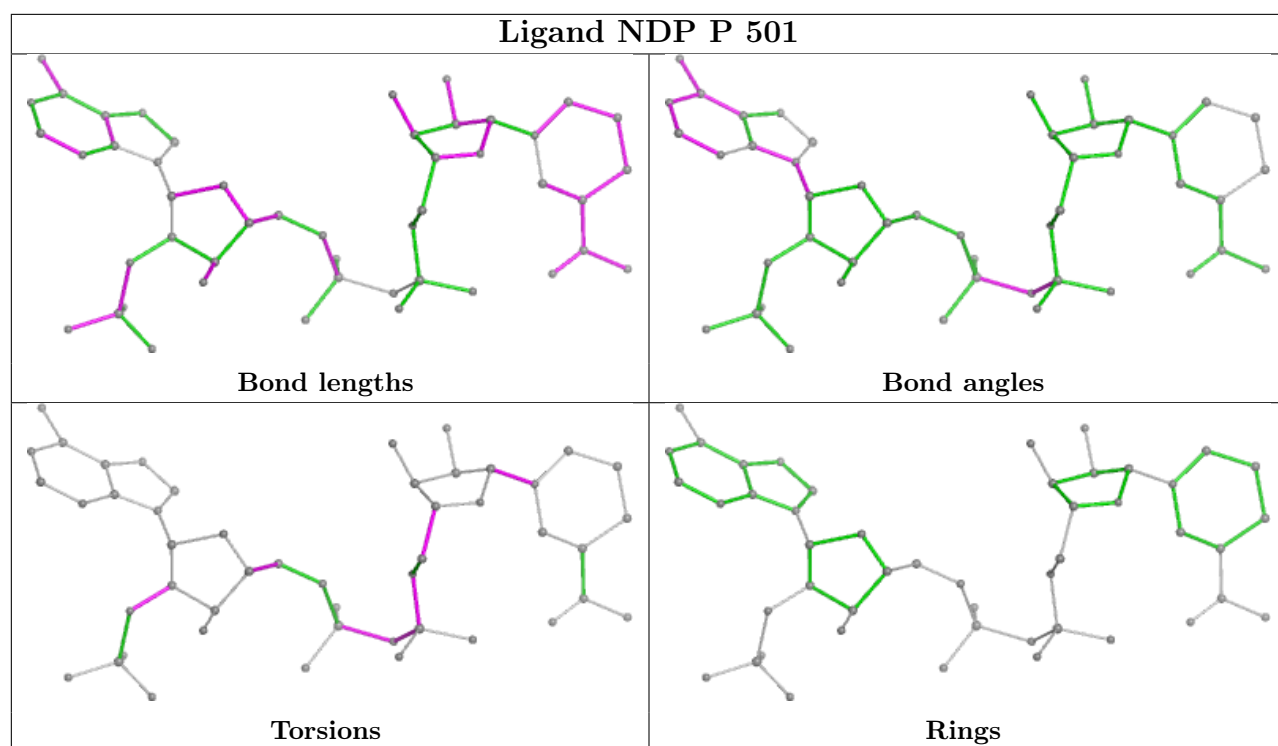




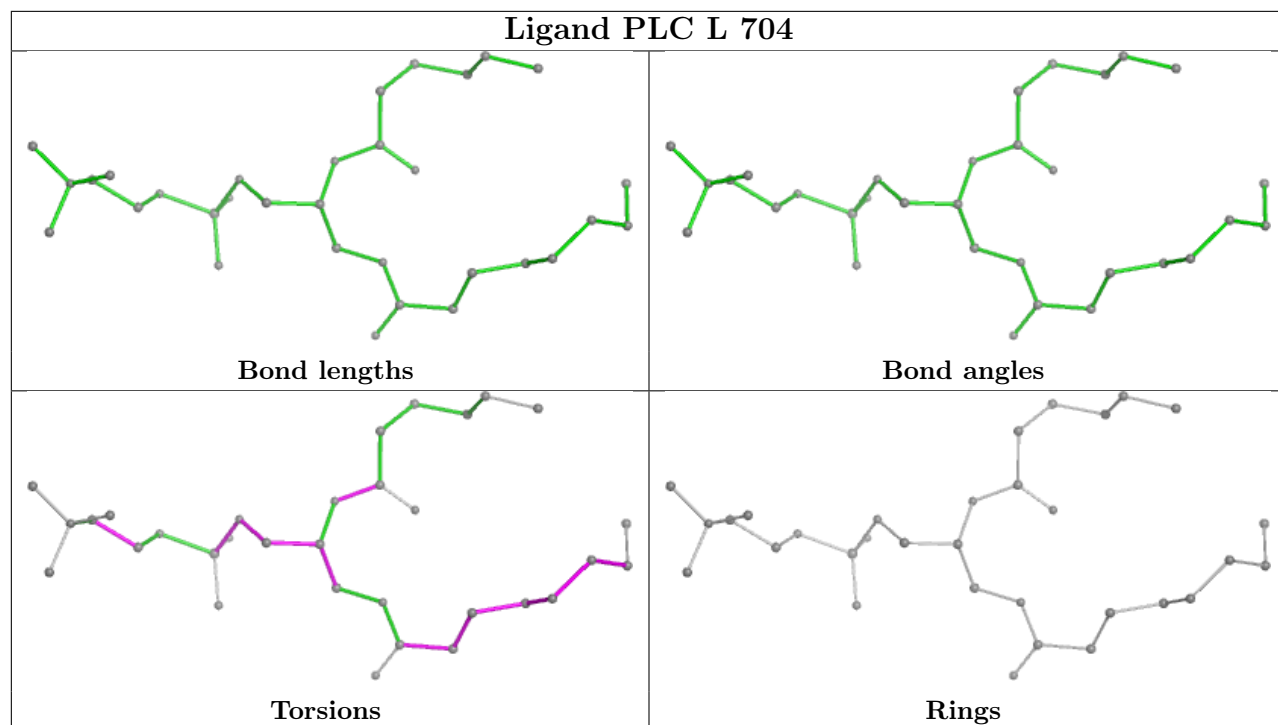




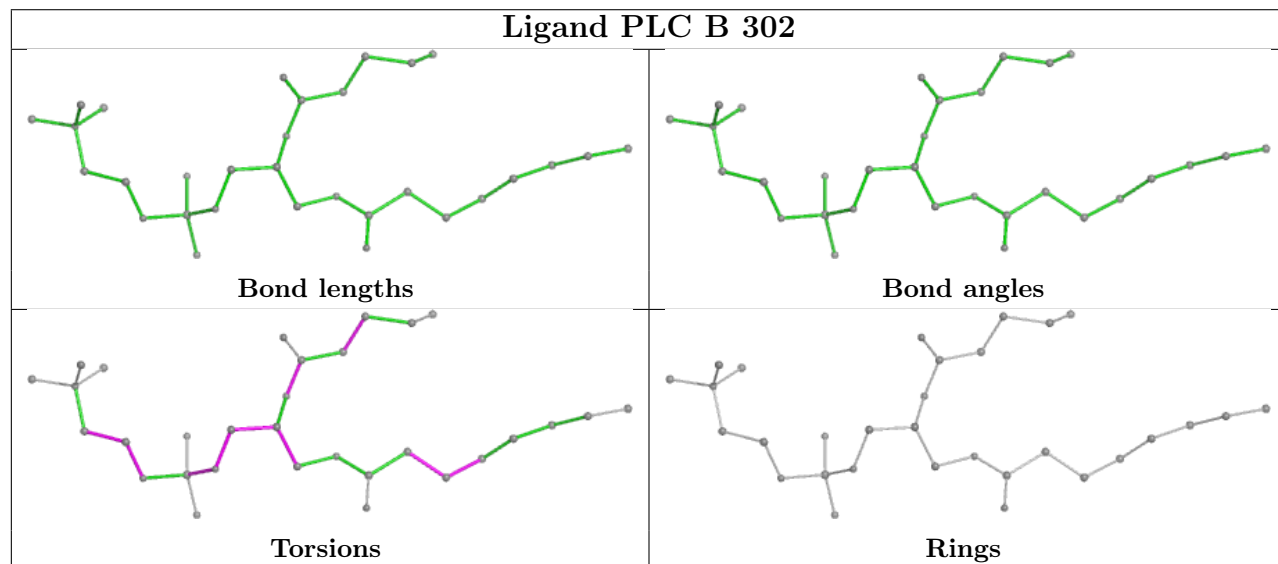


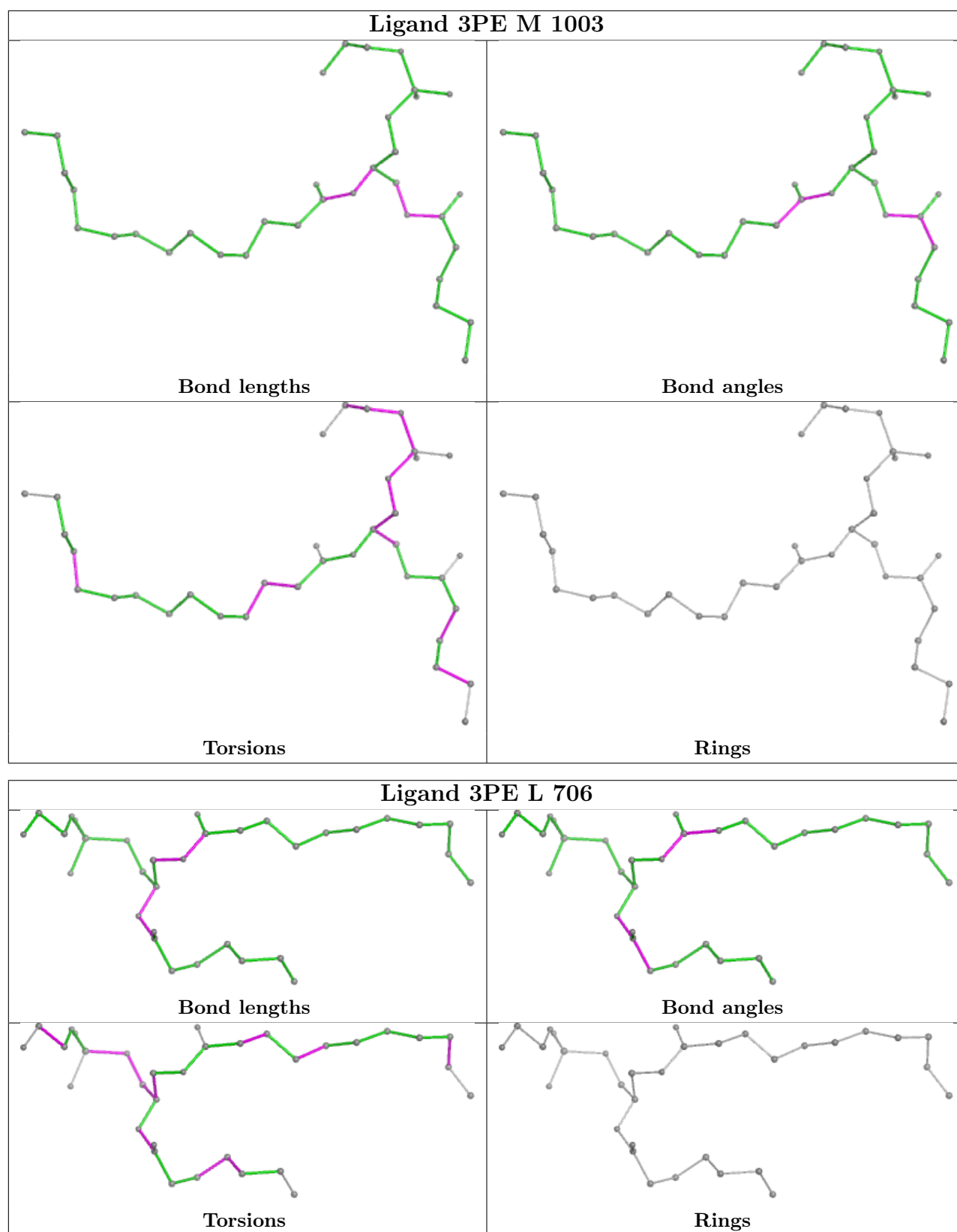


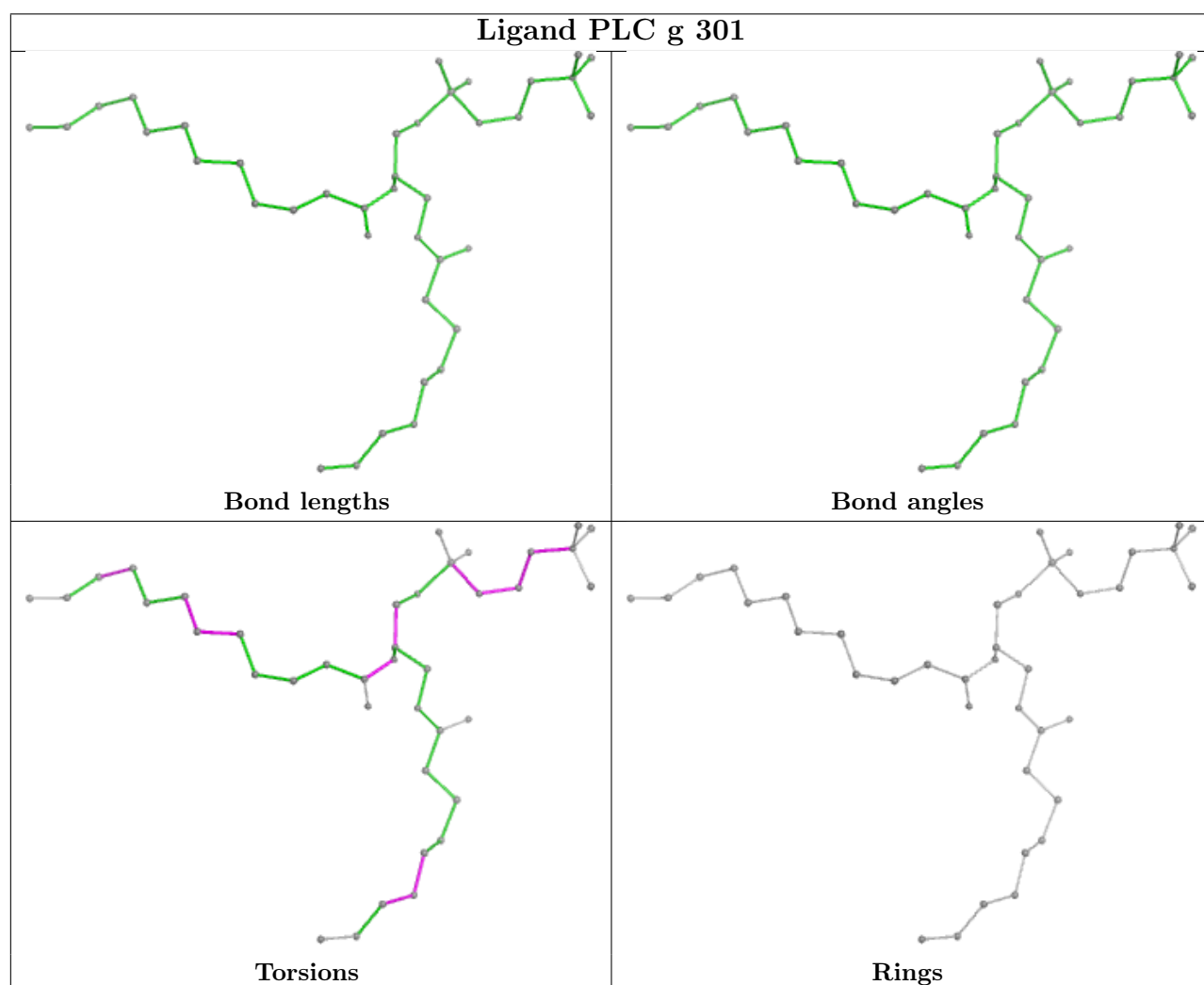
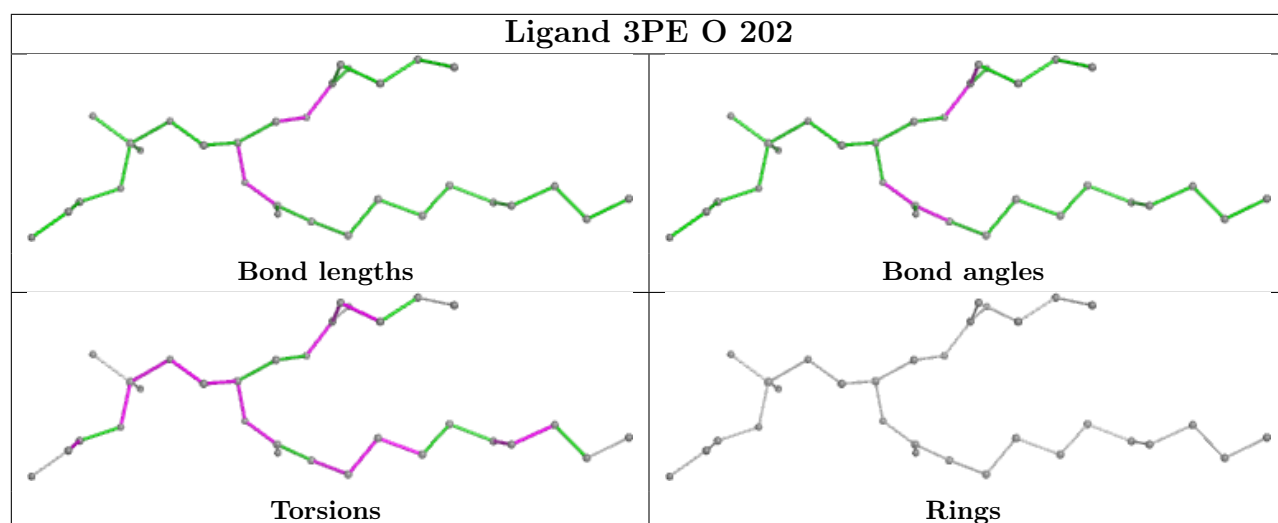
## Ligand PLC L 704

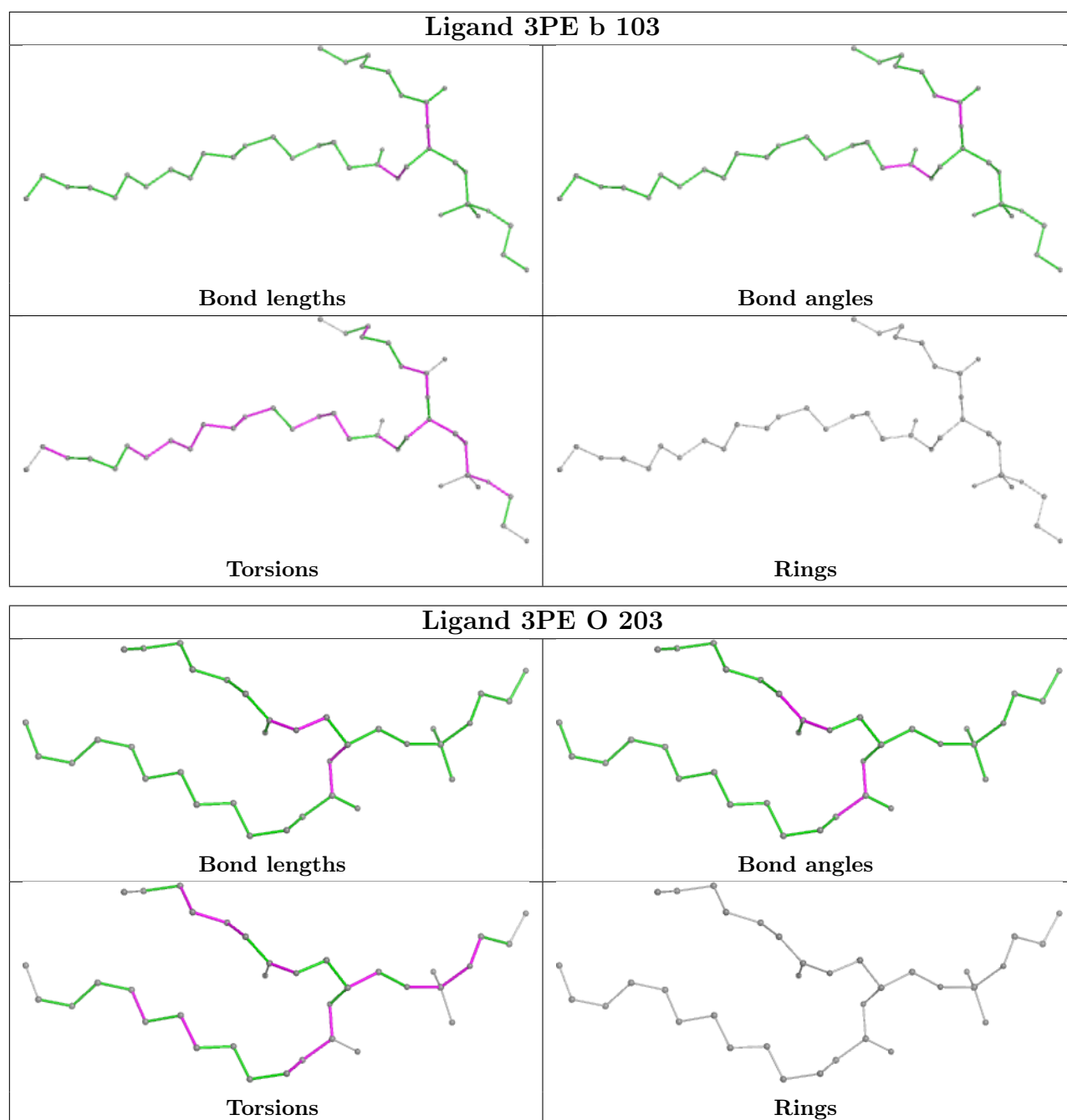


## Ligand PLC B 302

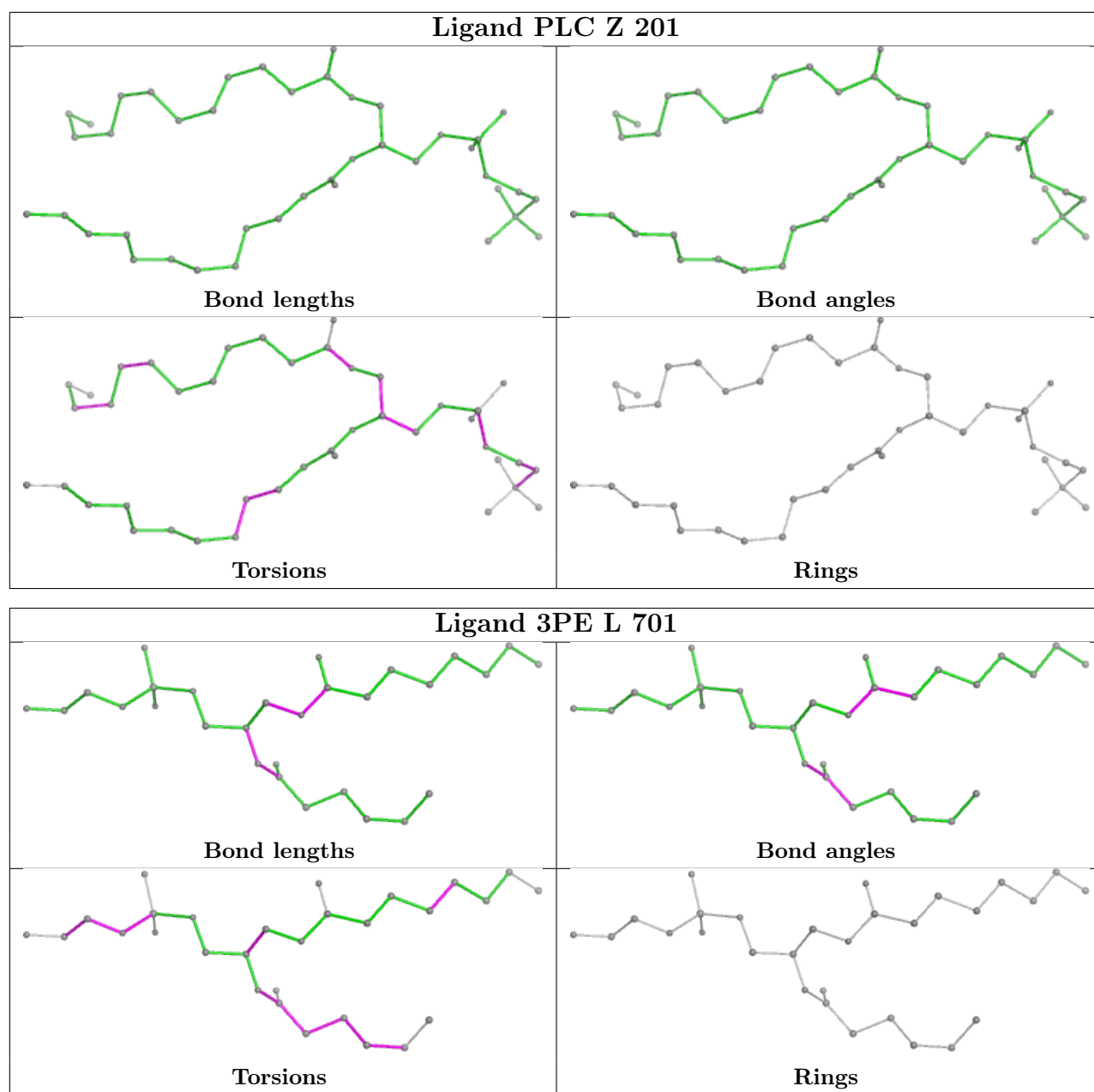


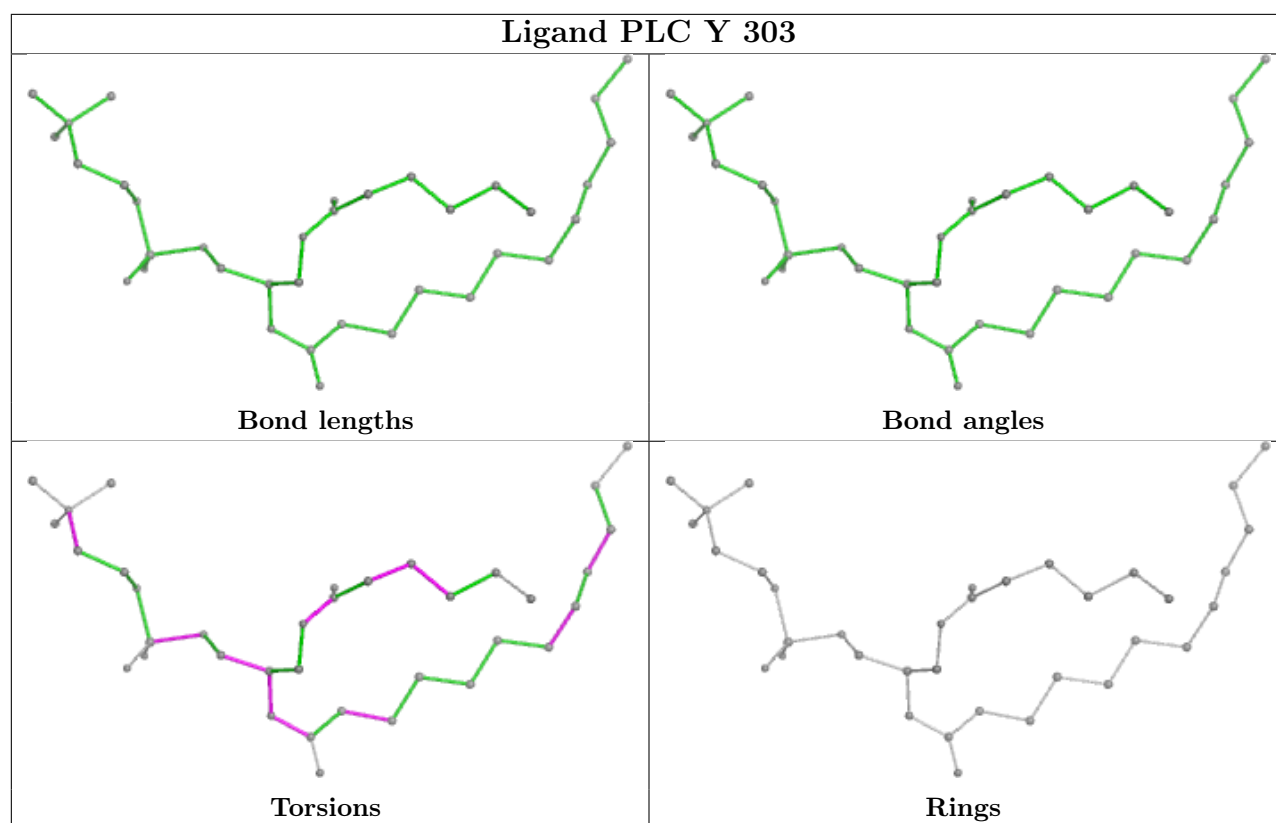












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

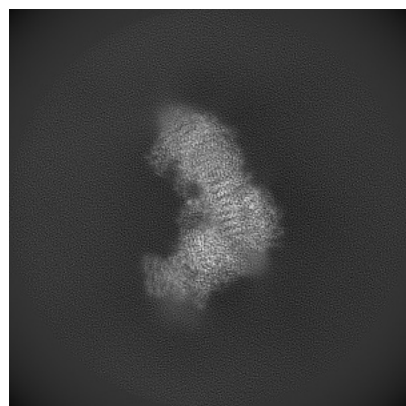
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52877. These allow visual inspection of the internal detail of the map and identification of artifacts.

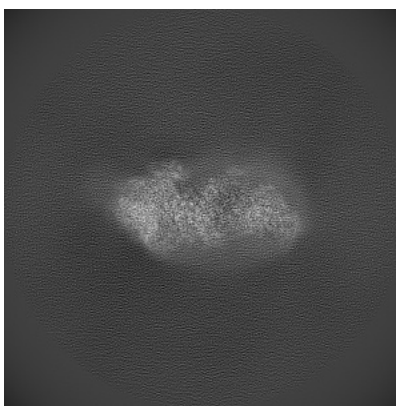
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

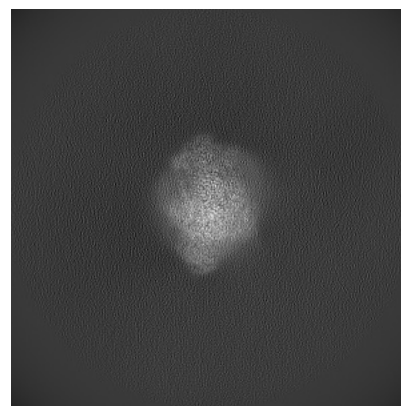
#### 6.1.1 Primary map



X

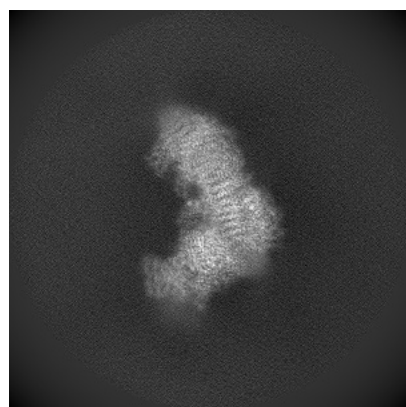


Y

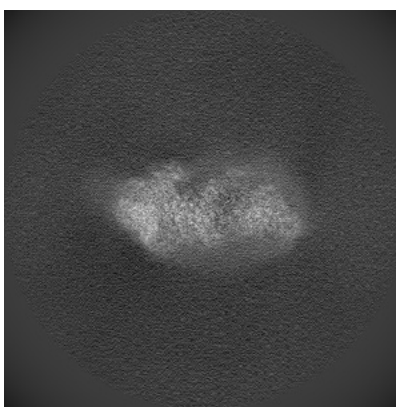


Z

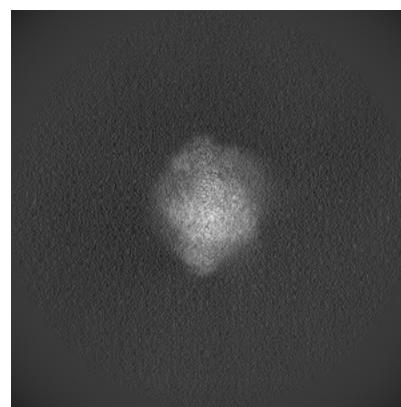
#### 6.1.2 Raw map



X



Y

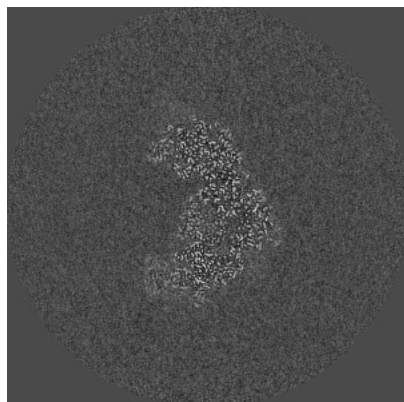


Z

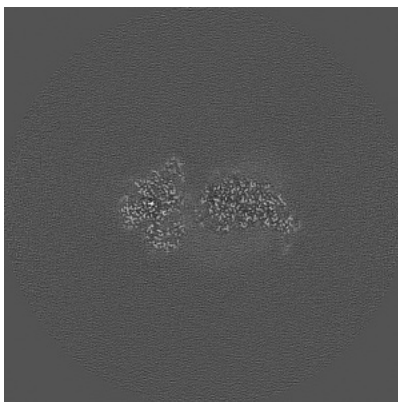
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

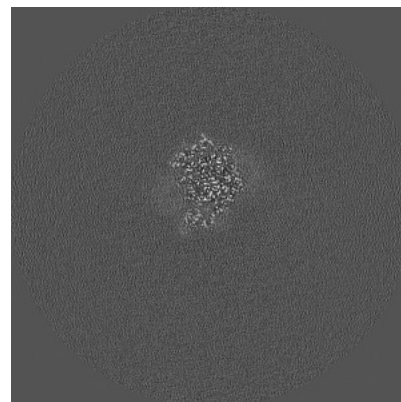
### 6.2.1 Primary map



X Index: 270

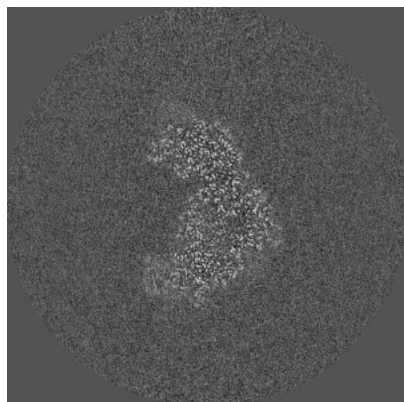


Y Index: 270

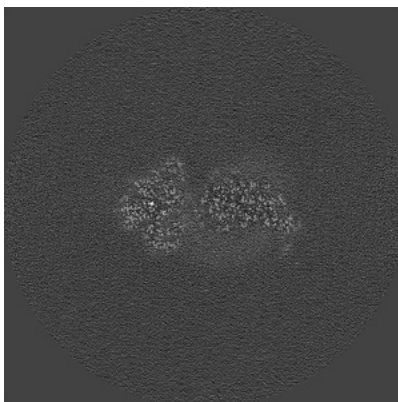


Z Index: 270

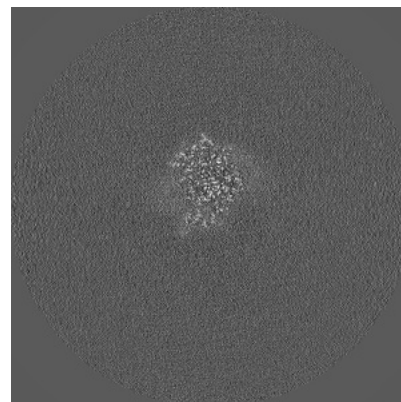
### 6.2.2 Raw map



X Index: 270



Y Index: 270

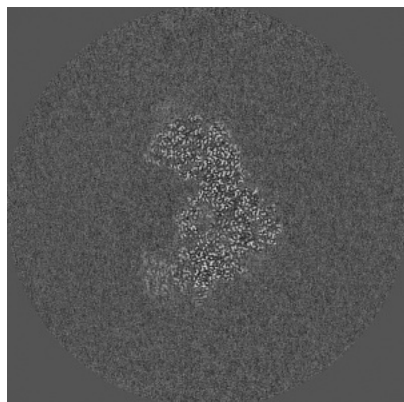


Z Index: 270

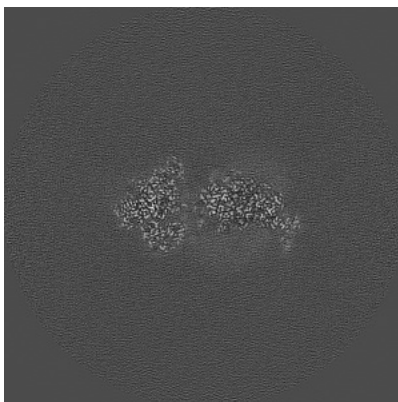
The images above show central slices of the map in three orthogonal directions.

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

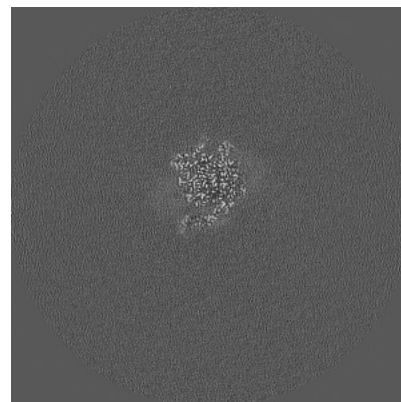
### 6.3.1 Primary map



X Index: 265

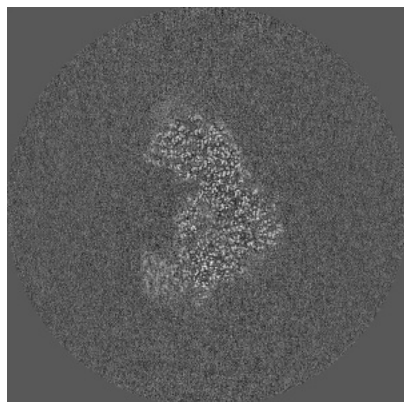


Y Index: 268

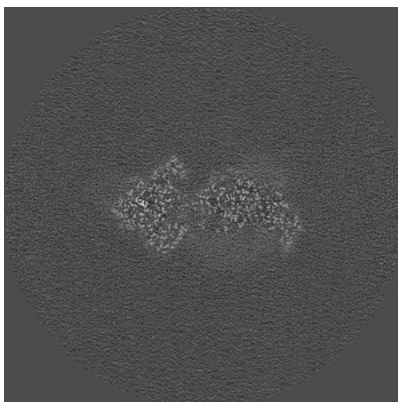


Z Index: 273

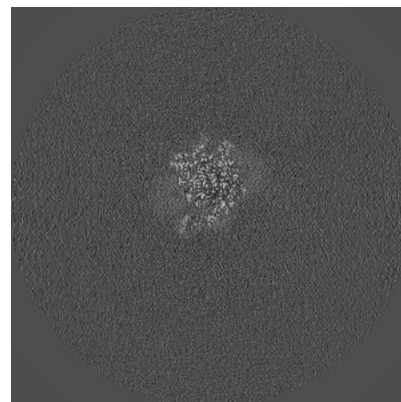
### 6.3.2 Raw map



X Index: 265



Y Index: 266



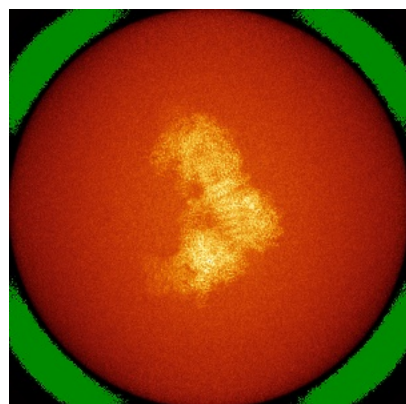
Z Index: 273

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

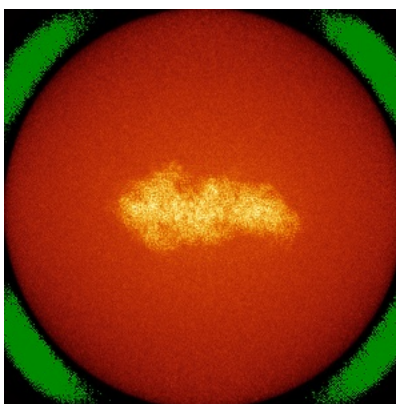


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

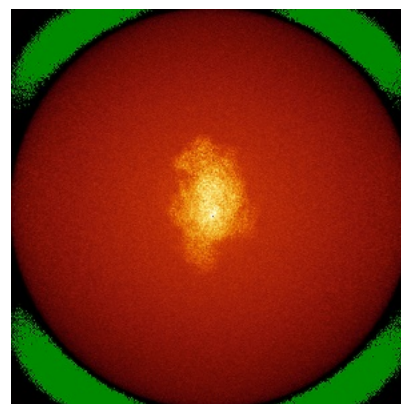
### 6.4.1 Primary map



X

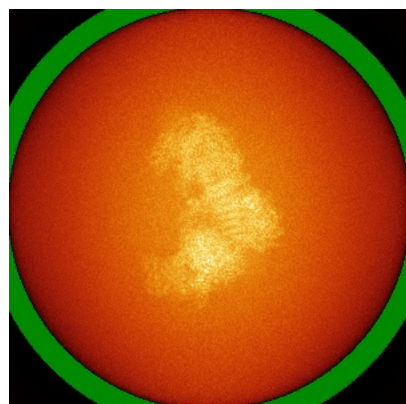


Y

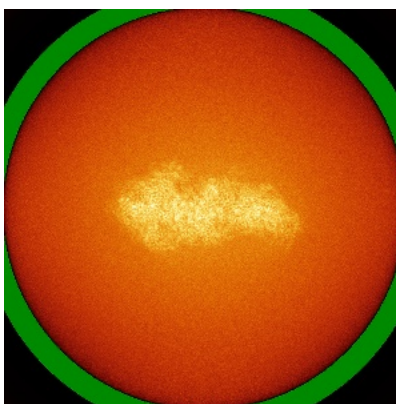


Z

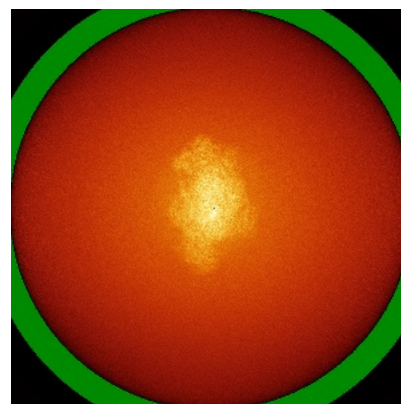
### 6.4.2 Raw map



X



Y

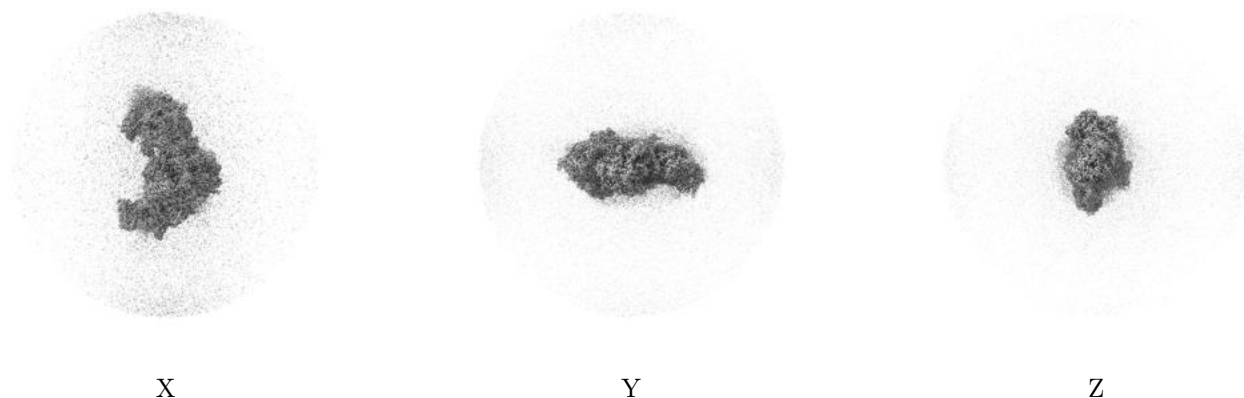


Z

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

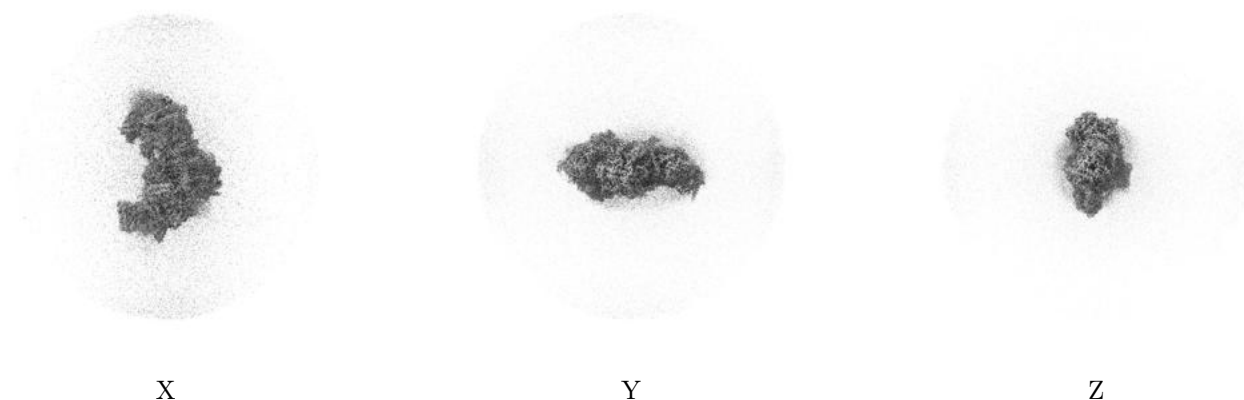
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0127. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

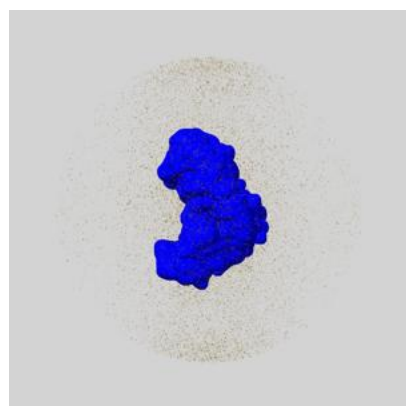
## 6.6 Mask visualisation [i](#)

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

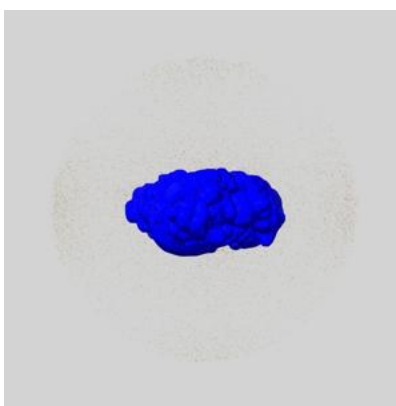
A mask typically either:

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

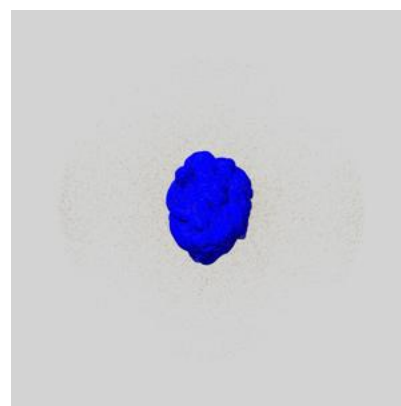
### 6.6.1 emd\_52877\_msk\_1.map [i](#)



X



Y



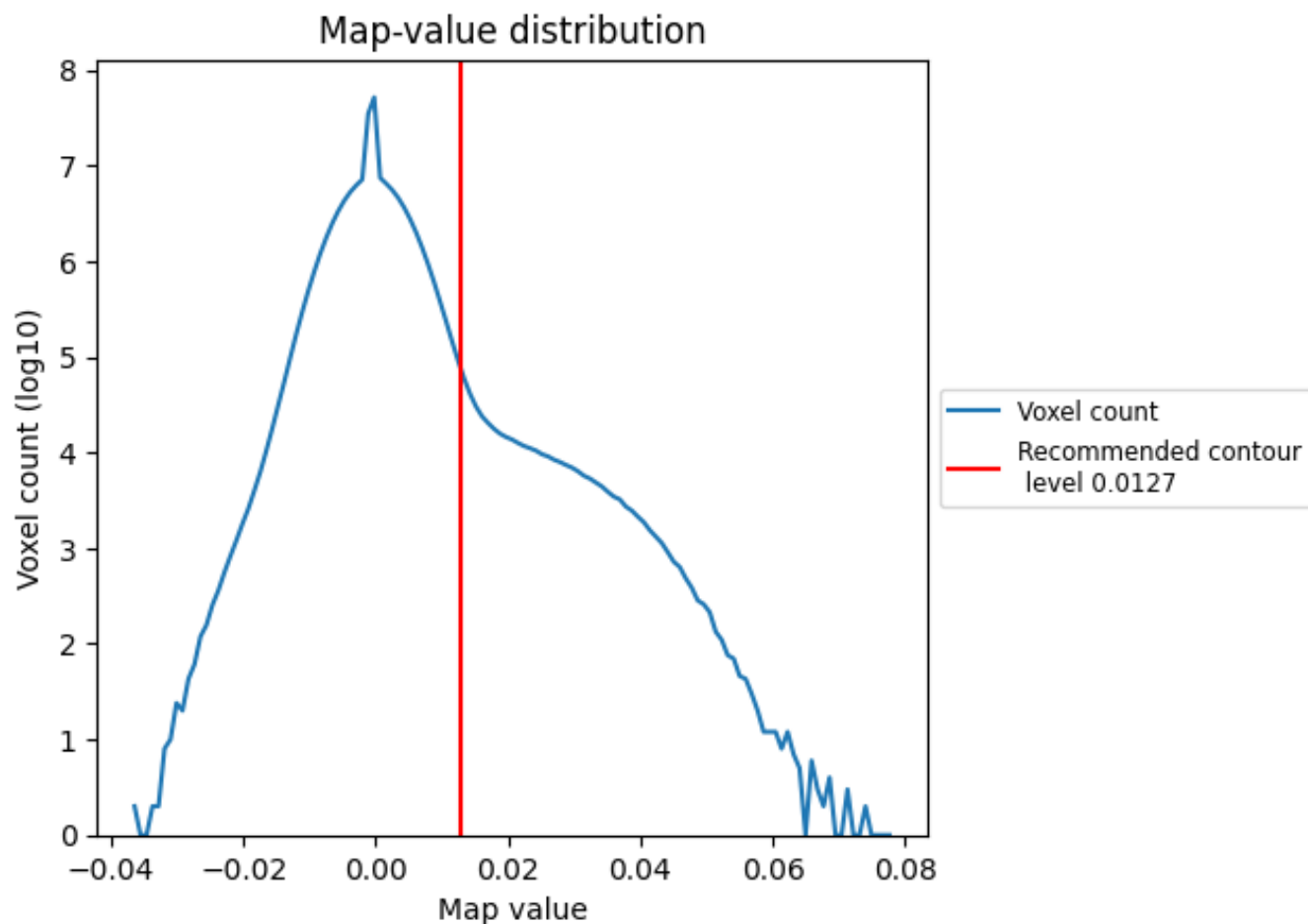
Z



## 7 Map analysis [i](#)

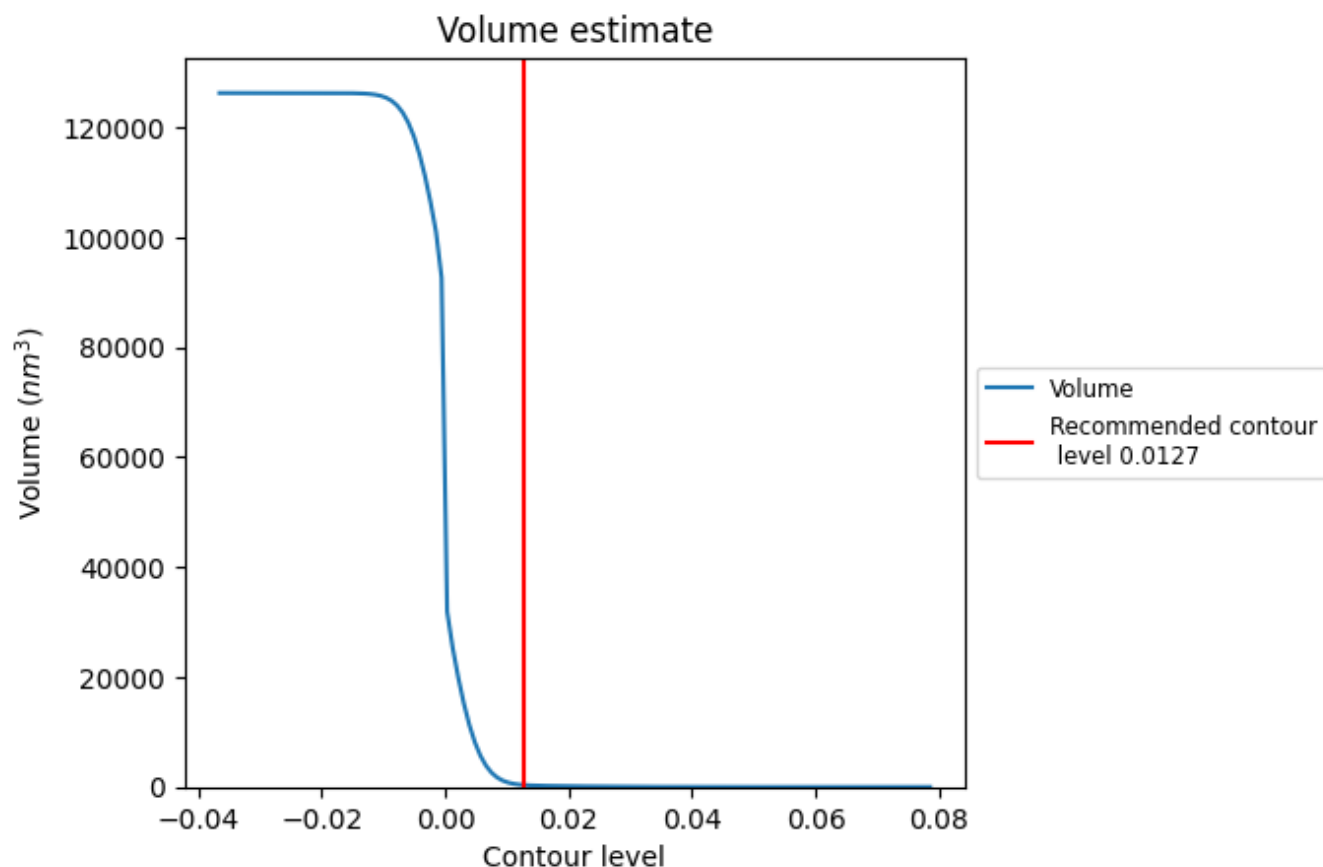
This section contains the results of statistical analysis of the map.

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



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

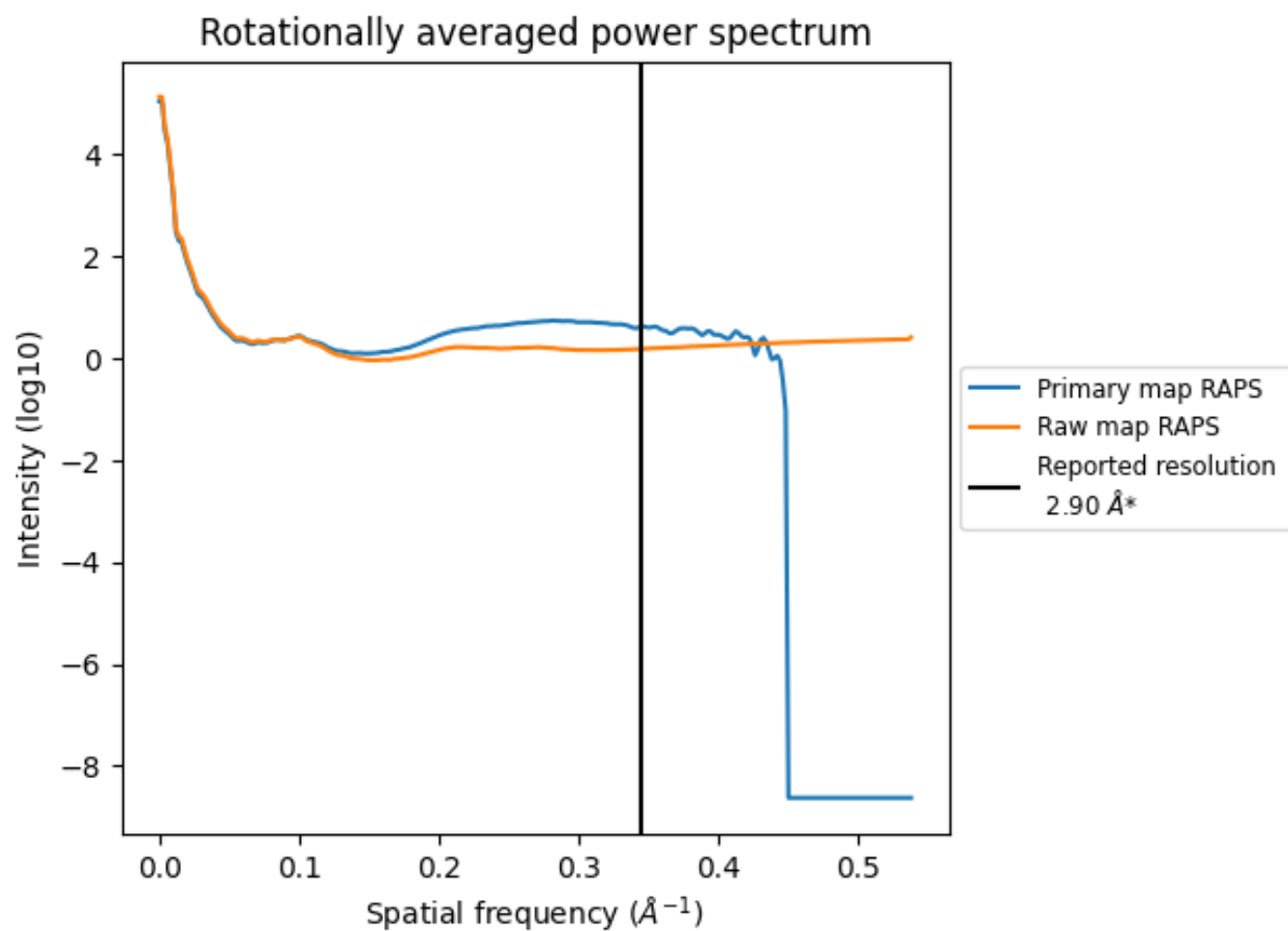
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm<sup>3</sup>; this corresponds to an approximate mass of 327 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

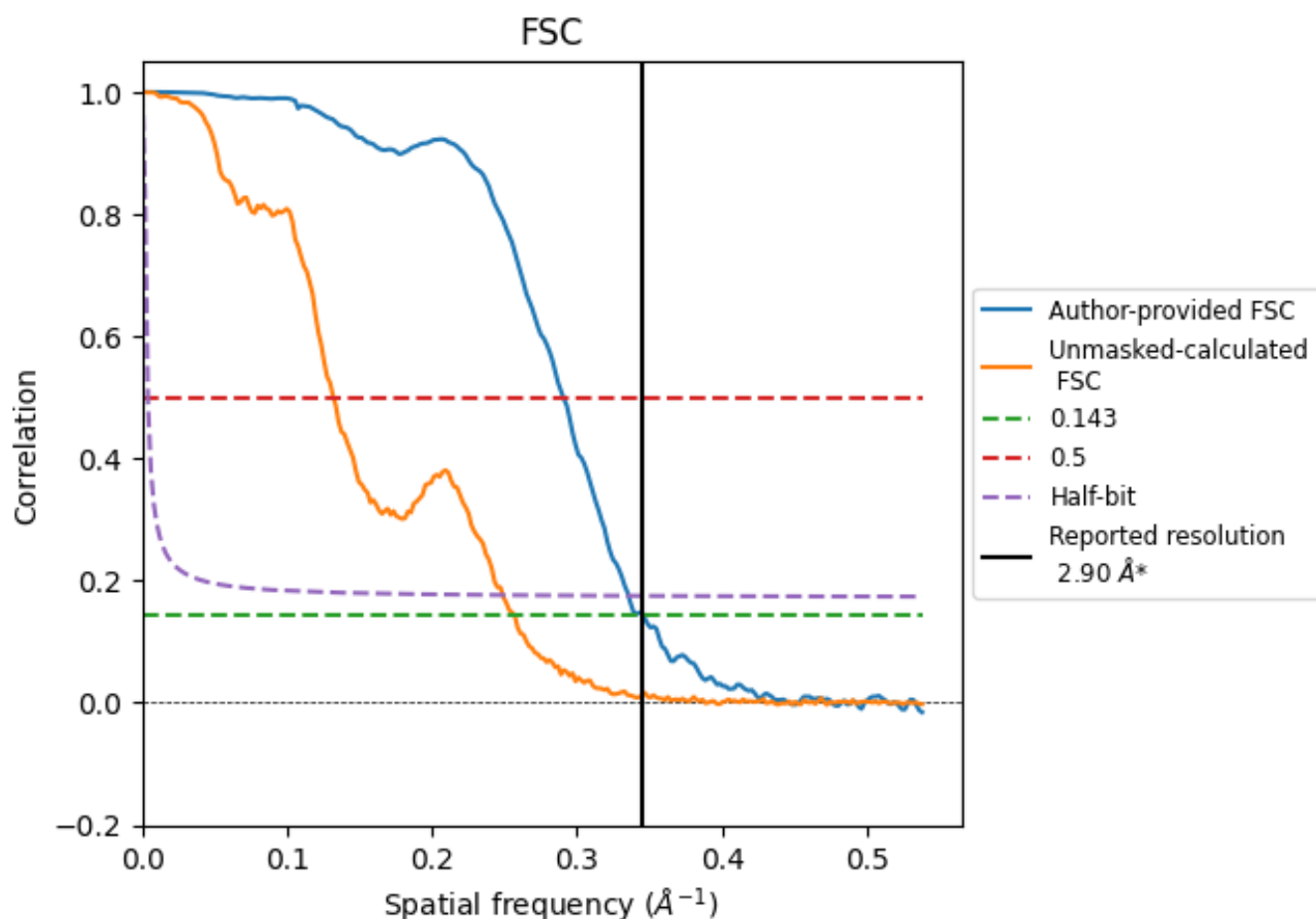


\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

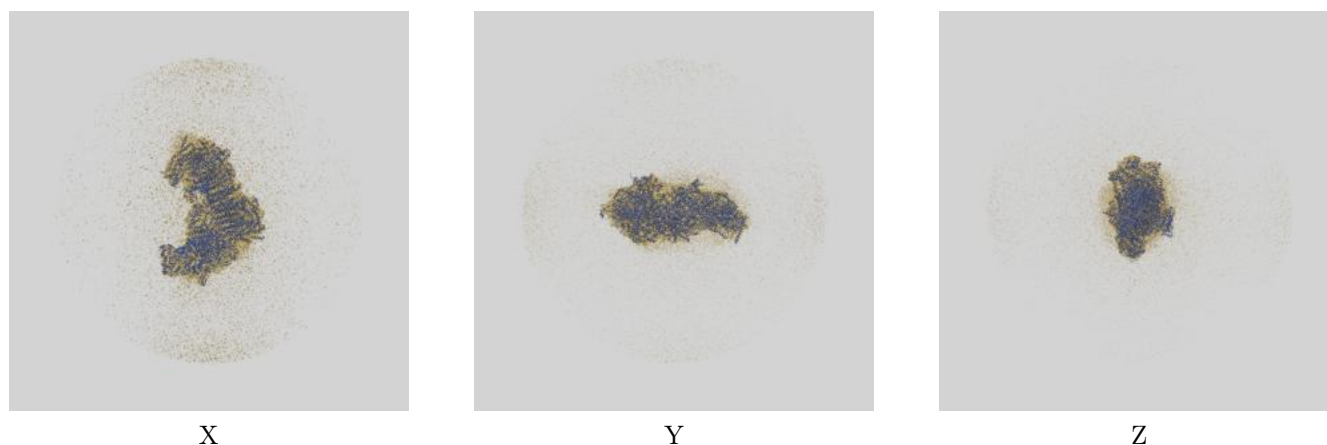
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | 2.89                               | 3.44 | 2.98     |
| Unmasked-calculated*      | 3.89                               | 7.58 | 4.02     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 2.9 by more than 10 %

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

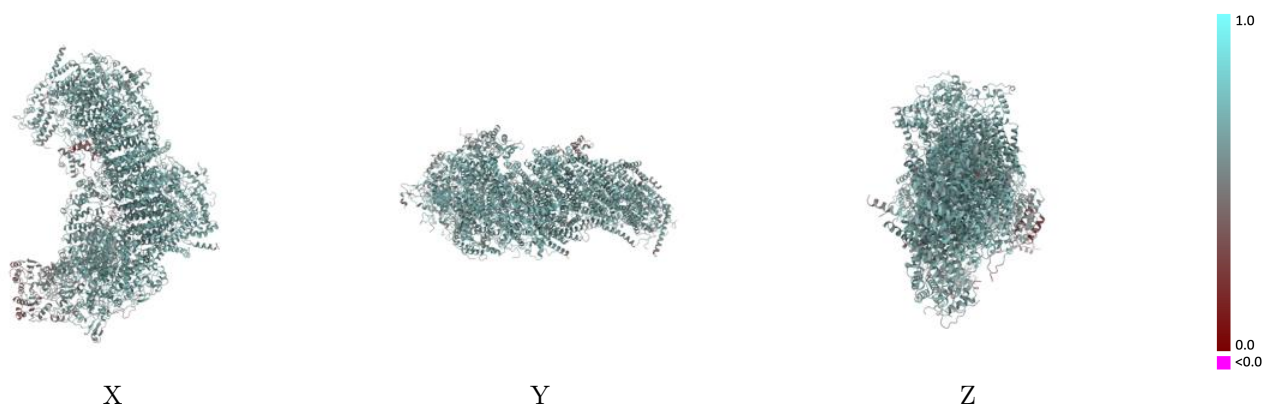
This section contains information regarding the fit between EMDB map EMD-52877 and PDB model 9IHQ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



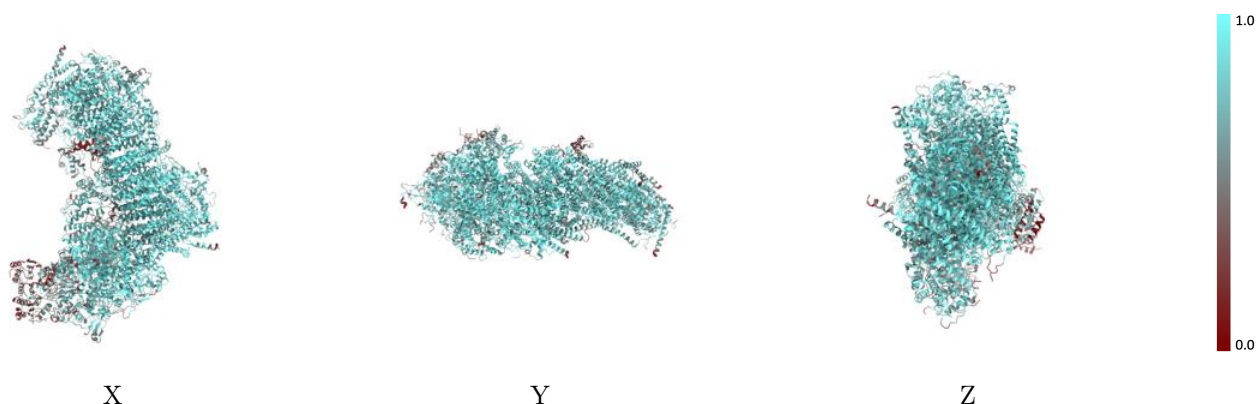
The images above show the 3D surface view of the map at the recommended contour level 0.0127 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



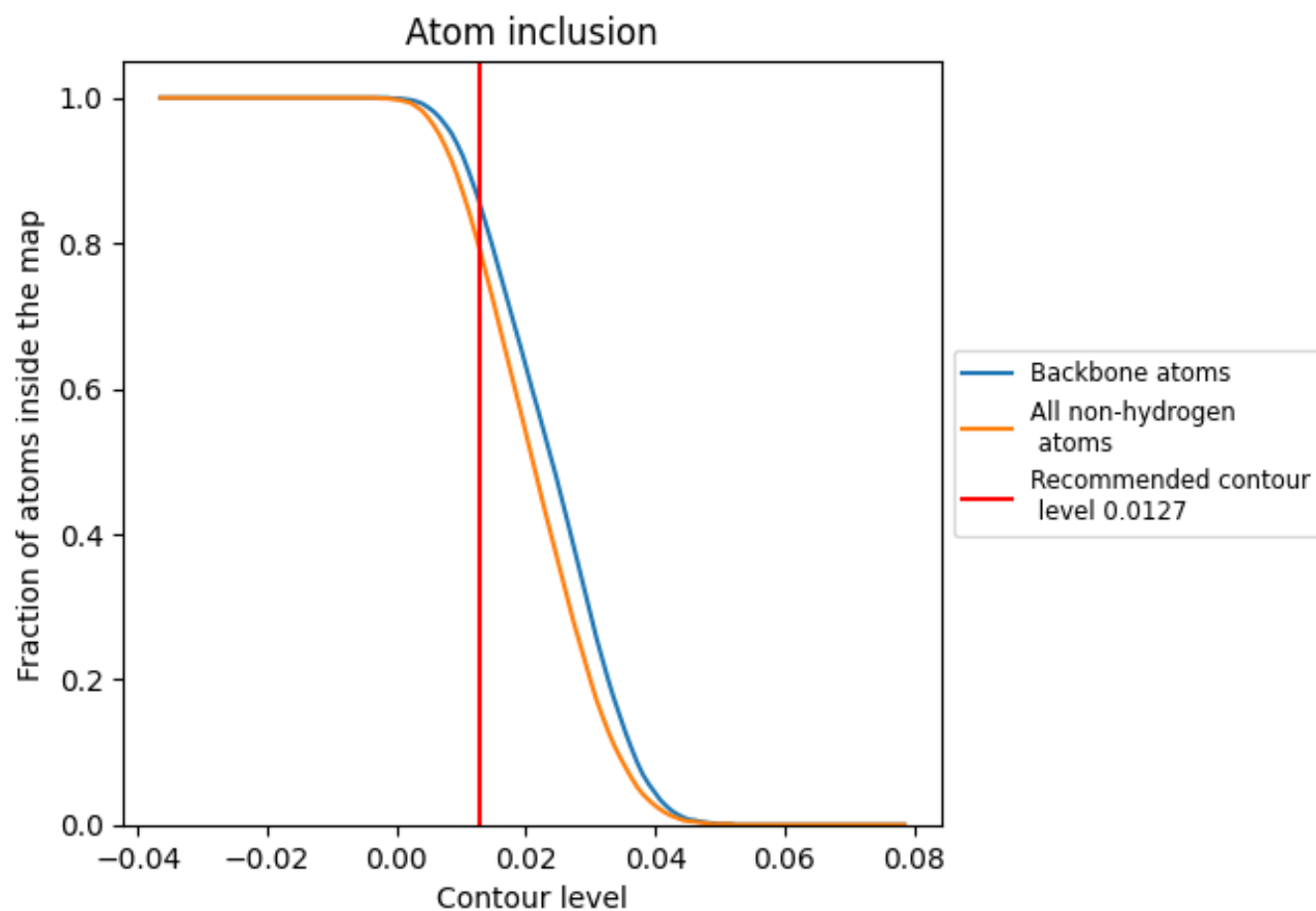
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0127).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.0127) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7970   |  0.6120   |
| 1     |  0.6520   |  0.5430   |
| A     |  0.8100   |  0.6270   |
| B     |  0.9030   |  0.6560   |
| C     |  0.7930   |  0.6130   |
| D     |  0.8920   |  0.6470   |
| G     |  0.5550   |  0.5120   |
| H     |  0.8610   |  0.6410   |
| I     |  0.8850   |  0.6480   |
| J     |  0.8140   |  0.6110   |
| K     |  0.8420   |  0.6450   |
| L     |  0.8630   |  0.6400   |
| M     |  0.9140   |  0.6600   |
| N     |  0.9080   |  0.6560   |
| O     |  0.8180  |  0.6270  |
| P     |  0.8140 |  0.6120 |
| Q     |  0.7960 |  0.6070 |
| R     |  0.6990 |  0.5680 |
| S     |  0.2940 |  0.4080 |
| T     |  0.7420 |  0.5970 |
| U     |  0.6550 |  0.5540 |
| V     |  0.7450 |  0.5850 |
| W     |  0.8380 |  0.6240 |
| X     |  0.8630 |  0.6360 |
| Y     |  0.8080 |  0.6260 |
| Z     |  0.8530 |  0.6320 |
| a     |  0.8670 |  0.6420 |
| b     |  0.8040 |  0.6300 |
| c     |  0.6010 |  0.5480 |
| d     |  0.8540 |  0.6430 |
| e     |  0.8660 |  0.6450 |
| f     |  0.7960 |  0.6140 |
| g     |  0.5330 |  0.5200 |
| h     |  0.7790 |  0.6030 |
| i     |  0.7290 |  0.5810 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| j     |  0.6740 |  0.5720 |
| k     |  0.7290 |  0.5730 |
| l     |  0.8180 |  0.6140 |
| m     |  0.7920 |  0.6150 |
| n     |  0.7450 |  0.5780 |
| o     |  0.7640 |  0.5900 |
| p     |  0.8770 |  0.6420 |
| q     |  0.8210 |  0.6170 |