



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:05 PM UTC

PDB ID : 9IHO / pdb\_00009iho  
EMDB ID : EMD-52875  
Title : Open state without NUQM and without flavoprotein (classification state 4) of Pichia pastoris mitochondrial complex I in cMSP26 nanodiscs  
Authors : Grba, D.N.; Hirst, J.  
Deposited on : 2025-02-21  
Resolution : 3.80 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:

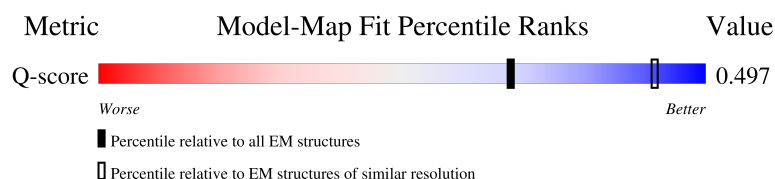
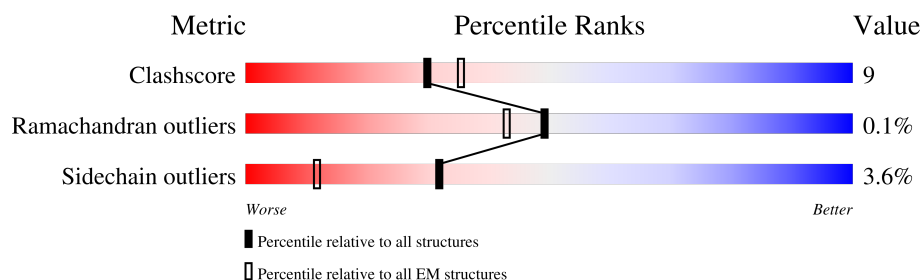
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 10198 ( 3.30 - 4.30 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                           |
|-----|-------|--------|----------------------------------------------------------------------------|
| 1   | A     | 141    | <div> <div>35%</div> <div>65%</div> <div>29%</div> <div>• •</div> </div>   |
| 2   | B     | 204    | <div> <div>9%</div> <div>62%</div> <div>22%</div> <div>• 14%</div> </div>  |
| 3   | C     | 289    | <div> <div>26%</div> <div>55%</div> <div>24%</div> <div>• 19%</div> </div> |
| 4   | D     | 482    | <div> <div>15%</div> <div>70%</div> <div>19%</div> <div>• 9%</div> </div>  |

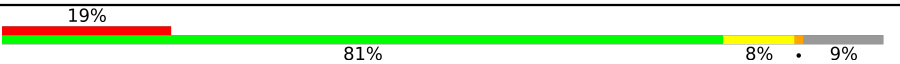
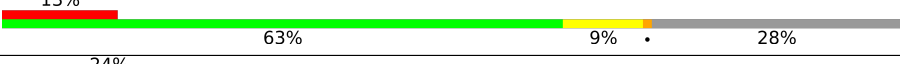
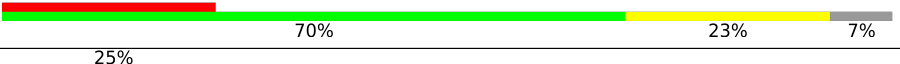
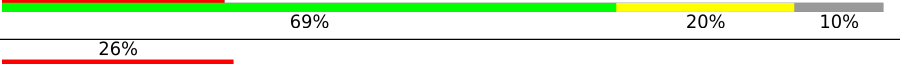
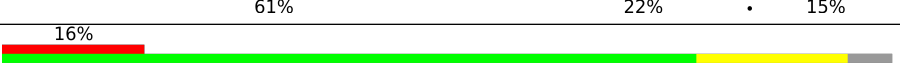
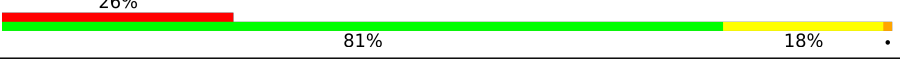
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | G     | 726    |                  |
| 6   | H     | 353    |                  |
| 7   | I     | 222    |                  |
| 8   | J     | 161    |                  |
| 9   | K     | 82     |                  |
| 10  | L     | 642    |                  |
| 11  | M     | 491    |                  |
| 12  | N     | 523    |                  |
| 13  | O     | 193    |                  |
| 14  | P     | 384    |                  |
| 15  | Q     | 159    |                  |
| 16  | R     | 139    |                  |
| 17  | S     | 90     |                  |
| 18  | T     | 138    |                  |
| 19  | U     | 130    |                  |
| 20  | V     | 134    |                  |
| 21  | W     | 122    |                  |
| 22  | X     | 184    |                  |
| 23  | Y     | 216    |                  |
| 24  | Z     | 147    |                  |
| 25  | a     | 150    |                  |
| 26  | b     | 79     |                  |
| 27  | c     | 182    |                  |
| 28  | d     | 78     |                  |
| 29  | e     | 106    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 30  | f     | 86     |    |
| 31  | g     | 239    |    |
| 32  | h     | 182    |    |
| 33  | i     | 74     |    |
| 34  | j     | 59     |    |
| 35  | k     | 61     |    |
| 36  | l     | 156    |    |
| 37  | m     | 81     |    |
| 38  | n     | 111    |    |
| 39  | o     | 87     |    |
| 40  | p     | 92     |   |
| 41  | 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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 42  | SF4  | G     | 801 | -         | -        | X       | -                |
| 42  | SF4  | G     | 802 | -         | -        | X       | -                |
| 42  | SF4  | I     | 302 | -         | -        | X       | -                |

## 2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 61836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1099  | 745 | 159 | 191 | 4 |         |       |

- Molecule 2 is a protein called BA75\_00622T0.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1407  | 901 | 241 | 249 | 16 |         |       |

- Molecule 3 is a protein called NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | C     | 233      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1922  | 1242 | 324 | 351 | 5 |         |       |

- Molecule 4 is a protein called NUCM (49 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 440      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3536  | 2259 | 602 | 657 | 18 |         |       |

- Molecule 5 is a protein called NUAM (75 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | G     | 556      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4295  | 2693 | 751 | 836 | 15 |         |       |

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | H     | 353      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2809  | 1903 | 414 | 478 | 14 |         |       |

- Molecule 7 is a protein called NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | I     | 192      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1556  | 988 | 259 | 299 | 10 |         |       |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | J     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1250  | 836 | 174 | 237 | 3 |         |       |

- Molecule 9 is a protein called NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 9   | K     | 80       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 617   | 400 | 93 | 118 | 6 |         |       |

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | L     | 642      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5115  | 3454 | 766 | 866 | 29 |         |       |

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11  | M     | 491      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3868  | 2597 | 593 | 663 | 15 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | N     | 506      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4045  | 2723 | 594 | 714 | 14 |         |       |

- Molecule 13 is a protein called NUXM subunit of mitochondrial NADH:ubiquinone oxidore-

ductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | 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 14 is a protein called NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | P     | 359      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2851  | 1821 | 496 | 531 | 3 |         |       |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | Q     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 727   | 462 | 122 | 141 | 2 |         |       |

- Molecule 16 is a protein called NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | R     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 978   | 610 | 179 | 186 | 3 |         |       |

- Molecule 17 is a protein called NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 17  | 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 18 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 730   | 459 | 116 | 154 | 1 |         |       |

- Molecule 19 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | U     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 681   | 427 | 102 | 152 |   |         |       |

- Molecule 20 is a protein called NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | V     | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1025  | 658 | 165 | 201 | 1 |         |       |

- Molecule 21 is a protein called BA75\_04796T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 979   | 626 | 177 | 171 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 22  | 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 23 is a protein called NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 23  | Y     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1578  | 1012 | 274 | 289 | 3 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 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 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | a     | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1215  | 756 | 228 | 225 | 6 |         |       |

- Molecule 26 is a protein called NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | b     | 78       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 419 | 111 | 109 | 2 |         |       |

- Molecule 27 is a protein called BA75\_00589T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | c     | 146      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1143  | 727 | 203 | 211 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 28 is a protein called Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | d     | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 616   | 406 | 106 | 103 | 1 |         |       |

- Molecule 29 is a protein called BA75\_05084T0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | e     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 848   | 531 | 154 | 157 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 30  | f     | 78       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 642   | 428 | 113 | 101 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | g     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1280  | 815 | 210 | 252 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 32  | h     | 131      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1078  | 699 | 183 | 196 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 33  | i     | 69       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 552   | 358 | 95 | 97 | 2 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 34  | j     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 460   | 319 | 76 | 64 | 1 |         |       |

- Molecule 35 is a protein called NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 35  | k     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 368   | 240 | 71 | 56 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | l     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1082  | 706 | 175 | 200 | 1 |         |       |

- Molecule 37 is a protein called NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | m     | 77       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 642   | 418 | 116 | 108 |   |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | n     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 861   | 550 | 155 | 155 | 1 |         |       |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | o     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 682   | 428 | 126 | 122 | 6 |         |       |

- Molecule 40 is a protein called NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | p     | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 740   | 457 | 135 | 144 | 4 |         |       |

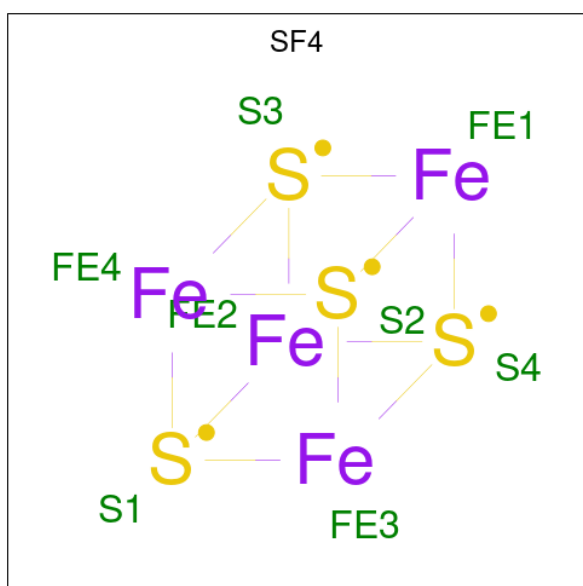
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | q     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1156  | 741 | 201 | 211 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

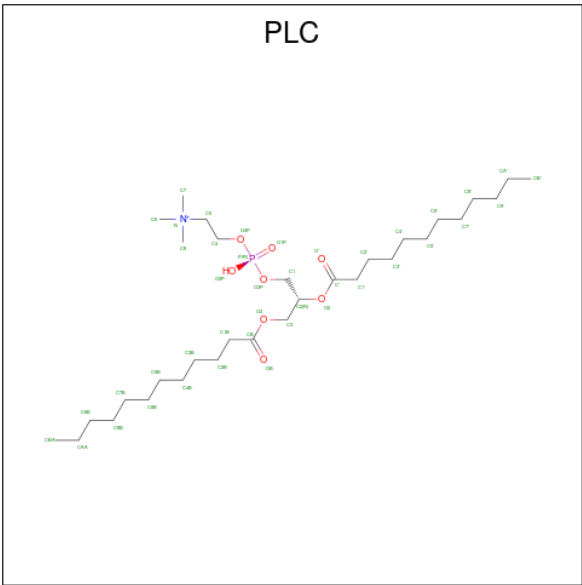
| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| q     | 0       | ACE      | -      | acetylation | UNP E1UWE0 |

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 42  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 42  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 42  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 42  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 42  | I     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 43 is DIUNDECYL PHOSPHATIDYL CHOLINE (CCD ID: PLC) (formula:  $\text{C}_{32}\text{H}_{65}\text{NO}_8\text{P}$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 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 |         |
| 43  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 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  | 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 |         |

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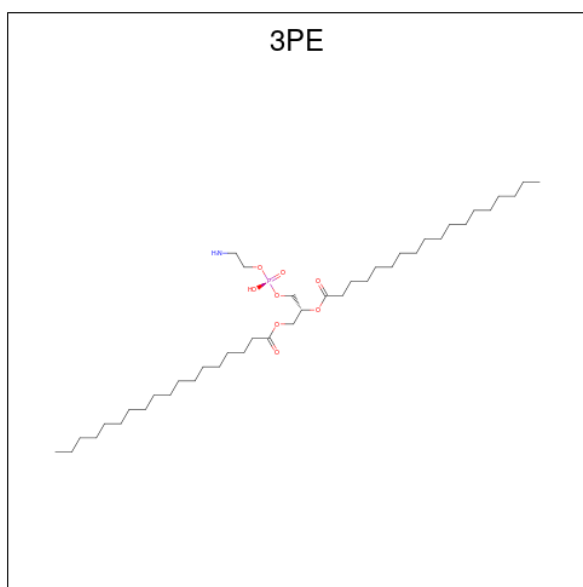
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| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 43  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 22    | 12 | 1 | 8 | 1 |         |
| 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  | 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 POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 44  | G     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



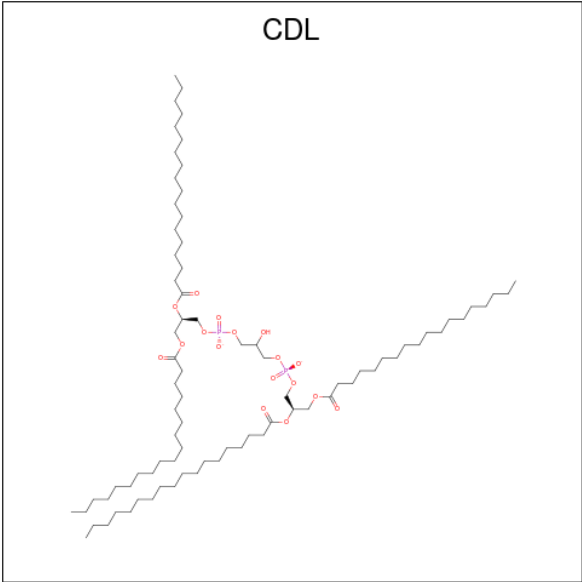
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |

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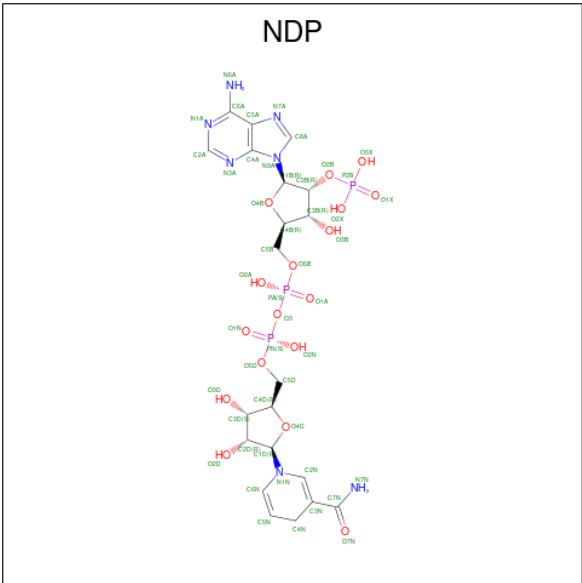
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 45  | L     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | M     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 45  | N     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 45  | Y     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 25    | 15 | 1 | 8 | 1 |         |
| 45  | Z     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 36    | 26 | 1 | 8 | 1 |         |
| 45  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 45  | b     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 45  | h     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 45  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 27    | 17 | 1 | 8 | 1 |         |
| 45  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 46  | O     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 75    | 56 | 17 | 2 |         |
| 46  | Z     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 30 | 17 | 2 |         |
| 46  | b     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 59    | 40 | 17 | 2 |         |
| 46  | q     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 60    | 41 | 17 | 2 |         |

- Molecule 47 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

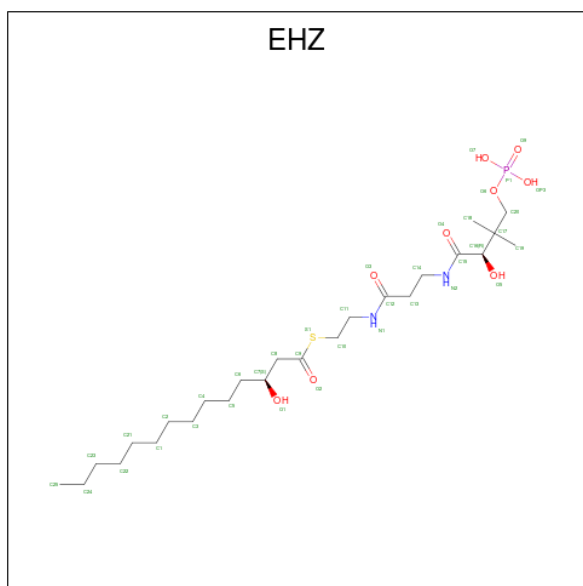


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 47  | P     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 48  | R     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 49 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-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).

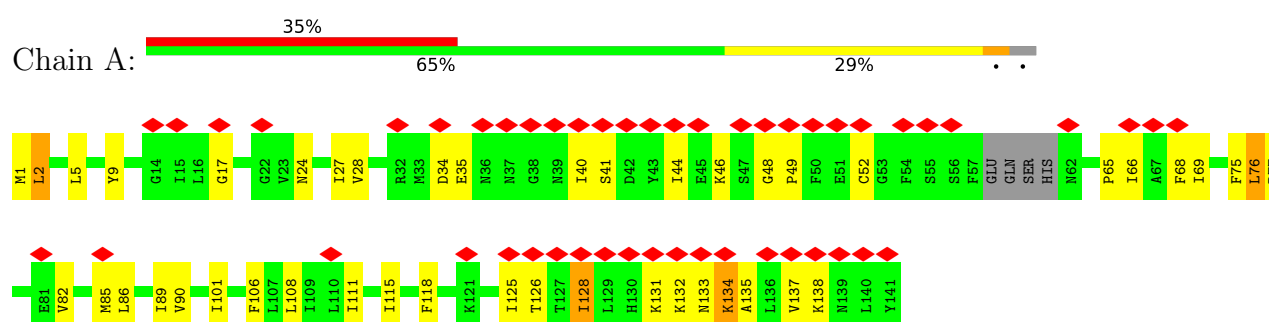


| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 49  | T     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 49  | U     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |

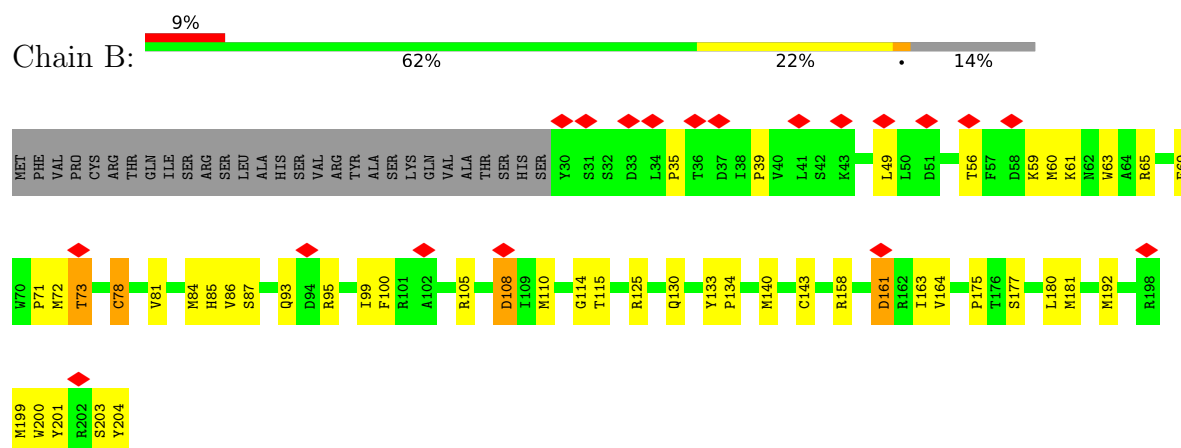
### 3 Residue-property plots

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

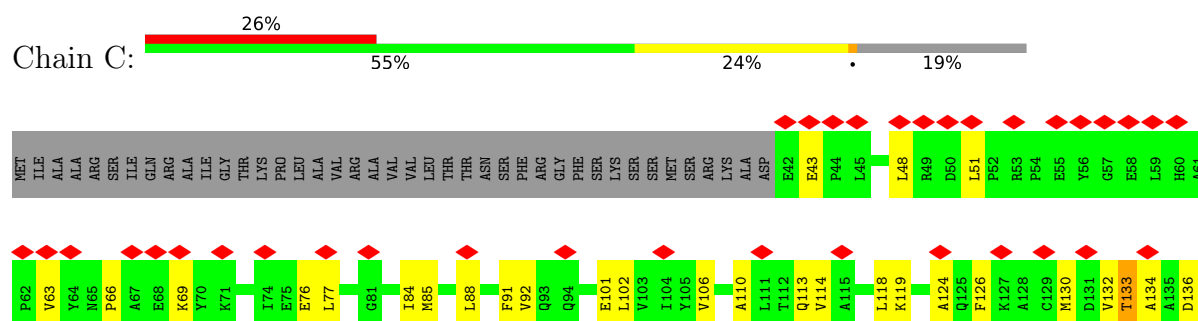
#### • Molecule 1: NADH-ubiquinone oxidoreductase chain 3

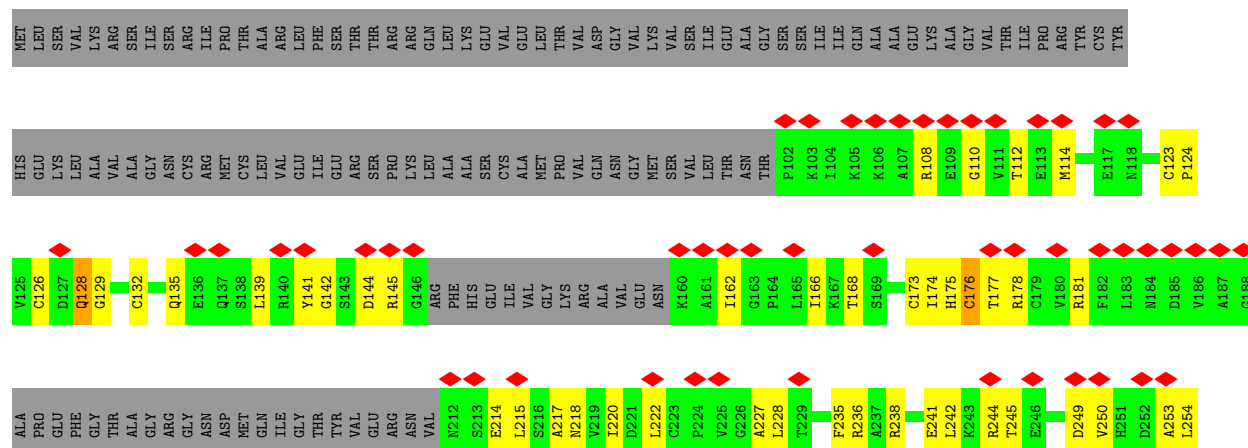


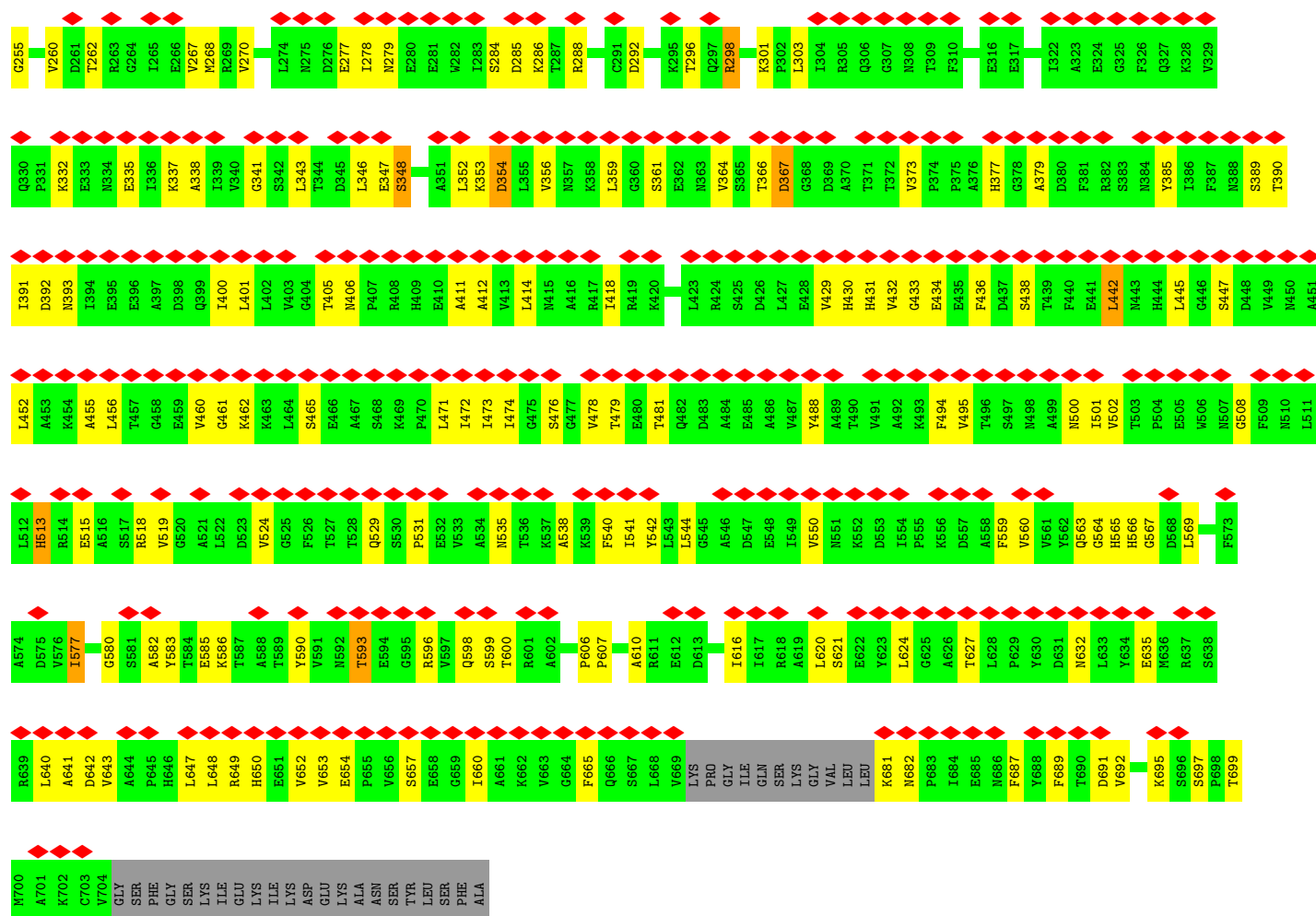
#### • Molecule 2: BA75\_00622T0



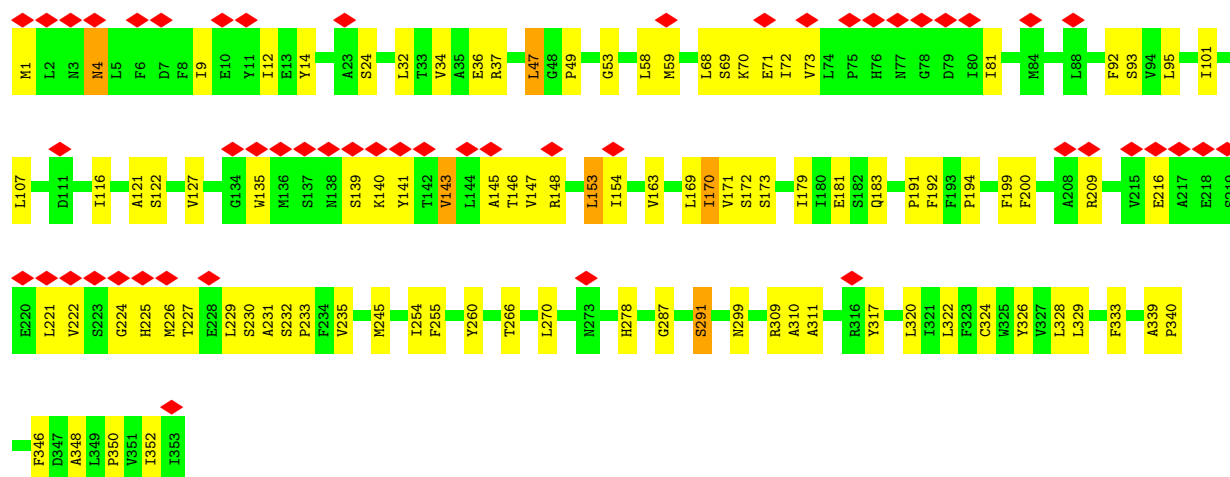
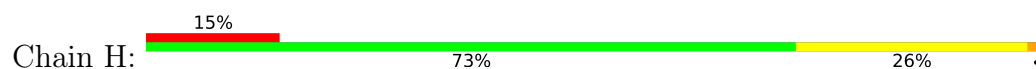
#### • Molecule 3: NUGM (30 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



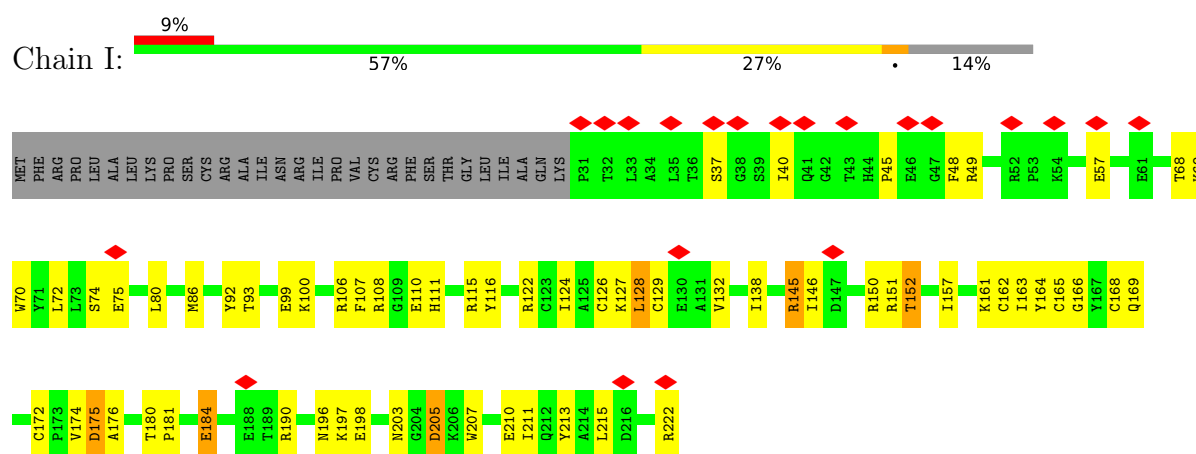




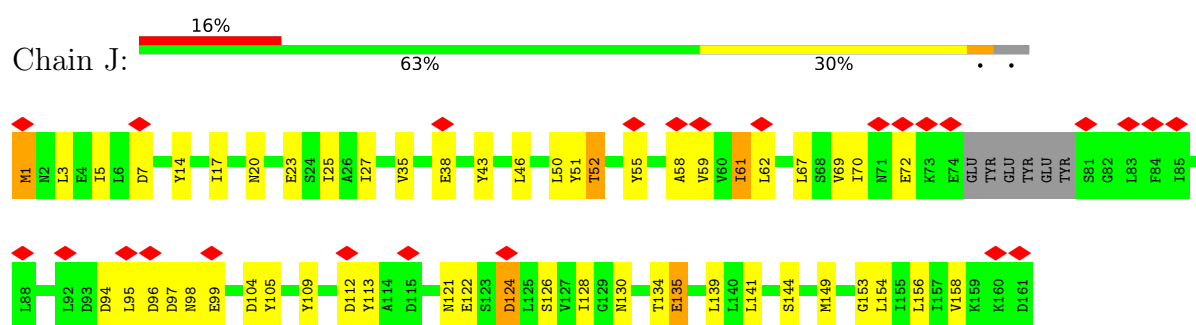
• Molecule 6: NADH-ubiquinone oxidoreductase chain 1



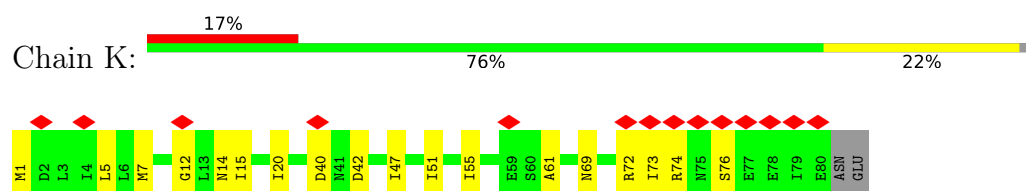
• Molecule 7: NUIM (TYKY) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



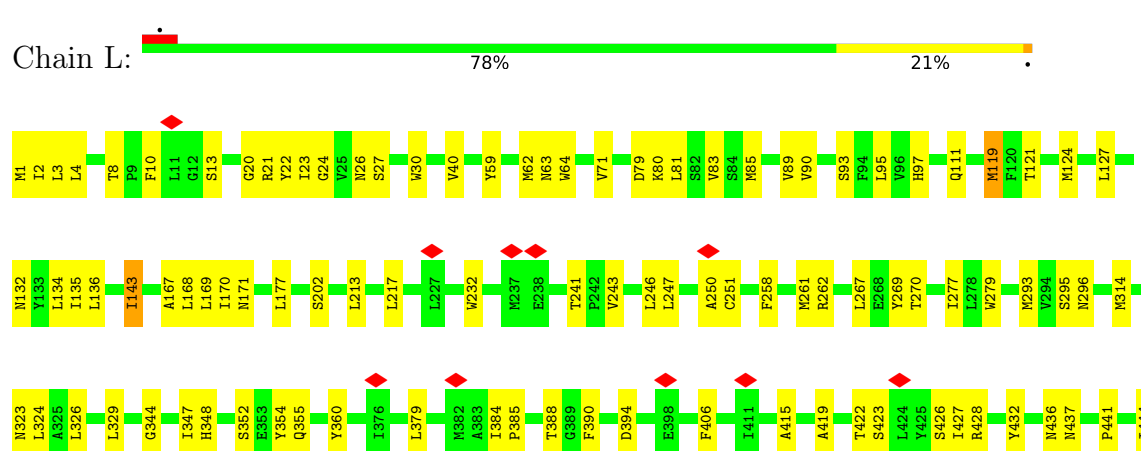
• Molecule 8: NADH-ubiquinone oxidoreductase chain 6

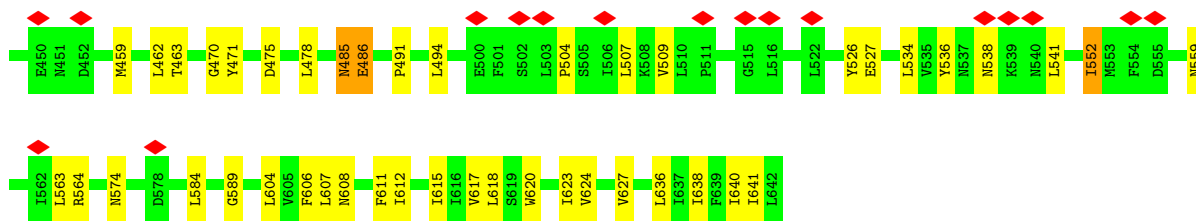


• Molecule 9: NULM (ND4L) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

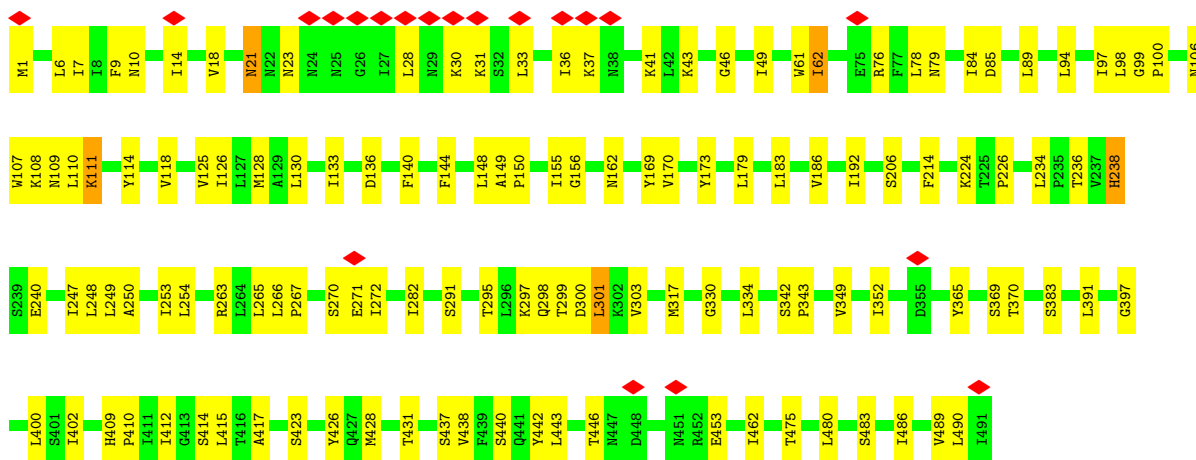
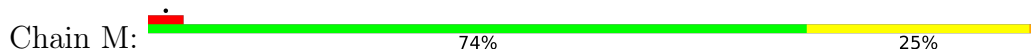


• Molecule 10: NADH-ubiquinone oxidoreductase chain 5

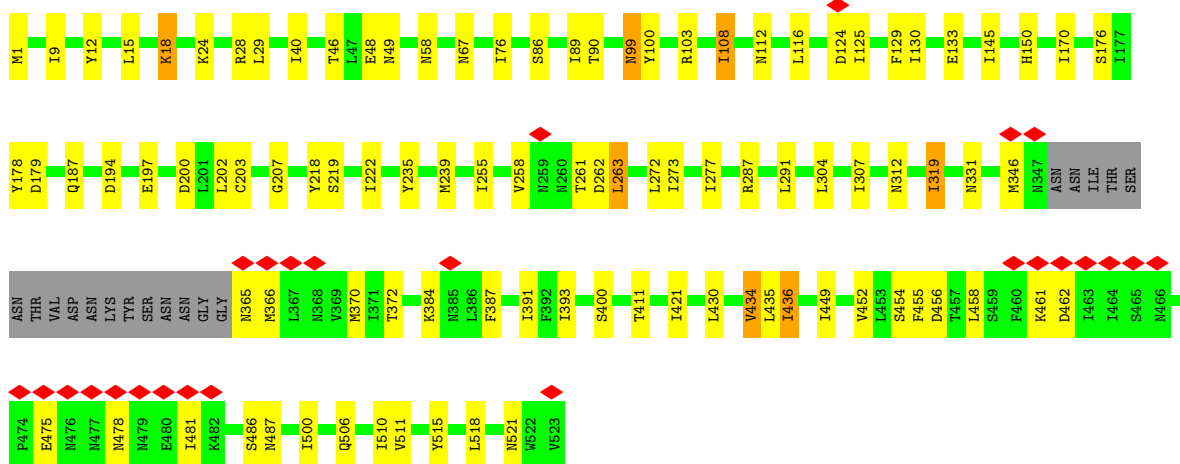
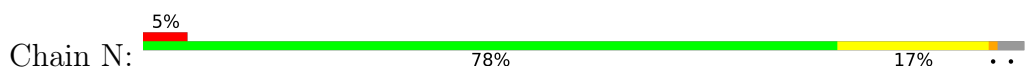




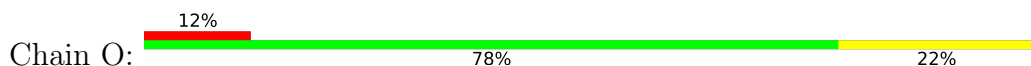
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4

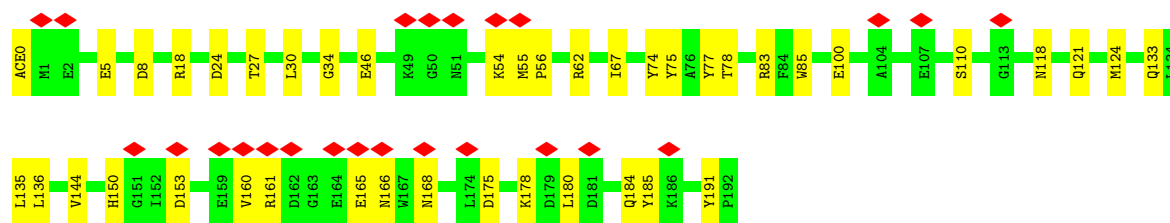


• Molecule 12: NADH-ubiquinone oxidoreductase chain 2



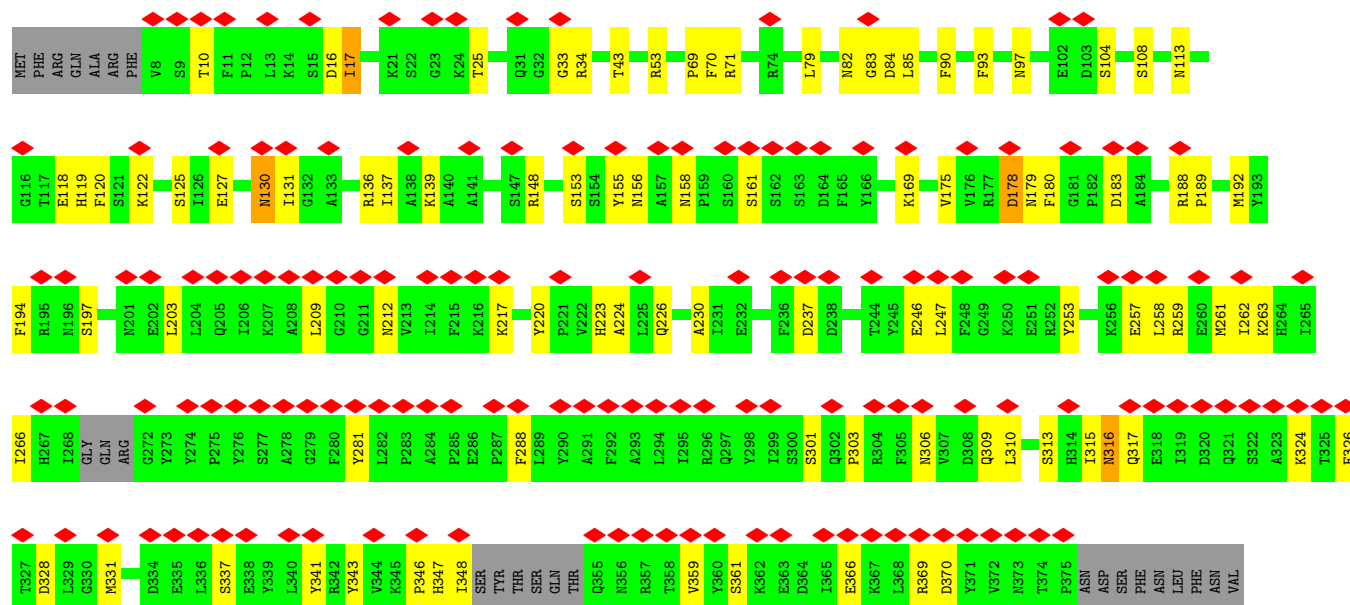
• Molecule 13: NUXM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



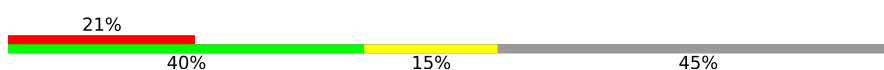


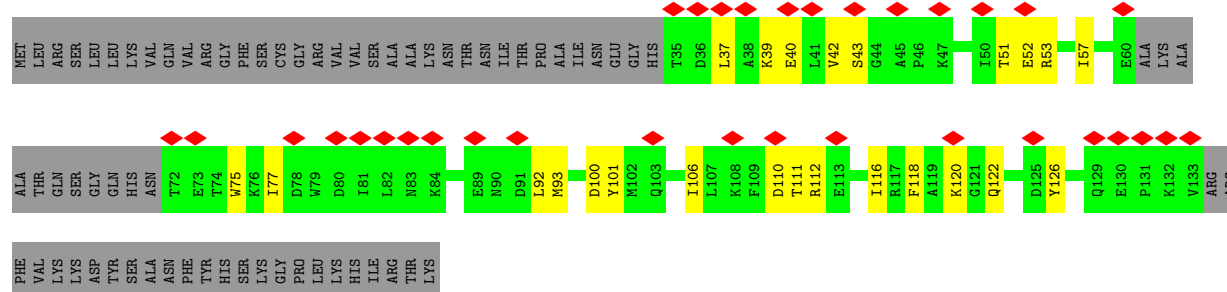
- Molecule 14: NUEM (39 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

Chain P: 



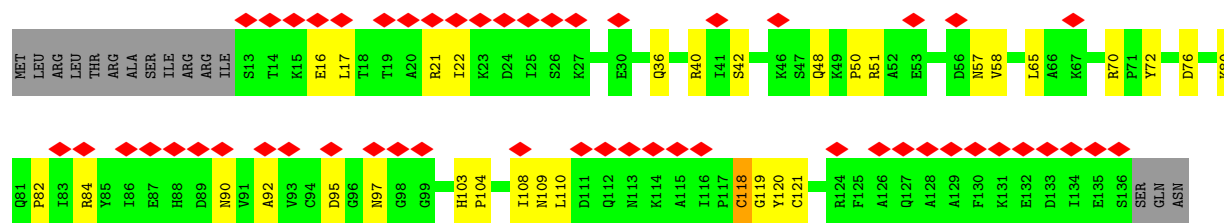
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q: 

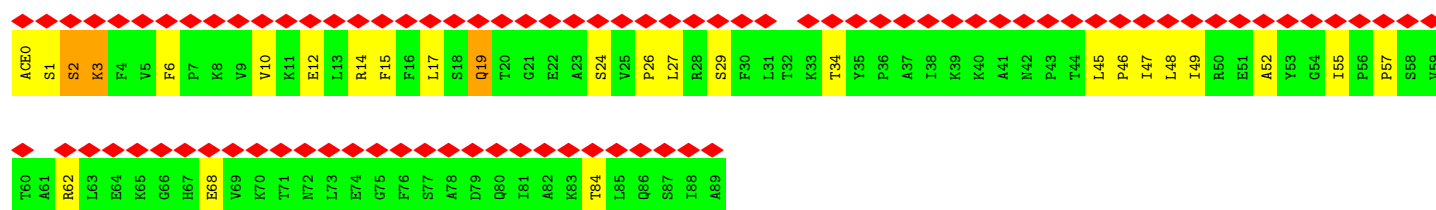


- Molecule 16: NUMM (13 kDa) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

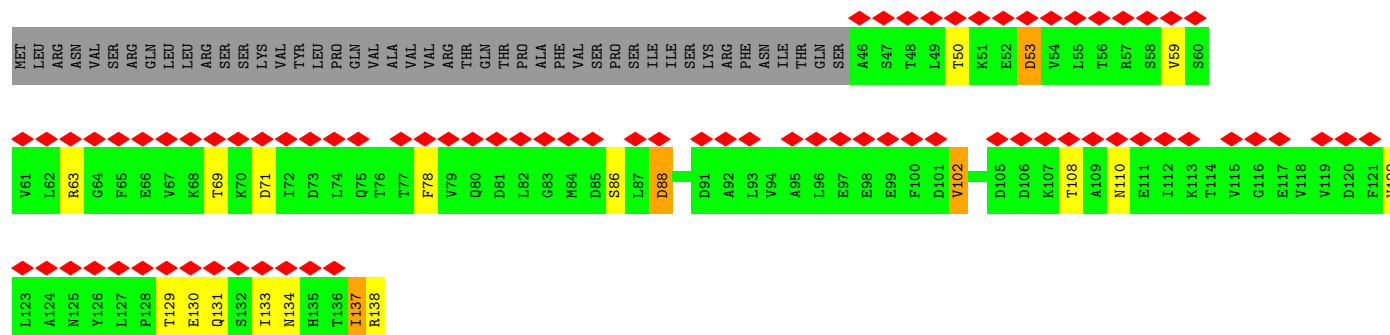
Chain R: 



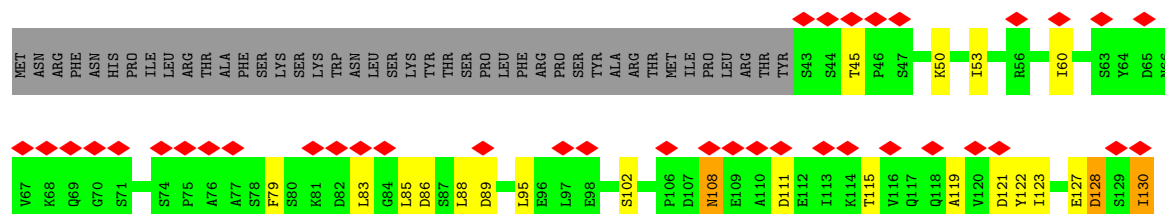
- Molecule 17: NI8M (B8) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 18: Acyl carrier protein

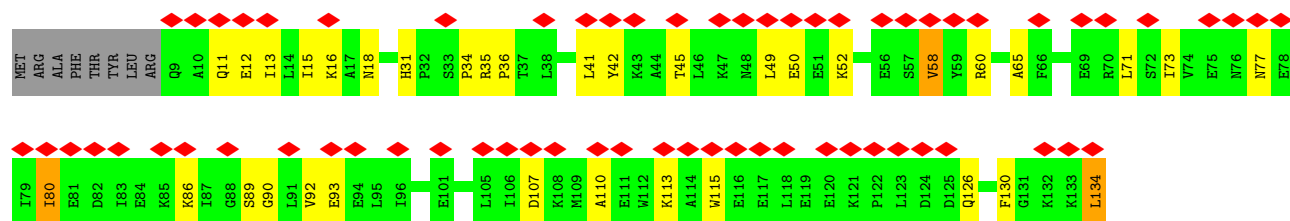


- Molecule 19: Acyl carrier protein

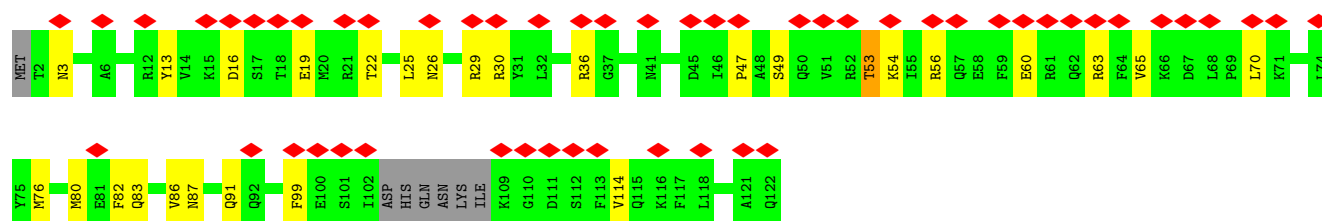
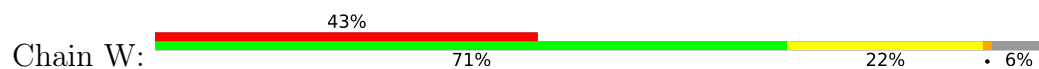


- Molecule 20: NUFM (B13) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

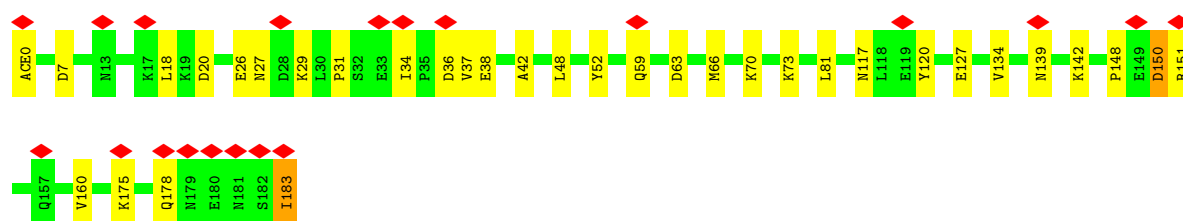
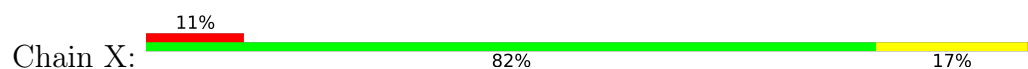




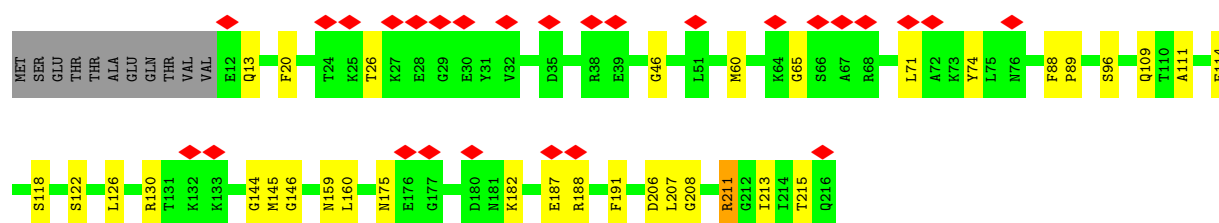
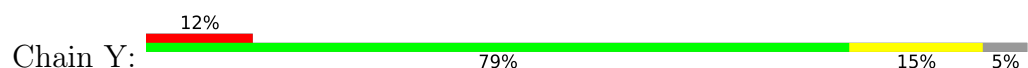
• Molecule 21: BA75\_04796T0



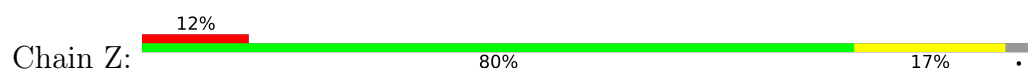
• Molecule 22: NADH-ubiquinone oxidoreductase

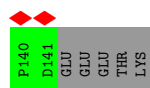


• Molecule 23: NUJM (B14.7) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

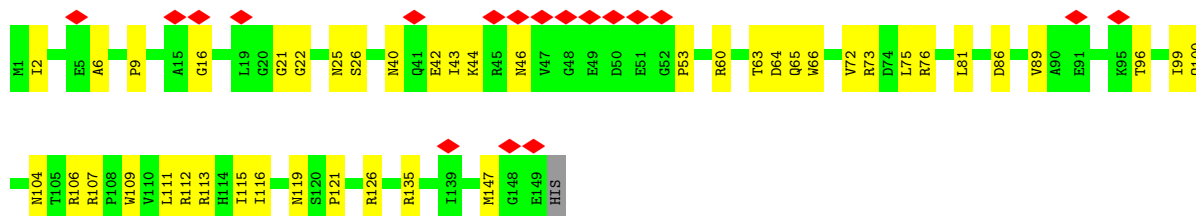


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

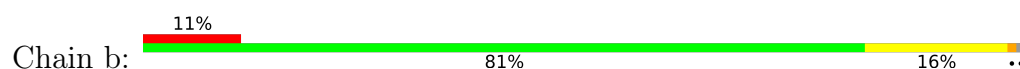




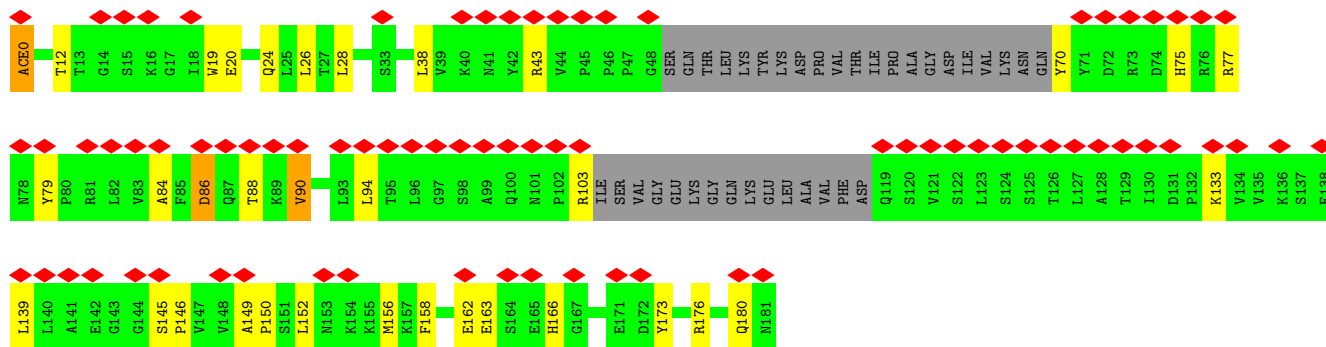
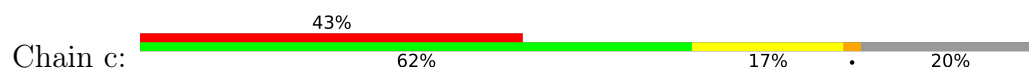
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



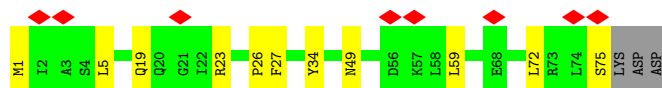
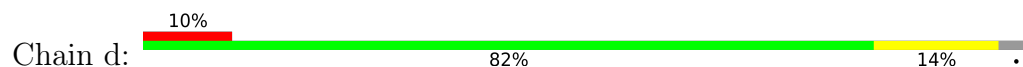
- Molecule 26: NI9M (B9) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



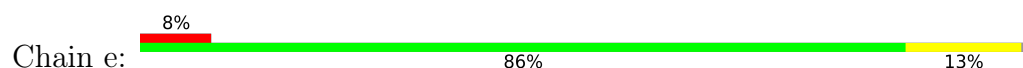
- Molecule 27: BA75\_00589T0

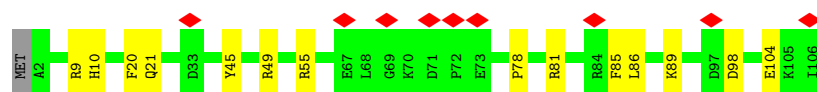


- Molecule 28: Pichia pastoris NADH-ubiquinone oxidoreductase subunit NEBM

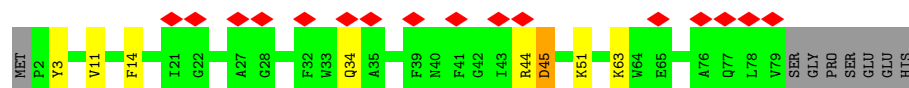
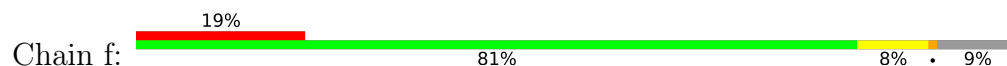


- Molecule 29: BA75\_05084T0

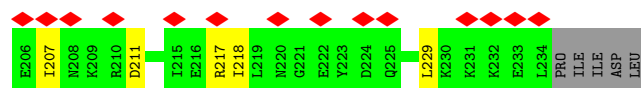
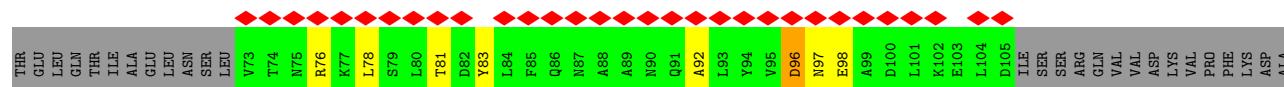
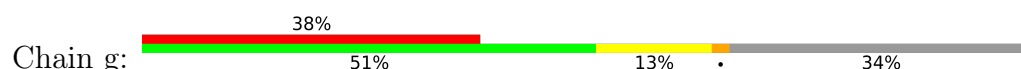




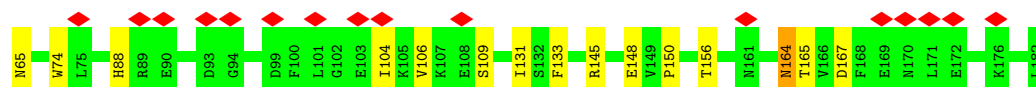
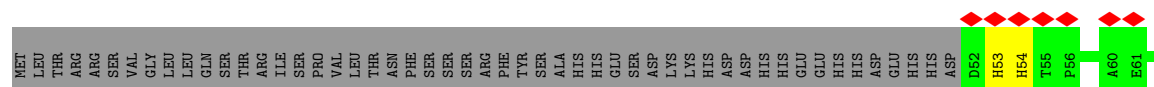
- Molecule 30: NUTM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 31: NESM (ESSS) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 32: NUSM subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



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

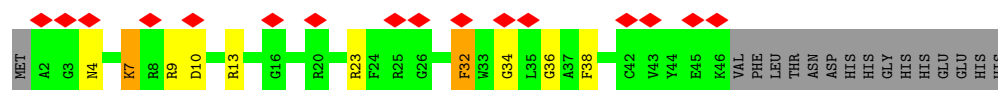




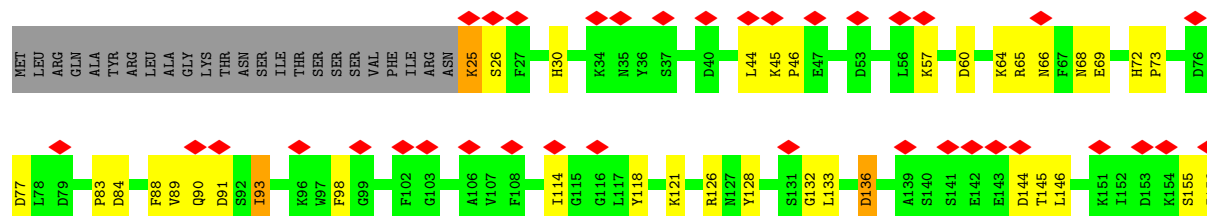
- Molecule 34: Subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



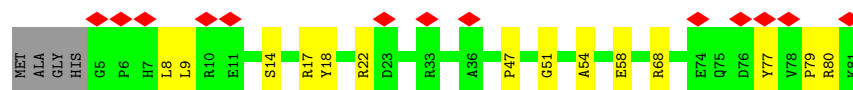
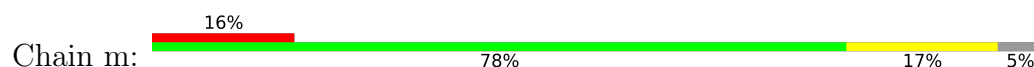
- Molecule 35: NB2M (B12) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



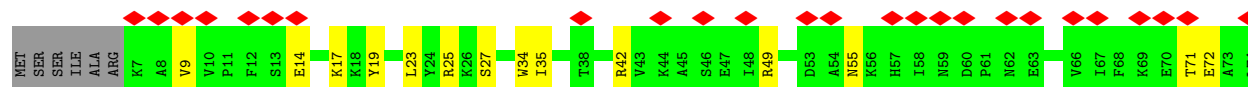
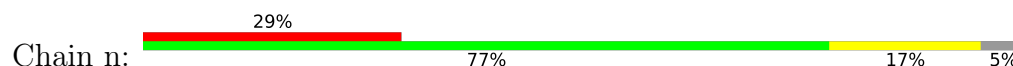
- Molecule 36: NIAM (ASHI) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)

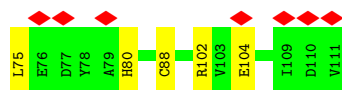


- Molecule 37: NB5M (B15) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

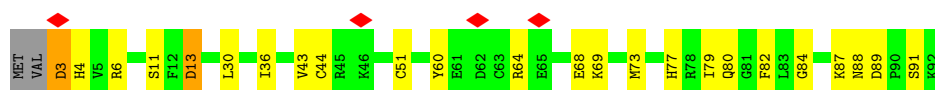




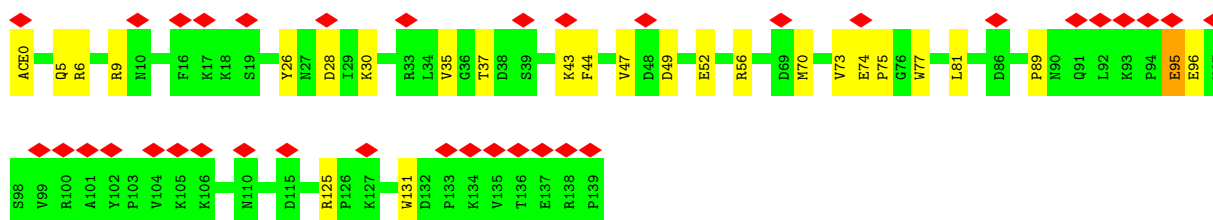
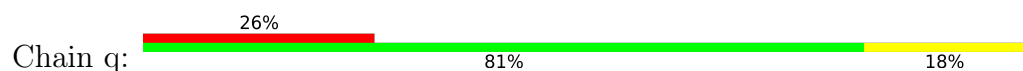
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 40: NIDM (PDSW) subunit of mitochondrial NADH:ubiquinone oxidoreductase (Complex I)



- Molecule 41: 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             | 18608                   | 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                    | 0.072                   | Depositor |
| Minimum map value                    | -0.025                  | Depositor |
| Average map value                    | -0.000                  | Depositor |
| Map value standard deviation         | 0.002                   | Depositor |
| Recommended contour level            | 0.012                   | 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: 2MR, K, ACE, ZN, NDP, CDL, FME, PLC, EHZ, SF4, 3PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |               | Bond angles |             |
|-----|-------|--------------|---------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.19         | 0/1115        | 0.30        | 0/1514      |
| 2   | B     | 0.20         | 0/1450        | 0.28        | 0/1969      |
| 3   | C     | 0.17         | 0/1981        | 0.26        | 0/2694      |
| 4   | D     | 0.19         | 0/3612        | 0.28        | 0/4892      |
| 5   | G     | 0.14         | 0/4371        | 0.28        | 0/5932      |
| 6   | H     | 0.21         | 0/2880        | 0.28        | 0/3939      |
| 7   | I     | 0.24         | 0/1596        | 0.33        | 0/2164      |
| 8   | J     | 0.22         | 0/1262        | 0.28        | 0/1723      |
| 9   | K     | 0.22         | 0/610         | 0.25        | 0/828       |
| 10  | L     | 0.21         | 0/5236        | 0.28        | 0/7128      |
| 11  | M     | 0.23         | 0/3940        | 0.29        | 0/5379      |
| 12  | N     | 0.23         | 0/4110        | 0.27        | 0/5609      |
| 13  | O     | 0.24         | 1/1621 (0.1%) | 0.30        | 0/2199      |
| 14  | P     | 0.15         | 0/2911        | 0.27        | 0/3932      |
| 15  | Q     | 0.16         | 0/742         | 0.26        | 0/1000      |
| 16  | R     | 0.15         | 0/998         | 0.26        | 0/1350      |
| 17  | S     | 0.26         | 1/710 (0.1%)  | 0.27        | 0/961       |
| 18  | T     | 0.11         | 0/737         | 0.24        | 0/1001      |
| 19  | U     | 0.14         | 0/688         | 0.26        | 0/936       |
| 20  | V     | 0.14         | 0/1044        | 0.27        | 0/1411      |
| 21  | W     | 0.14         | 0/999         | 0.26        | 0/1340      |
| 22  | X     | 0.24         | 1/1475 (0.1%) | 0.28        | 0/1990      |
| 23  | Y     | 0.18         | 0/1615        | 0.27        | 0/2175      |
| 24  | Z     | 0.26         | 1/1210 (0.1%) | 0.25        | 0/1639      |
| 25  | a     | 0.19         | 0/1241        | 0.26        | 0/1670      |
| 26  | b     | 0.16         | 0/666         | 0.25        | 0/911       |
| 27  | c     | 0.23         | 1/1167 (0.1%) | 0.27        | 0/1581      |
| 28  | d     | 0.19         | 0/633         | 0.22        | 0/854       |
| 29  | e     | 0.20         | 0/865         | 0.25        | 0/1158      |
| 30  | f     | 0.17         | 0/663         | 0.22        | 0/896       |
| 31  | g     | 0.15         | 0/1293        | 0.26        | 0/1735      |
| 32  | h     | 0.18         | 0/1114        | 0.27        | 0/1516      |

| Mol | Chain | Bond lengths |                | Bond angles |         |
|-----|-------|--------------|----------------|-------------|---------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5 |
| 33  | i     | 0.16         | 0/571          | 0.25        | 0/777   |
| 34  | j     | 0.15         | 0/484          | 0.26        | 0/658   |
| 35  | k     | 0.14         | 0/382          | 0.24        | 0/514   |
| 36  | l     | 0.17         | 0/1119         | 0.29        | 0/1520  |
| 37  | m     | 0.18         | 0/661          | 0.27        | 0/893   |
| 38  | n     | 0.14         | 0/884          | 0.23        | 0/1197  |
| 39  | o     | 0.14         | 0/696          | 0.27        | 0/933   |
| 40  | p     | 0.20         | 0/756          | 0.25        | 0/1020  |
| 41  | q     | 0.25         | 1/1192 (0.1%)  | 0.29        | 0/1620  |
| All | All   | 0.20         | 6/61300 (0.0%) | 0.27        | 0/83158 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 17  | S     | 0   | ACE  | C-N   | 6.20 | 1.45        | 1.33     |
| 27  | c     | 0   | ACE  | C-N   | 6.14 | 1.45        | 1.33     |
| 22  | X     | 0   | ACE  | C-N   | 6.11 | 1.45        | 1.33     |
| 41  | q     | 0   | ACE  | C-N   | 6.06 | 1.45        | 1.33     |
| 24  | Z     | 0   | ACE  | C-N   | 6.03 | 1.45        | 1.33     |
| 13  | O     | 0   | ACE  | C-N   | 5.85 | 1.45        | 1.33     |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1099  | 0        | 1140     | 38      | 0            |
| 2   | B     | 1407  | 0        | 1372     | 42      | 0            |
| 3   | C     | 1922  | 0        | 1861     | 61      | 0            |
| 4   | D     | 3536  | 0        | 3437     | 79      | 0            |
| 5   | G     | 4295  | 0        | 4257     | 133     | 0            |
| 6   | H     | 2809  | 0        | 2880     | 66      | 0            |
| 7   | I     | 1556  | 0        | 1499     | 60      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | J     | 1250  | 0        | 1274     | 44      | 0            |
| 9   | K     | 617   | 0        | 657      | 16      | 0            |
| 10  | L     | 5115  | 0        | 5338     | 98      | 0            |
| 11  | M     | 3868  | 0        | 4127     | 88      | 0            |
| 12  | N     | 4045  | 0        | 4327     | 68      | 0            |
| 13  | O     | 1575  | 0        | 1523     | 27      | 0            |
| 14  | P     | 2851  | 0        | 2847     | 69      | 0            |
| 15  | Q     | 727   | 0        | 701      | 13      | 0            |
| 16  | R     | 978   | 0        | 964      | 19      | 0            |
| 17  | S     | 697   | 0        | 736      | 20      | 0            |
| 18  | T     | 730   | 0        | 721      | 16      | 0            |
| 19  | U     | 681   | 0        | 664      | 15      | 0            |
| 20  | V     | 1025  | 0        | 1035     | 30      | 0            |
| 21  | W     | 979   | 0        | 980      | 19      | 0            |
| 22  | X     | 1450  | 0        | 1422     | 23      | 0            |
| 23  | Y     | 1578  | 0        | 1567     | 25      | 0            |
| 24  | Z     | 1176  | 0        | 1165     | 19      | 0            |
| 25  | a     | 1215  | 0        | 1197     | 41      | 0            |
| 26  | b     | 641   | 0        | 620      | 13      | 0            |
| 27  | c     | 1143  | 0        | 1165     | 29      | 0            |
| 28  | d     | 616   | 0        | 624      | 8       | 0            |
| 29  | e     | 848   | 0        | 830      | 11      | 0            |
| 30  | f     | 642   | 0        | 640      | 9       | 0            |
| 31  | g     | 1280  | 0        | 1302     | 27      | 0            |
| 32  | h     | 1078  | 0        | 1036     | 12      | 0            |
| 33  | i     | 552   | 0        | 540      | 12      | 0            |
| 34  | j     | 460   | 0        | 455      | 8       | 0            |
| 35  | k     | 368   | 0        | 348      | 8       | 0            |
| 36  | l     | 1082  | 0        | 1033     | 26      | 0            |
| 37  | m     | 642   | 0        | 635      | 12      | 0            |
| 38  | n     | 861   | 0        | 866      | 13      | 0            |
| 39  | o     | 682   | 0        | 677      | 15      | 0            |
| 40  | p     | 740   | 0        | 700      | 20      | 0            |
| 41  | q     | 1156  | 0        | 1115     | 17      | 0            |
| 42  | B     | 8     | 0        | 0        | 1       | 0            |
| 42  | G     | 16    | 0        | 0        | 6       | 0            |
| 42  | I     | 16    | 0        | 0        | 3       | 0            |
| 43  | B     | 31    | 0        | 36       | 3       | 0            |
| 43  | D     | 42    | 0        | 64       | 3       | 0            |
| 43  | H     | 24    | 0        | 22       | 0       | 0            |
| 43  | L     | 151   | 0        | 210      | 13      | 0            |
| 43  | M     | 84    | 0        | 128      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | P     | 62    | 0        | 72       | 3       | 0            |
| 43  | Y     | 72    | 0        | 98       | 4       | 0            |
| 43  | Z     | 42    | 0        | 64       | 3       | 0            |
| 43  | a     | 22    | 0        | 18       | 0       | 0            |
| 43  | b     | 39    | 0        | 55       | 0       | 0            |
| 43  | d     | 84    | 0        | 128      | 3       | 0            |
| 43  | g     | 39    | 0        | 55       | 5       | 0            |
| 43  | q     | 78    | 0        | 113      | 5       | 0            |
| 44  | G     | 1     | 0        | 0        | 0       | 0            |
| 45  | J     | 51    | 0        | 82       | 4       | 0            |
| 45  | L     | 259   | 0        | 380      | 19      | 0            |
| 45  | M     | 86    | 0        | 126      | 6       | 0            |
| 45  | N     | 40    | 0        | 57       | 1       | 0            |
| 45  | Y     | 25    | 0        | 24       | 1       | 0            |
| 45  | Z     | 36    | 0        | 46       | 1       | 0            |
| 45  | b     | 71    | 0        | 93       | 3       | 0            |
| 45  | h     | 46    | 0        | 69       | 5       | 0            |
| 45  | j     | 27    | 0        | 28       | 4       | 0            |
| 45  | m     | 46    | 0        | 69       | 4       | 0            |
| 46  | O     | 75    | 0        | 97       | 3       | 0            |
| 46  | Z     | 49    | 0        | 42       | 1       | 0            |
| 46  | b     | 59    | 0        | 62       | 3       | 0            |
| 46  | q     | 60    | 0        | 64       | 5       | 0            |
| 47  | P     | 48    | 0        | 25       | 2       | 0            |
| 48  | R     | 1     | 0        | 0        | 0       | 0            |
| 49  | T     | 37    | 0        | 0        | 0       | 0            |
| 49  | U     | 37    | 0        | 0        | 2       | 0            |
| All | All   | 61836 | 0        | 62604    | 1133    | 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 9.

All (1133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 5:G:175:HIS:HA    | 42:G:801:SF4:S4 | 1.96                     | 1.04              |
| 7:I:111:HIS:CD2   | 7:I:168:CYS:SG  | 2.49                     | 1.03              |
| 7:I:111:HIS:CE1   | 42:I:302:SF4:S2 | 2.55                     | 0.97              |
| 14:P:156:ASN:HD21 | 14:P:317:GLN:HA | 1.39                     | 0.86              |
| 16:R:103:HIS:CD2  | 16:R:121:CYS:SG | 2.68                     | 0.86              |
| 5:G:175:HIS:CA    | 42:G:801:SF4:S4 | 2.69                     | 0.80              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:388:THR:HG22 | 10:L:470:GLY:H    | 1.48                     | 0.78              |
| 7:I:172:CYS:SG    | 7:I:176:ALA:N     | 2.56                     | 0.77              |
| 12:N:312:ASN:ND2  | 32:h:133:PHE:O    | 2.17                     | 0.76              |
| 27:c:86:ASP:N     | 27:c:86:ASP:OD1   | 2.18                     | 0.76              |
| 26:b:41:MET:HE2   | 45:b:103:3PE:H272 | 1.68                     | 0.75              |
| 5:G:177:THR:N     | 42:G:801:SF4:S4   | 2.60                     | 0.75              |
| 7:I:48:PHE:O      | 27:c:176:ARG:NH1  | 2.20                     | 0.75              |
| 1:A:76:LEU:HD23   | 8:J:62:LEU:HD12   | 1.69                     | 0.74              |
| 4:D:77:GLU:HG2    | 10:L:606:PHE:HA   | 1.68                     | 0.74              |
| 16:R:16:GLU:HG2   | 16:R:42:SER:HB3   | 1.68                     | 0.74              |
| 19:U:102:SER:HB2  | 19:U:130:ILE:HD11 | 1.68                     | 0.74              |
| 5:G:337:LYS:HB3   | 5:G:541:ILE:HG12  | 1.71                     | 0.73              |
| 5:G:236:ARG:NH1   | 5:G:268:MET:SD    | 2.61                     | 0.73              |
| 4:D:105:PRO:HB3   | 4:D:113:VAL:HG12  | 1.69                     | 0.72              |
| 6:H:226:MET:HG2   | 6:H:229:LEU:HD12  | 1.72                     | 0.72              |
| 11:M:106:ASN:ND2  | 11:M:109:ASN:OD1  | 2.21                     | 0.72              |
| 2:B:86:VAL:HG12   | 2:B:93:GLN:HB3    | 1.72                     | 0.71              |
| 6:H:127:VAL:HG13  | 6:H:153:LEU:HD13  | 1.70                     | 0.71              |
| 5:G:649:ARG:HB3   | 5:G:652:VAL:HB    | 1.72                     | 0.71              |
| 43:L:701:PLC:H61  | 11:M:370:THR:HA   | 1.74                     | 0.70              |
| 11:M:297:LYS:NZ   | 36:l:77:ASP:OD1   | 2.25                     | 0.70              |
| 5:G:583:TYR:HA    | 5:G:586:LYS:HE2   | 1.74                     | 0.70              |
| 11:M:442:TYR:OH   | 36:l:65:ARG:NH1   | 2.25                     | 0.70              |
| 39:o:14:GLU:O     | 39:o:18:ASN:ND2   | 2.25                     | 0.70              |
| 6:H:36:GLU:OE2    | 6:H:309:ARG:NH1   | 2.25                     | 0.69              |
| 7:I:196:ASN:ND2   | 7:I:198:GLU:OE1   | 2.24                     | 0.69              |
| 4:D:313:ARG:NH2   | 4:D:355:GLU:OE2   | 2.25                     | 0.69              |
| 7:I:111:HIS:HE1   | 42:I:302:SF4:S2   | 2.04                     | 0.69              |
| 14:P:263:LYS:NZ   | 14:P:281:TYR:OH   | 2.26                     | 0.69              |
| 3:C:119:LYS:NZ    | 3:C:177:LEU:O     | 2.25                     | 0.69              |
| 5:G:338:ALA:HB3   | 5:G:364:VAL:HG12  | 1.74                     | 0.69              |
| 10:L:296:ASN:OD1  | 10:L:428:ARG:NH2  | 2.26                     | 0.69              |
| 4:D:90:PRO:HD3    | 12:N:370:MET:HE1  | 1.74                     | 0.69              |
| 5:G:531:PRO:O     | 5:G:535:ASN:ND2   | 2.26                     | 0.69              |
| 14:P:148:ARG:NH1  | 14:P:237:ASP:O    | 2.27                     | 0.68              |
| 4:D:231:GLU:OE2   | 27:c:43:ARG:NH1   | 2.26                     | 0.68              |
| 10:L:23:ILE:O     | 10:L:27:SER:OG    | 2.11                     | 0.68              |
| 33:i:25:ASN:O     | 33:i:29:ASN:ND2   | 2.27                     | 0.68              |
| 7:I:108:ARG:NH1   | 7:I:165:CYS:O     | 2.27                     | 0.67              |
| 7:I:172:CYS:HA    | 42:I:301:SF4:S2   | 2.34                     | 0.67              |
| 43:L:701:PLC:O2P  | 33:i:16:THR:OG1   | 2.12                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:69:LYS:HE2    | 43:Z:202:PLC:H12  | 1.76                     | 0.67              |
| 7:I:152:THR:O     | 7:I:197:LYS:NZ    | 2.27                     | 0.67              |
| 2:B:163:ILE:HG22  | 2:B:164:VAL:HG13  | 1.75                     | 0.67              |
| 10:L:4:LEU:O      | 10:L:8:THR:OG1    | 2.11                     | 0.67              |
| 13:O:24:ASP:OD2   | 13:O:83:ARG:NH1   | 2.27                     | 0.67              |
| 20:V:31:HIS:HB3   | 20:V:34:PRO:HG3   | 1.77                     | 0.67              |
| 10:L:324:LEU:HD23 | 10:L:478:LEU:HD22 | 1.76                     | 0.67              |
| 14:P:192:MET:H    | 47:P:501:NDP:H71N | 1.42                     | 0.67              |
| 5:G:286:LYS:NZ    | 5:G:687:PHE:O     | 2.27                     | 0.66              |
| 21:W:83:GLN:O     | 21:W:87:ASN:ND2   | 2.27                     | 0.66              |
| 10:L:202:SER:O    | 37:m:68:ARG:NH2   | 2.28                     | 0.66              |
| 7:I:126:CYS:HB2   | 7:I:128:LEU:H     | 1.61                     | 0.66              |
| 45:L:705:3PE:H231 | 23:Y:46:GLY:HA3   | 1.77                     | 0.66              |
| 5:G:277:GLU:OE1   | 5:G:596:ARG:NH1   | 2.27                     | 0.65              |
| 16:R:36:GLN:NE2   | 16:R:48:GLN:OE1   | 2.28                     | 0.65              |
| 22:X:150:ASP:OD1  | 22:X:150:ASP:N    | 2.28                     | 0.65              |
| 10:L:526:TYR:OH   | 43:L:708:PLC:O1P  | 2.12                     | 0.65              |
| 22:X:175:LYS:HA   | 22:X:178:GLN:HB2  | 1.78                     | 0.65              |
| 36:l:30:HIS:NE2   | 36:l:91:ASP:OD2   | 2.27                     | 0.65              |
| 5:G:176:CYS:O     | 5:G:181:ARG:NH2   | 2.28                     | 0.65              |
| 14:P:175:VAL:O    | 14:P:179:ASN:ND2  | 2.27                     | 0.65              |
| 5:G:660:ILE:HD11  | 17:S:17:LEU:HD11  | 1.79                     | 0.65              |
| 2:B:161:ASP:OD2   | 7:I:190:ARG:NH1   | 2.24                     | 0.65              |
| 13:O:185:TYR:O    | 26:b:67:ASN:ND2   | 2.29                     | 0.65              |
| 22:X:27:ASN:OD1   | 24:Z:137:ARG:NH1  | 2.29                     | 0.65              |
| 5:G:168:THR:HG22  | 5:G:228:LEU:HD22  | 1.79                     | 0.65              |
| 15:Q:120:LYS:NZ   | 15:Q:126:TYR:OH   | 2.30                     | 0.65              |
| 19:U:111:ASP:OD1  | 38:n:25:ARG:NH1   | 2.30                     | 0.65              |
| 12:N:331:ASN:OD1  | 12:N:400:SER:OG   | 2.15                     | 0.64              |
| 27:c:94:LEU:O     | 27:c:103:ARG:NH2  | 2.30                     | 0.64              |
| 24:Z:121:LYS:NZ   | 24:Z:136:ASN:O    | 2.31                     | 0.64              |
| 5:G:431:HIS:HB2   | 5:G:442:LEU:HD22  | 1.80                     | 0.64              |
| 24:Z:100:GLU:HB2  | 25:a:147:MET:HE2  | 1.80                     | 0.64              |
| 31:g:76:ARG:HH22  | 31:g:97:ASN:HB2   | 1.62                     | 0.64              |
| 14:P:70:PHE:HE2   | 14:P:90:PHE:HB3   | 1.61                     | 0.64              |
| 5:G:515:GLU:HB2   | 5:G:518:ARG:HG2   | 1.79                     | 0.64              |
| 2:B:158:ARG:NH1   | 3:C:227:GLU:OE1   | 2.31                     | 0.64              |
| 5:G:260:VAL:HG22  | 5:G:270:VAL:HG22  | 1.79                     | 0.64              |
| 12:N:312:ASN:OD1  | 12:N:521:ASN:ND2  | 2.31                     | 0.64              |
| 22:X:73:LYS:NZ    | 32:h:165:THR:O    | 2.28                     | 0.64              |
| 26:b:47:ARG:NH2   | 26:b:54:ASP:OD1   | 2.31                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:G:303:LEU:HB2   | 5:G:577:ILE:HB    | 1.80                     | 0.64              |
| 5:G:135:GLN:NE2   | 42:G:802:SF4:S3   | 2.71                     | 0.63              |
| 17:S:12:GLU:HA    | 17:S:46:PRO:HG2   | 1.80                     | 0.63              |
| 6:H:93:SER:OG     | 6:H:122:SER:O     | 2.17                     | 0.63              |
| 23:Y:208:GLY:O    | 23:Y:211:ARG:NH2  | 2.31                     | 0.63              |
| 24:Z:136:ASN:ND2  | 24:Z:138:PHE:O    | 2.31                     | 0.63              |
| 17:S:15:PHE:HB2   | 17:S:49:ILE:HG13  | 1.78                     | 0.63              |
| 3:C:133:THR:HG23  | 3:C:147:VAL:HB    | 1.80                     | 0.63              |
| 8:J:121:ASN:HD21  | 25:a:66:TRP:CD1   | 2.17                     | 0.63              |
| 1:A:138:LYS:HB3   | 20:V:13:ILE:HB    | 1.80                     | 0.63              |
| 43:B:302:PLC:H3A1 | 43:q:201:PLC:H9'1 | 1.81                     | 0.63              |
| 5:G:565:HIS:O     | 5:G:566:HIS:ND1   | 2.32                     | 0.63              |
| 6:H:37:ARG:HH12   | 6:H:59:MET:HE2    | 1.64                     | 0.63              |
| 5:G:389:SER:O     | 5:G:393:ASN:ND2   | 2.32                     | 0.63              |
| 7:I:165:CYS:SG    | 7:I:166:GLY:N     | 2.72                     | 0.63              |
| 45:L:704:3PE:H341 | 45:Y:301:3PE:H361 | 1.80                     | 0.63              |
| 11:M:76:ARG:NH2   | 11:M:79:ASN:OD1   | 2.32                     | 0.63              |
| 18:T:69:THR:HG22  | 18:T:71:ASP:H     | 1.62                     | 0.62              |
| 4:D:387:ARG:NH2   | 7:I:172:CYS:O     | 2.32                     | 0.62              |
| 4:D:414:GLU:OE1   | 4:D:429:TYR:OH    | 2.17                     | 0.62              |
| 10:L:295:SER:O    | 10:L:428:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:128:ILE:O     | 1:A:132:LYS:NZ    | 2.30                     | 0.62              |
| 10:L:3:LEU:HD11   | 45:h:201:3PE:H262 | 1.80                     | 0.62              |
| 7:I:129:CYS:HB3   | 7:I:138:ILE:HG21  | 1.81                     | 0.62              |
| 25:a:65:GLN:HG3   | 29:e:10:HIS:HE2   | 1.63                     | 0.62              |
| 36:l:25:LYS:NZ    | 36:l:26:SER:OG    | 2.33                     | 0.62              |
| 22:X:117:ASN:OD1  | 25:a:60:ARG:NH1   | 2.29                     | 0.62              |
| 30:f:45:ASP:OD1   | 30:f:45:ASP:N     | 2.33                     | 0.62              |
| 31:g:161:ASP:OD1  | 31:g:161:ASP:N    | 2.25                     | 0.62              |
| 3:C:173:SER:N     | 3:C:197:GLU:O     | 2.33                     | 0.62              |
| 33:i:64:LEU:HD13  | 40:p:51:CYS:HA    | 1.81                     | 0.62              |
| 38:n:102:ARG:NH1  | 38:n:104:GLU:OE1  | 2.32                     | 0.62              |
| 6:H:107:LEU:HD11  | 25:a:25:ASN:HD22  | 1.65                     | 0.62              |
| 14:P:223:HIS:HE2  | 14:P:343:TYR:HH   | 1.43                     | 0.62              |
| 21:W:16:ASP:OD2   | 21:W:19:GLU:N     | 2.31                     | 0.62              |
| 5:G:255:GLY:O     | 5:G:598:GLN:NE2   | 2.32                     | 0.62              |
| 14:P:217:LYS:NZ   | 14:P:315:ILE:O    | 2.32                     | 0.62              |
| 11:M:85:ASP:OD2   | 11:M:263:ARG:NH2  | 2.33                     | 0.62              |
| 25:a:42:GLU:O     | 25:a:46:ASN:ND2   | 2.32                     | 0.62              |
| 5:G:348:SER:HB3   | 5:G:544:LEU:HD21  | 1.82                     | 0.61              |
| 19:U:89:ASP:OD1   | 38:n:49:ARG:NH2   | 2.33                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Y:109:GLN:NE2  | 23:Y:114:GLU:OE2  | 2.33                     | 0.61              |
| 2:B:140:MET:HG2   | 2:B:175:PRO:HG2   | 1.83                     | 0.61              |
| 10:L:80:LYS:HB2   | 10:L:486:GLU:HG3  | 1.82                     | 0.61              |
| 9:K:69:ASN:OD1    | 9:K:72:ARG:NH1    | 2.33                     | 0.61              |
| 41:q:95:GLU:HG2   | 41:q:96:GLU:HG3   | 1.82                     | 0.61              |
| 1:A:135:ALA:HB2   | 20:V:18:ASN:HB3   | 1.82                     | 0.61              |
| 10:L:608:ASN:ND2  | 18:T:138:ARG:O    | 2.34                     | 0.61              |
| 2:B:56:THR:OG1    | 43:B:302:PLC:O'   | 2.18                     | 0.61              |
| 7:I:126:CYS:HB3   | 7:I:128:LEU:HD23  | 1.82                     | 0.61              |
| 12:N:29:LEU:HD22  | 13:O:67:ILE:HD12  | 1.82                     | 0.61              |
| 49:U:201:EHZ:O2   | 49:U:201:EHZ:O1   | 2.17                     | 0.61              |
| 12:N:9:ILE:HD11   | 13:O:67:ILE:HD11  | 1.83                     | 0.60              |
| 41:q:6:ARG:NH2    | 41:q:28:ASP:OD1   | 2.34                     | 0.60              |
| 28:d:59:LEU:HD11  | 32:h:131:ILE:HD11 | 1.81                     | 0.60              |
| 6:H:216:GLU:HA    | 6:H:224:GLY:HA3   | 1.83                     | 0.60              |
| 16:R:65:LEU:O     | 16:R:70:ARG:NH2   | 2.31                     | 0.60              |
| 28:d:1:MET:HE3    | 28:d:49:ASN:HB2   | 1.82                     | 0.60              |
| 31:g:33:GLU:HG2   | 31:g:37:LYS:HE3   | 1.83                     | 0.60              |
| 14:P:118:GLU:OE1  | 14:P:309:GLN:NE2  | 2.34                     | 0.60              |
| 17:S:12:GLU:HB3   | 17:S:62:ARG:HB3   | 1.84                     | 0.60              |
| 7:I:100:LYS:NZ    | 7:I:184:GLU:OE2   | 2.35                     | 0.60              |
| 22:X:20:ASP:OD1   | 29:e:81:ARG:NH2   | 2.34                     | 0.60              |
| 2:B:203:SER:O     | 14:P:71:ARG:NH1   | 2.33                     | 0.60              |
| 5:G:390:THR:OG1   | 5:G:392:ASP:OD1   | 2.18                     | 0.60              |
| 19:U:127:GLU:OE1  | 19:U:127:GLU:N    | 2.30                     | 0.60              |
| 10:L:459:MET:O    | 10:L:463:THR:OG1  | 2.16                     | 0.60              |
| 4:D:228:LYS:HD2   | 4:D:266:TRP:HD1   | 1.66                     | 0.60              |
| 6:H:181:GLU:OE2   | 6:H:260:TYR:OH    | 2.13                     | 0.60              |
| 10:L:20:GLY:O     | 10:L:111:GLN:NE2  | 2.34                     | 0.60              |
| 14:P:43:THR:HG1   | 14:P:108:SER:HG   | 1.50                     | 0.60              |
| 5:G:175:HIS:C     | 42:G:801:SF4:S4   | 2.84                     | 0.60              |
| 13:O:62:ARG:NH2   | 46:b:102:CDL:OA4  | 2.33                     | 0.60              |
| 4:D:254:ASP:OD1   | 4:D:255:LEU:N     | 2.34                     | 0.59              |
| 8:J:104:ASP:OD1   | 30:f:63:LYS:NZ    | 2.33                     | 0.59              |
| 12:N:384:LYS:NZ   | 12:N:456:ASP:OD2  | 2.29                     | 0.59              |
| 16:R:92:ALA:HB3   | 16:R:108:ILE:HB   | 1.84                     | 0.59              |
| 4:D:191:THR:OG1   | 4:D:328:ASP:O     | 2.20                     | 0.59              |
| 4:D:428:VAL:HG12  | 4:D:443:ILE:HG12  | 1.84                     | 0.59              |
| 11:M:155:ILE:HD12 | 11:M:170:VAL:HG11 | 1.84                     | 0.59              |
| 14:P:257:GLU:OE2  | 14:P:369:ARG:NE   | 2.36                     | 0.59              |
| 16:R:21:ARG:O     | 16:R:40:ARG:NH2   | 2.34                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:o:8:GLU:O      | 39:o:30:ARG:NH1   | 2.35                     | 0.59              |
| 2:B:35:PRO:O      | 14:P:136:ARG:NH1  | 2.36                     | 0.59              |
| 20:V:134:LEU:HD12 | 27:c:84:ALA:HB2   | 1.83                     | 0.59              |
| 4:D:433:ASP:OD1   | 4:D:433:ASP:N     | 2.31                     | 0.59              |
| 7:I:99:GLU:OE2    | 41:q:26:TYR:OH    | 2.18                     | 0.59              |
| 7:I:210:GLU:HA    | 7:I:213:TYR:HD2   | 1.68                     | 0.59              |
| 11:M:31:LYS:HB3   | 31:g:92:ALA:HA    | 1.85                     | 0.59              |
| 11:M:130:LEU:HD23 | 11:M:133:ILE:HD11 | 1.83                     | 0.59              |
| 31:g:32:LYS:NZ    | 31:g:32:LYS:O     | 2.35                     | 0.59              |
| 5:G:400:ILE:HB    | 5:G:429:VAL:HG22  | 1.85                     | 0.59              |
| 4:D:103:PHE:HB3   | 4:D:116:LEU:HB3   | 1.85                     | 0.59              |
| 4:D:461:HIS:HD2   | 4:D:469:ILE:HD11  | 1.68                     | 0.59              |
| 8:J:156:LEU:HD13  | 12:N:145:ILE:HD12 | 1.85                     | 0.59              |
| 28:d:23:ARG:NH1   | 43:d:102:PLC:O1P  | 2.34                     | 0.59              |
| 45:L:703:3PE:H2I2 | 12:N:434:VAL:HG13 | 1.86                     | 0.58              |
| 12:N:487:ASN:OD1  | 28:d:19:GLN:NE2   | 2.34                     | 0.58              |
| 16:R:57:ASN:OD1   | 16:R:58:VAL:N     | 2.33                     | 0.58              |
| 17:S:45:LEU:HD12  | 17:S:46:PRO:HD2   | 1.85                     | 0.58              |
| 10:L:538:ASN:HB3  | 10:L:541:LEU:HB2  | 1.85                     | 0.58              |
| 32:h:53:HIS:O     | 32:h:54:HIS:ND1   | 2.37                     | 0.58              |
| 9:K:40:ASP:OD2    | 29:e:49:ARG:NH2   | 2.35                     | 0.58              |
| 15:Q:110:ASP:OD1  | 15:Q:111:THR:N    | 2.37                     | 0.58              |
| 20:V:110:ALA:HA   | 20:V:115:TRP:HZ3  | 1.68                     | 0.58              |
| 13:O:168:ASN:O    | 13:O:168:ASN:ND2  | 2.35                     | 0.58              |
| 23:Y:20:PHE:HE1   | 43:Y:302:PLC:H12  | 1.68                     | 0.58              |
| 5:G:242:LEU:O     | 5:G:244:ARG:NH1   | 2.37                     | 0.58              |
| 16:R:82:PRO:O     | 16:R:84:ARG:NH1   | 2.36                     | 0.58              |
| 3:C:218:LYS:HE3   | 4:D:439:TYR:CZ    | 2.39                     | 0.58              |
| 5:G:166:ILE:HG12  | 5:G:220:ILE:HD11  | 1.85                     | 0.58              |
| 45:J:201:3PE:H3A1 | 30:f:11:VAL:HG23  | 1.85                     | 0.58              |
| 6:H:172:SER:HB2   | 6:H:350:PRO:HG2   | 1.84                     | 0.58              |
| 11:M:412:ILE:HD12 | 37:m:54:ALA:HB2   | 1.86                     | 0.58              |
| 32:h:88:HIS:O     | 32:h:88:HIS:ND1   | 2.34                     | 0.58              |
| 3:C:261:VAL:HG11  | 4:D:411:PRO:HG3   | 1.85                     | 0.57              |
| 12:N:197:GLU:OE1  | 25:a:135:ARG:NH1  | 2.36                     | 0.57              |
| 8:J:134:THR:HB    | 13:O:124:MET:HE2  | 1.84                     | 0.57              |
| 10:L:534:LEU:HD22 | 38:n:35:ILE:HG12  | 1.87                     | 0.57              |
| 14:P:257:GLU:HG2  | 14:P:261:MET:HE2  | 1.85                     | 0.57              |
| 1:A:27:ILE:O      | 2:B:61:LYS:NZ     | 2.38                     | 0.57              |
| 10:L:277:ILE:HG23 | 10:L:314:MET:HE3  | 1.86                     | 0.57              |
| 11:M:14:ILE:HG21  | 43:M:504:PLC:H5A2 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:131:ILE:HG23 | 14:P:175:VAL:HG11 | 1.85                     | 0.57              |
| 40:p:44:CYS:SG    | 40:p:69:LYS:NZ    | 2.68                     | 0.57              |
| 12:N:170:ILE:HG13 | 12:N:207:GLY:HA3  | 1.86                     | 0.57              |
| 22:X:48:LEU:O     | 22:X:120:TYR:OH   | 2.15                     | 0.57              |
| 31:g:136:GLU:N    | 31:g:139:GLU:OE2  | 2.34                     | 0.57              |
| 41:q:44:PHE:HZ    | 41:q:73:VAL:HG13  | 1.69                     | 0.57              |
| 38:n:19:TYR:OH    | 38:n:72:GLU:OE2   | 2.22                     | 0.57              |
| 6:H:32:LEU:HD21   | 6:H:245:MET:HE2   | 1.86                     | 0.57              |
| 6:H:121:ALA:HB1   | 8:J:52:THR:HB     | 1.86                     | 0.57              |
| 10:L:269:TYR:HH   | 40:p:60:TYR:HH    | 1.53                     | 0.57              |
| 1:A:108:LEU:HD23  | 1:A:111:ILE:HD12  | 1.86                     | 0.57              |
| 2:B:108:ASP:OD1   | 2:B:108:ASP:N     | 2.34                     | 0.57              |
| 3:C:154:ARG:NH2   | 20:V:89:SER:O     | 2.38                     | 0.57              |
| 5:G:353:LYS:NZ    | 17:S:12:GLU:OE1   | 2.37                     | 0.57              |
| 10:L:627:VAL:HG21 | 12:N:262:ASP:HB3  | 1.86                     | 0.57              |
| 13:O:118:ASN:OD1  | 13:O:121:GLN:NE2  | 2.38                     | 0.57              |
| 14:P:188:ARG:HB2  | 14:P:246:GLU:HG2  | 1.87                     | 0.57              |
| 1:A:138:LYS:HB2   | 20:V:15:ILE:HD11  | 1.87                     | 0.57              |
| 12:N:304:LEU:HD23 | 12:N:307:ILE:HD12 | 1.87                     | 0.57              |
| 11:M:144:PHE:CZ   | 11:M:224:LYS:HG3  | 2.40                     | 0.56              |
| 31:g:164:SER:OG   | 31:g:166:ASP:OD1  | 2.17                     | 0.56              |
| 3:C:223:THR:HG21  | 3:C:244:LEU:HD11  | 1.86                     | 0.56              |
| 6:H:148:ARG:HH21  | 6:H:221:LEU:HD11  | 1.69                     | 0.56              |
| 9:K:51:ILE:HD13   | 12:N:130:ILE:HD11 | 1.85                     | 0.56              |
| 24:Z:71:GLN:NE2   | 24:Z:75:ASP:OD1   | 2.38                     | 0.56              |
| 3:C:133:THR:OG1   | 3:C:134:ALA:N     | 2.38                     | 0.56              |
| 5:G:249:ASP:OD1   | 5:G:250:VAL:N     | 2.38                     | 0.56              |
| 8:J:20:ASN:ND2    | 8:J:23:GLU:OE1    | 2.38                     | 0.56              |
| 12:N:124:ASP:OD1  | 12:N:125:ILE:N    | 2.39                     | 0.56              |
| 14:P:209:LEU:HD21 | 14:P:288:PHE:HE2  | 1.69                     | 0.56              |
| 20:V:42:TYR:HB3   | 20:V:71:LEU:HD22  | 1.86                     | 0.56              |
| 12:N:112:ASN:HD22 | 12:N:235:TYR:HE2  | 1.53                     | 0.56              |
| 2:B:161:ASP:OD1   | 2:B:161:ASP:N     | 2.26                     | 0.56              |
| 45:L:702:3PE:H3D1 | 45:L:705:3PE:H2F1 | 1.87                     | 0.56              |
| 5:G:432:VAL:HG22  | 5:G:445:LEU:HD12  | 1.87                     | 0.56              |
| 17:S:52:ALA:HB3   | 17:S:55:ILE:HG12  | 1.88                     | 0.56              |
| 22:X:26:GLU:HG3   | 24:Z:81:ARG:HG2   | 1.88                     | 0.56              |
| 17:S:27:LEU:HD22  | 17:S:57:PRO:HB3   | 1.87                     | 0.56              |
| 11:M:128:MET:HE1  | 11:M:248:LEU:HD22 | 1.88                     | 0.56              |
| 3:C:150:LEU:HB2   | 3:C:159:ILE:HG22  | 1.87                     | 0.55              |
| 11:M:110:LEU:HB2  | 11:M:114:TYR:CZ   | 2.41                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:X:27:ASN:HD21  | 29:e:78:PRO:HG2   | 1.71                     | 0.55              |
| 3:C:88:LEU:HD13   | 3:C:114:VAL:HG22  | 1.89                     | 0.55              |
| 11:M:437:SER:OG   | 11:M:438:VAL:N    | 2.39                     | 0.55              |
| 14:P:130:ASN:HD22 | 14:P:169:LYS:HG2  | 1.71                     | 0.55              |
| 22:X:29:LYS:HG2   | 25:a:96:THR:HG21  | 1.88                     | 0.55              |
| 22:X:42:ALA:O     | 25:a:73:ARG:NH1   | 2.36                     | 0.55              |
| 5:G:108:ARG:HB3   | 5:G:141:TYR:HB3   | 1.88                     | 0.55              |
| 10:L:620:TRP:CE2  | 25:a:121:PRO:HG3  | 2.41                     | 0.55              |
| 41:q:37:THR:HG22  | 41:q:43:LYS:HA    | 1.89                     | 0.55              |
| 5:G:241:GLU:OE1   | 7:I:127:LYS:NZ    | 2.35                     | 0.55              |
| 10:L:379:LEU:HD22 | 10:L:384:ILE:HG13 | 1.89                     | 0.55              |
| 24:Z:23:ARG:HG2   | 27:c:28:LEU:HD22  | 1.87                     | 0.55              |
| 36:l:118:TYR:O    | 37:m:80:ARG:NH2   | 2.40                     | 0.55              |
| 5:G:112:THR:HG21  | 5:G:142:GLY:HA3   | 1.89                     | 0.55              |
| 5:G:173:CYS:SG    | 5:G:174:ILE:N     | 2.79                     | 0.55              |
| 6:H:53:GLY:HA3    | 6:H:58:LEU:HB2    | 1.88                     | 0.55              |
| 45:J:201:3PE:H391 | 45:J:201:3PE:H331 | 1.88                     | 0.55              |
| 10:L:170:ILE:HD12 | 10:L:232:TRP:HB3  | 1.88                     | 0.55              |
| 14:P:34:ARG:NH1   | 14:P:83:GLY:O     | 2.39                     | 0.55              |
| 1:A:75:PHE:HE2    | 8:J:58:ALA:HA     | 1.72                     | 0.55              |
| 7:I:151:ARG:NH2   | 16:R:120:TYR:O    | 2.34                     | 0.55              |
| 3:C:77:LEU:HD22   | 3:C:102:LEU:HB2   | 1.88                     | 0.55              |
| 4:D:433:ASP:HB3   | 20:V:130:PHE:CZ   | 2.42                     | 0.55              |
| 4:D:196:ILE:HG23  | 4:D:229:LEU:HD22  | 1.88                     | 0.55              |
| 11:M:78:LEU:H     | 45:M:502:3PE:HN3  | 1.54                     | 0.55              |
| 11:M:301:LEU:HD22 | 11:M:349:VAL:HG13 | 1.89                     | 0.55              |
| 45:M:501:3PE:H392 | 45:h:201:3PE:H382 | 1.89                     | 0.55              |
| 28:d:72:LEU:O     | 28:d:75:SER:OG    | 2.25                     | 0.55              |
| 5:G:175:HIS:O     | 5:G:176:CYS:HB3   | 2.06                     | 0.55              |
| 5:G:235:PHE:HB3   | 7:I:150:ARG:HG3   | 1.88                     | 0.55              |
| 41:q:70:MET:HE1   | 41:q:81:LEU:HD23  | 1.89                     | 0.55              |
| 1:A:106:PHE:CD1   | 8:J:144:SER:HB3   | 2.42                     | 0.54              |
| 5:G:456:LEU:HD13  | 5:G:494:PHE:HB2   | 1.89                     | 0.54              |
| 11:M:352:ILE:HD11 | 11:M:453:GLU:HB3  | 1.90                     | 0.54              |
| 13:O:30:LEU:O     | 13:O:34:GLY:N     | 2.37                     | 0.54              |
| 22:X:59:GLN:NE2   | 22:X:63:ASP:OD2   | 2.40                     | 0.54              |
| 7:I:115:ARG:NH2   | 16:R:72:TYR:O     | 2.40                     | 0.54              |
| 11:M:111:LYS:HE2  | 12:N:458:LEU:HD13 | 1.90                     | 0.54              |
| 40:p:3:ASP:OD1    | 40:p:3:ASP:N      | 2.41                     | 0.54              |
| 3:C:130:MET:HE3   | 4:D:444:ARG:HH21  | 1.72                     | 0.54              |
| 5:G:332:LYS:H     | 5:G:335:GLU:HB2   | 1.72                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:261:MET:HE1  | 10:L:326:LEU:HD13 | 1.89                     | 0.54              |
| 11:M:226:PRO:HG3  | 11:M:234:LEU:HD22 | 1.90                     | 0.54              |
| 12:N:12:TYR:HD1   | 46:b:102:CDL:HA61 | 1.72                     | 0.54              |
| 23:Y:159:ASN:OD1  | 23:Y:160:LEU:N    | 2.40                     | 0.54              |
| 36:l:126:ARG:NH2  | 39:o:26:ASP:OD2   | 2.39                     | 0.54              |
| 7:I:169:GLN:OE1   | 7:I:222:ARG:NH2   | 2.40                     | 0.54              |
| 3:C:142:ASN:HB2   | 20:V:126:GLN:HE22 | 1.73                     | 0.54              |
| 29:e:21:GLN:NE2   | 32:h:150:PRO:O    | 2.40                     | 0.54              |
| 1:A:35:GLU:O      | 14:P:53:ARG:NH2   | 2.35                     | 0.54              |
| 3:C:204:ARG:NH2   | 3:C:211:PHE:O     | 2.39                     | 0.54              |
| 43:D:501:PLC:H42  | 7:I:70:TRP:HE1    | 1.73                     | 0.54              |
| 10:L:491:PRO:O    | 36:l:128:TYR:OH   | 2.23                     | 0.54              |
| 3:C:101:GLU:OE1   | 3:C:160:ARG:NH2   | 2.33                     | 0.54              |
| 3:C:170:PRO:HB3   | 3:C:195:PHE:HD2   | 1.72                     | 0.54              |
| 8:J:25:ILE:HD13   | 9:K:20:ILE:HD11   | 1.89                     | 0.54              |
| 8:J:124:ASP:N     | 8:J:124:ASP:OD1   | 2.40                     | 0.54              |
| 11:M:6:LEU:O      | 11:M:10:ASN:ND2   | 2.38                     | 0.54              |
| 35:k:32:PHE:O     | 35:k:36:GLY:N     | 2.41                     | 0.54              |
| 5:G:379:ALA:HA    | 5:G:385:TYR:HE2   | 1.71                     | 0.54              |
| 11:M:267:PRO:O    | 40:p:87:LYS:NZ    | 2.41                     | 0.54              |
| 22:X:31:PRO:HD2   | 22:X:34:ILE:HD12  | 1.90                     | 0.54              |
| 6:H:81:ILE:HD11   | 30:f:14:PHE:HB3   | 1.90                     | 0.54              |
| 10:L:485:ASN:OD1  | 10:L:485:ASN:N    | 2.40                     | 0.54              |
| 26:b:3:ILE:HD13   | 26:b:3:ILE:H      | 1.73                     | 0.54              |
| 9:K:7:MET:HB3     | 25:a:119:ASN:HD22 | 1.71                     | 0.53              |
| 10:L:618:LEU:HD13 | 45:L:702:3PE:H3E2 | 1.89                     | 0.53              |
| 24:Z:23:ARG:NH1   | 27:c:28:LEU:O     | 2.40                     | 0.53              |
| 14:P:120:PHE:HB2  | 14:P:125:SER:HA   | 1.90                     | 0.53              |
| 39:o:52:GLU:OE1   | 39:o:52:GLU:N     | 2.40                     | 0.53              |
| 4:D:221:TRP:CZ2   | 7:I:86:MET:HG3    | 2.43                     | 0.53              |
| 4:D:313:ARG:NH1   | 4:D:320:ASP:OD1   | 2.41                     | 0.53              |
| 10:L:437:ASN:ND2  | 35:k:13:ARG:O     | 2.30                     | 0.53              |
| 10:L:584:LEU:O    | 10:L:589:GLY:HA3  | 2.08                     | 0.53              |
| 11:M:330:GLY:HA3  | 11:M:400:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:28:VAL:HG12   | 6:H:69:SER:HA     | 1.91                     | 0.53              |
| 4:D:40:ASP:OD1    | 4:D:40:ASP:N      | 2.39                     | 0.53              |
| 11:M:97:ILE:HD13  | 31:g:150:MET:HE1  | 1.90                     | 0.53              |
| 17:S:15:PHE:N     | 17:S:48:LEU:O     | 2.37                     | 0.53              |
| 3:C:106:VAL:HG11  | 3:C:114:VAL:HG21  | 1.91                     | 0.53              |
| 10:L:10:PHE:HE1   | 43:L:701:PLC:H9A1 | 1.74                     | 0.53              |
| 10:L:59:TYR:HE2   | 45:h:201:3PE:H251 | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:S:17:LEU:HB3   | 17:S:27:LEU:HD23  | 1.90                     | 0.53              |
| 7:I:110:GLU:OE2   | 7:I:203:ASN:ND2   | 2.41                     | 0.53              |
| 8:J:5:ILE:HD12    | 30:f:34:GLN:HE22  | 1.72                     | 0.53              |
| 16:R:95:ASP:OD1   | 16:R:95:ASP:N     | 2.40                     | 0.53              |
| 3:C:126:PHE:CD1   | 3:C:152:SER:HB2   | 2.44                     | 0.53              |
| 2:B:199:MET:HG3   | 2:B:203:SER:HB2   | 1.90                     | 0.53              |
| 6:H:169:LEU:HD21  | 6:H:340:PRO:HG3   | 1.90                     | 0.53              |
| 34:j:55:HIS:N     | 34:j:58:GLU:OE1   | 2.42                     | 0.53              |
| 7:I:57:GLU:OE2    | 26:b:15:ARG:NH2   | 2.40                     | 0.52              |
| 8:J:105:TYR:HA    | 29:e:55:ARG:HD3   | 1.91                     | 0.52              |
| 4:D:201:ASN:HD21  | 4:D:423:LYS:HE3   | 1.73                     | 0.52              |
| 4:D:391:LYS:HB3   | 16:R:104:PRO:HA   | 1.91                     | 0.52              |
| 5:G:217:ALA:O     | 5:G:288:ARG:NH1   | 2.42                     | 0.52              |
| 6:H:9:ILE:HA      | 6:H:12:ILE:HG22   | 1.89                     | 0.52              |
| 45:h:201:3PE:H2I2 | 33:i:40:CYS:HB3   | 1.90                     | 0.52              |
| 8:J:112:ASP:O     | 25:a:100:GLN:NE2  | 2.43                     | 0.52              |
| 12:N:387:PHE:CD1  | 12:N:454:SER:HB3  | 2.45                     | 0.52              |
| 13:O:165:GLU:OE1  | 13:O:165:GLU:N    | 2.37                     | 0.52              |
| 36:l:144:ASP:O    | 36:l:146:LEU:N    | 2.42                     | 0.52              |
| 5:G:379:ALA:HA    | 5:G:385:TYR:CE2   | 2.45                     | 0.52              |
| 8:J:43:TYR:OH     | 25:a:106:ARG:O    | 2.24                     | 0.52              |
| 4:D:166:ASN:ND2   | 4:D:426:MET:SD    | 2.82                     | 0.52              |
| 14:P:192:MET:HB3  | 14:P:224:ALA:HB2  | 1.92                     | 0.52              |
| 1:A:133:ASN:OD1   | 1:A:134:LYS:N     | 2.42                     | 0.52              |
| 3:C:242:LEU:HD23  | 15:Q:101:TYR:HB3  | 1.92                     | 0.52              |
| 4:D:230:MET:HE2   | 4:D:240:ARG:HE    | 1.75                     | 0.52              |
| 5:G:238:ARG:HG3   | 7:I:127:LYS:HB2   | 1.92                     | 0.52              |
| 5:G:356:VAL:HG13  | 5:G:361:SER:HB3   | 1.91                     | 0.52              |
| 6:H:154:ILE:HD11  | 8:J:61:ILE:HG12   | 1.91                     | 0.52              |
| 12:N:461:LYS:NZ   | 12:N:462:ASP:OD1  | 2.38                     | 0.52              |
| 36:l:133:LEU:HD11 | 39:o:25:ARG:HB2   | 1.91                     | 0.52              |
| 6:H:324:CYS:HA    | 6:H:328:LEU:HB2   | 1.92                     | 0.52              |
| 3:C:243:GLU:HG3   | 14:P:33:GLY:HA3   | 1.90                     | 0.52              |
| 5:G:567:GLY:HA3   | 41:q:131:TRP:CD1  | 2.44                     | 0.52              |
| 5:G:606:PRO:HB2   | 5:G:610:ALA:HB3   | 1.91                     | 0.52              |
| 3:C:229:ARG:NH2   | 3:C:240:GLU:OE2   | 2.40                     | 0.52              |
| 5:G:128:GLN:HE22  | 5:G:132:CYS:HB3   | 1.75                     | 0.52              |
| 5:G:541:ILE:O     | 5:G:560:VAL:HA    | 2.10                     | 0.52              |
| 14:P:266:ILE:HG23 | 14:P:348:ILE:HA   | 1.92                     | 0.52              |
| 19:U:122:TYR:HD1  | 19:U:123:ILE:HD13 | 1.75                     | 0.52              |
| 33:i:26:TRP:O     | 33:i:30:THR:OG1   | 2.21                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:236:VAL:O     | 7:I:106:ARG:NH1   | 2.42                     | 0.52              |
| 5:G:401:LEU:HD23  | 5:G:472:ILE:HG23  | 1.90                     | 0.52              |
| 9:K:73:ILE:O      | 9:K:76:SER:OG     | 2.19                     | 0.52              |
| 45:L:702:3PE:H2H1 | 12:N:272:LEU:HD11 | 1.92                     | 0.52              |
| 12:N:28:ARG:HG2   | 12:N:86:SER:OG    | 2.10                     | 0.52              |
| 17:S:2:SER:OG     | 17:S:3:LYS:N      | 2.42                     | 0.52              |
| 5:G:389:SER:O     | 5:G:390:THR:OG1   | 2.28                     | 0.51              |
| 45:L:704:3PE:H282 | 23:Y:144:GLY:HA3  | 1.92                     | 0.51              |
| 28:d:27:PHE:O     | 28:d:34:TYR:OH    | 2.19                     | 0.51              |
| 4:D:285:ARG:NE    | 7:I:75:GLU:OE2    | 2.29                     | 0.51              |
| 5:G:292:ASP:OD1   | 5:G:697:SER:OG    | 2.27                     | 0.51              |
| 8:J:95:LEU:O      | 30:f:44:ARG:NH1   | 2.43                     | 0.51              |
| 22:X:70:LYS:HE3   | 26:b:65:LEU:HD13  | 1.90                     | 0.51              |
| 4:D:156:ASP:N     | 4:D:156:ASP:OD1   | 2.41                     | 0.51              |
| 5:G:478:VAL:O     | 5:G:481:THR:OG1   | 2.24                     | 0.51              |
| 1:A:48:GLY:O      | 2:B:105:ARG:NH2   | 2.30                     | 0.51              |
| 5:G:347:GLU:N     | 5:G:347:GLU:OE1   | 2.44                     | 0.51              |
| 5:G:596:ARG:HG3   | 5:G:653:VAL:HG22  | 1.93                     | 0.51              |
| 8:J:5:ILE:HD12    | 30:f:34:GLN:NE2   | 2.26                     | 0.51              |
| 8:J:23:GLU:O      | 8:J:27:ILE:HG12   | 2.10                     | 0.51              |
| 20:V:35:ARG:HB2   | 20:V:36:PRO:HD3   | 1.93                     | 0.51              |
| 4:D:123:GLU:OE2   | 6:H:148:ARG:NH1   | 2.35                     | 0.51              |
| 5:G:128:GLN:O     | 5:G:128:GLN:NE2   | 2.44                     | 0.51              |
| 5:G:279:ASN:OD1   | 5:G:279:ASN:N     | 2.44                     | 0.51              |
| 12:N:46:THR:OG1   | 12:N:49:ASN:OD1   | 2.28                     | 0.51              |
| 14:P:212:ASN:OD1  | 14:P:212:ASN:N    | 2.43                     | 0.51              |
| 4:D:85:ASP:HB2    | 12:N:372:THR:HG21 | 1.93                     | 0.51              |
| 45:L:706:3PE:H31  | 36:l:83:PRO:HG3   | 1.93                     | 0.51              |
| 22:X:66:MET:HB3   | 26:b:65:LEU:HD21  | 1.92                     | 0.51              |
| 40:p:64:ARG:NH1   | 40:p:68:GLU:HB2   | 2.25                     | 0.51              |
| 5:G:124:PRO:O     | 5:G:238:ARG:NH2   | 2.44                     | 0.51              |
| 18:T:88:ASP:OD1   | 21:W:56:ARG:NH2   | 2.44                     | 0.51              |
| 6:H:4:ASN:O       | 6:H:4:ASN:ND2     | 2.39                     | 0.51              |
| 8:J:70:ILE:HG23   | 18:T:133:ILE:HD11 | 1.92                     | 0.51              |
| 2:B:114:GLY:HA2   | 42:B:301:SF4:S2   | 2.50                     | 0.51              |
| 2:B:200:TRP:HA    | 2:B:204:TYR:HB2   | 1.93                     | 0.51              |
| 8:J:1:FME:HE2     | 8:J:3:LEU:HD21    | 1.93                     | 0.51              |
| 8:J:154:LEU:HD11  | 9:K:61:ALA:HB1    | 1.93                     | 0.51              |
| 9:K:12:GLY:O      | 18:T:138:ARG:NH2  | 2.43                     | 0.51              |
| 11:M:36:ILE:HG22  | 11:M:37:LYS:HG3   | 1.93                     | 0.51              |
| 22:X:127:GLU:OE2  | 22:X:142:LYS:NZ   | 2.38                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:133:THR:HB    | 4:D:442:LYS:HG2   | 1.91                     | 0.51              |
| 18:T:88:ASP:OD1   | 18:T:88:ASP:N     | 2.42                     | 0.51              |
| 4:D:387:ARG:NH1   | 7:I:175:ASP:OD1   | 2.43                     | 0.50              |
| 5:G:540:PHE:HD1   | 5:G:559:PHE:HB3   | 1.76                     | 0.50              |
| 10:L:22:TYR:OH    | 32:h:65:ASN:ND2   | 2.44                     | 0.50              |
| 10:L:354:TYR:O    | 10:L:360:TYR:OH   | 2.26                     | 0.50              |
| 6:H:317:TYR:HA    | 6:H:320:LEU:HD12  | 1.94                     | 0.50              |
| 10:L:641:ILE:HD11 | 45:L:702:3PE:H272 | 1.93                     | 0.50              |
| 2:B:95:ARG:HA     | 6:H:49:PRO:HA     | 1.93                     | 0.50              |
| 21:W:54:LYS:HG2   | 21:W:99:PHE:CD1   | 2.46                     | 0.50              |
| 33:i:67:TRP:O     | 33:i:70:SER:OG    | 2.23                     | 0.50              |
| 6:H:291:SER:OG    | 25:a:21:GLY:HA3   | 2.11                     | 0.50              |
| 24:Z:43:TYR:HD1   | 45:Z:201:3PE:H242 | 1.77                     | 0.50              |
| 36:l:88:PHE:CD2   | 36:l:89:VAL:HG13  | 2.46                     | 0.50              |
| 16:R:118:CYS:SG   | 16:R:119:GLY:N    | 2.83                     | 0.50              |
| 26:b:19:TYR:O     | 26:b:23:THR:OG1   | 2.29                     | 0.50              |
| 35:k:10:ASP:OD2   | 38:n:42:ARG:NE    | 2.36                     | 0.50              |
| 3:C:170:PRO:HG3   | 21:W:13:TYR:CG    | 2.46                     | 0.50              |
| 4:D:229:LEU:HD21  | 4:D:266:TRP:CZ2   | 2.47                     | 0.50              |
| 10:L:241:THR:HG21 | 10:L:344:GLY:HA3  | 1.94                     | 0.50              |
| 12:N:116:LEU:HD11 | 12:N:239:MET:HB3  | 1.94                     | 0.50              |
| 14:P:130:ASN:OD1  | 14:P:130:ASN:N    | 2.44                     | 0.50              |
| 2:B:115:THR:HA    | 2:B:143:CYS:HB3   | 1.93                     | 0.50              |
| 9:K:5:LEU:HD22    | 10:L:617:VAL:HG12 | 1.93                     | 0.50              |
| 3:C:154:ARG:NH2   | 20:V:90:GLY:HA3   | 2.27                     | 0.50              |
| 5:G:474:ILE:HG23  | 5:G:478:VAL:HG21  | 1.93                     | 0.50              |
| 8:J:38:GLU:OE2    | 25:a:109:TRP:N    | 2.34                     | 0.50              |
| 14:P:306:ASN:OD1  | 14:P:306:ASN:N    | 2.42                     | 0.50              |
| 31:g:31:GLU:O     | 31:g:97:ASN:ND2   | 2.44                     | 0.50              |
| 2:B:69:PHE:O      | 2:B:71:PRO:HD3    | 2.11                     | 0.50              |
| 43:D:501:PLC:H7A2 | 6:H:194:PRO:HB3   | 1.94                     | 0.50              |
| 45:M:501:3PE:H3H1 | 43:g:301:PLC:H1A1 | 1.94                     | 0.50              |
| 25:a:115:ILE:HG23 | 25:a:116:ILE:HG13 | 1.93                     | 0.50              |
| 5:G:354:ASP:OD1   | 5:G:354:ASP:N     | 2.45                     | 0.49              |
| 5:G:436:PHE:CE2   | 5:G:438:SER:HB2   | 2.47                     | 0.49              |
| 10:L:217:LEU:HD13 | 10:L:277:ILE:HG12 | 1.93                     | 0.49              |
| 11:M:486:ILE:HD12 | 40:p:79:ILE:HG22  | 1.94                     | 0.49              |
| 2:B:39:PRO:HA     | 14:P:97:ASN:HD22  | 1.78                     | 0.49              |
| 3:C:191:LEU:HA    | 3:C:215:PRO:HD2   | 1.93                     | 0.49              |
| 11:M:43:LYS:NZ    | 11:M:107:TRP:O    | 2.43                     | 0.49              |
| 11:M:43:LYS:HD3   | 11:M:114:TYR:CD1  | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:N:202:LEU:HB2  | 12:N:263:LEU:HD11 | 1.94                     | 0.49              |
| 12:N:518:LEU:HD22 | 12:N:521:ASN:HB2  | 1.93                     | 0.49              |
| 14:P:230:ALA:HA   | 14:P:331:MET:HE1  | 1.92                     | 0.49              |
| 14:P:303:PRO:HA   | 43:P:503:PLC:H73  | 1.93                     | 0.49              |
| 18:T:53:ASP:OD1   | 18:T:53:ASP:N     | 2.43                     | 0.49              |
| 39:o:26:ASP:OD1   | 39:o:26:ASP:N     | 2.43                     | 0.49              |
| 2:B:105:ARG:HH21  | 6:H:73:VAL:HG11   | 1.77                     | 0.49              |
| 3:C:148:TYR:HB2   | 3:C:161:ILE:HB    | 1.94                     | 0.49              |
| 31:g:96:ASP:OD1   | 31:g:96:ASP:N     | 2.45                     | 0.49              |
| 5:G:462:LYS:O     | 5:G:465:SER:OG    | 2.20                     | 0.49              |
| 7:I:122:ARG:NH1   | 7:I:174:VAL:O     | 2.45                     | 0.49              |
| 10:L:40:VAL:HG22  | 10:L:90:VAL:HG12  | 1.95                     | 0.49              |
| 10:L:563:LEU:HD21 | 45:L:706:3PE:H242 | 1.94                     | 0.49              |
| 22:X:183:ILE:HD13 | 22:X:183:ILE:H    | 1.76                     | 0.49              |
| 23:Y:182:LYS:NZ   | 40:p:13:ASP:O     | 2.44                     | 0.49              |
| 4:D:320:ASP:HB3   | 4:D:323:LYS:HG2   | 1.93                     | 0.49              |
| 14:P:153:SER:O    | 14:P:189:PRO:HD2  | 2.12                     | 0.49              |
| 7:I:175:ASP:OD1   | 7:I:175:ASP:N     | 2.44                     | 0.49              |
| 12:N:366:MET:HA   | 12:N:366:MET:HE2  | 1.95                     | 0.49              |
| 24:Z:16:TRP:HE1   | 27:c:0:ACE:H2     | 1.78                     | 0.49              |
| 39:o:60:GLN:HE21  | 39:o:60:GLN:HA    | 1.78                     | 0.49              |
| 4:D:283:ASP:OD1   | 27:c:173:TYR:OH   | 2.25                     | 0.49              |
| 6:H:145:ALA:HB2   | 6:H:221:LEU:HD13  | 1.94                     | 0.49              |
| 8:J:109:TYR:CE1   | 25:a:104:ASN:HB3  | 2.47                     | 0.49              |
| 11:M:383:SER:OG   | 11:M:431:THR:OG1  | 2.31                     | 0.49              |
| 25:a:60:ARG:HG2   | 25:a:63:THR:HG22  | 1.94                     | 0.49              |
| 9:K:7:MET:HB3     | 25:a:119:ASN:ND2  | 2.27                     | 0.49              |
| 12:N:24:LYS:HD2   | 12:N:100:TYR:CZ   | 2.48                     | 0.49              |
| 10:L:436:ASN:OD1  | 10:L:437:ASN:N    | 2.45                     | 0.49              |
| 12:N:129:PHE:O    | 12:N:133:GLU:HG2  | 2.13                     | 0.49              |
| 15:Q:118:PHE:O    | 15:Q:122:GLN:HG2  | 2.13                     | 0.49              |
| 19:U:108:ASN:OD1  | 19:U:108:ASN:N    | 2.44                     | 0.49              |
| 2:B:87:SER:HA     | 2:B:93:GLN:HG2    | 1.93                     | 0.49              |
| 7:I:100:LYS:HE3   | 41:q:70:MET:HE2   | 1.94                     | 0.49              |
| 2:B:93:GLN:HE22   | 2:B:100:PHE:HD1   | 1.61                     | 0.48              |
| 3:C:48:LEU:HA     | 3:C:51:LEU:HG     | 1.94                     | 0.48              |
| 11:M:300:ASP:HB3  | 11:M:303:VAL:HB   | 1.95                     | 0.48              |
| 25:a:75:LEU:HB2   | 25:a:81:LEU:HD23  | 1.95                     | 0.48              |
| 39:o:3:VAL:HG11   | 39:o:31:LEU:HD11  | 1.94                     | 0.48              |
| 3:C:229:ARG:HD2   | 14:P:34:ARG:HH21  | 1.78                     | 0.48              |
| 7:I:146:ILE:HG21  | 16:R:22:ILE:HA    | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:14:TYR:HA     | 8:J:17:ILE:HG12   | 1.94                     | 0.48              |
| 14:P:220:TYR:N    | 14:P:317:GLN:OE1  | 2.46                     | 0.48              |
| 36:l:155:SER:O    | 39:o:27:ARG:NH2   | 2.46                     | 0.48              |
| 3:C:170:PRO:HB3   | 3:C:195:PHE:CD2   | 2.48                     | 0.48              |
| 17:S:24:SER:HA    | 17:S:57:PRO:HG3   | 1.94                     | 0.48              |
| 18:T:102:VAL:HG11 | 18:T:122:VAL:HG22 | 1.94                     | 0.48              |
| 19:U:60:ILE:HG12  | 35:k:9:ARG:HE     | 1.79                     | 0.48              |
| 27:c:163:GLU:HA   | 27:c:166:HIS:CE1  | 2.48                     | 0.48              |
| 3:C:118:LEU:HD12  | 3:C:161:ILE:HD11  | 1.96                     | 0.48              |
| 10:L:385:PRO:HB2  | 34:j:50:TRP:CZ3   | 2.48                     | 0.48              |
| 43:L:701:PLC:H42  | 33:i:18:GLY:HA3   | 1.94                     | 0.48              |
| 11:M:415:LEU:HD21 | 45:m:101:3PE:H2B1 | 1.95                     | 0.48              |
| 15:Q:57:ILE:HG22  | 15:Q:75:TRP:HE3   | 1.78                     | 0.48              |
| 41:q:47:VAL:HG11  | 41:q:52:GLU:HG3   | 1.95                     | 0.48              |
| 5:G:616:ILE:O     | 5:G:620:LEU:N     | 2.38                     | 0.48              |
| 6:H:24:SER:OG     | 25:a:16:GLY:O     | 2.28                     | 0.48              |
| 10:L:127:LEU:HD22 | 10:L:143:ILE:HD11 | 1.95                     | 0.48              |
| 12:N:176:SER:OG   | 12:N:200:ASP:OD2  | 2.23                     | 0.48              |
| 2:B:125:ARG:NH1   | 2:B:163:ILE:O     | 2.46                     | 0.48              |
| 5:G:657:SER:HB3   | 17:S:19:GLN:HB3   | 1.96                     | 0.48              |
| 14:P:34:ARG:NH2   | 14:P:82:ASN:O     | 2.47                     | 0.48              |
| 18:T:50:THR:OG1   | 18:T:53:ASP:OD1   | 2.32                     | 0.48              |
| 41:q:47:VAL:HG12  | 41:q:49:ASP:H     | 1.78                     | 0.48              |
| 8:J:97:ASP:O      | 25:a:112:ARG:HD2  | 2.13                     | 0.48              |
| 12:N:291:LEU:HD22 | 12:N:449:ILE:HD11 | 1.95                     | 0.48              |
| 23:Y:188:ARG:NH2  | 23:Y:206:ASP:OD1  | 2.42                     | 0.48              |
| 25:a:2:ILE:HD12   | 46:q:203:CDL:HB4  | 1.94                     | 0.48              |
| 5:G:430:HIS:CD2   | 5:G:460:VAL:HG13  | 2.48                     | 0.48              |
| 5:G:632:ASN:ND2   | 5:G:635:GLU:OE2   | 2.47                     | 0.48              |
| 6:H:34:VAL:HG22   | 6:H:59:MET:HB3    | 1.96                     | 0.48              |
| 6:H:47:LEU:HD12   | 7:I:93:THR:HB     | 1.96                     | 0.48              |
| 6:H:209:ARG:HH22  | 6:H:309:ARG:HH11  | 1.60                     | 0.48              |
| 10:L:552:ILE:HG22 | 36:l:98:PHE:HD1   | 1.78                     | 0.48              |
| 11:M:179:LEU:HB3  | 12:N:436:ILE:HD13 | 1.95                     | 0.48              |
| 11:M:334:LEU:HB2  | 11:M:397:GLY:HA3  | 1.95                     | 0.48              |
| 14:P:316:ASN:OD1  | 14:P:316:ASN:N    | 2.46                     | 0.48              |
| 17:S:14:ARG:HG2   | 17:S:48:LEU:HD12  | 1.96                     | 0.48              |
| 20:V:15:ILE:HG22  | 20:V:16:LYS:HG3   | 1.94                     | 0.48              |
| 39:o:7:PRO:HG3    | 39:o:31:LEU:HG    | 1.96                     | 0.48              |
| 5:G:262:THR:HG22  | 5:G:267:VAL:HG22  | 1.95                     | 0.48              |
| 7:I:37:SER:HB2    | 27:c:146:PRO:HG2  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:I:111:HIS:HD2   | 7:I:168:CYS:SG    | 2.18                     | 0.48              |
| 11:M:85:ASP:OD1   | 11:M:85:ASP:N     | 2.45                     | 0.48              |
| 1:A:2:LEU:HD11    | 25:a:81:LEU:HD12  | 1.96                     | 0.47              |
| 1:A:5:LEU:HD13    | 6:H:14:TYR:HD1    | 1.79                     | 0.47              |
| 4:D:380:PHE:HB2   | 5:G:144:ASP:HB2   | 1.96                     | 0.47              |
| 5:G:455:ALA:O     | 5:G:461:GLY:N     | 2.47                     | 0.47              |
| 20:V:110:ALA:HA   | 20:V:115:TRP:CZ3  | 2.49                     | 0.47              |
| 7:I:128:LEU:O     | 7:I:132:VAL:HG23  | 2.15                     | 0.47              |
| 14:P:69:PRO:HB2   | 14:P:93:PHE:CD1   | 2.49                     | 0.47              |
| 3:C:187:GLU:OE1   | 4:D:442:LYS:NZ    | 2.47                     | 0.47              |
| 5:G:373:VAL:HG21  | 5:G:531:PRO:HA    | 1.95                     | 0.47              |
| 6:H:70:LYS:HB2    | 6:H:231:ALA:HB2   | 1.95                     | 0.47              |
| 6:H:346:PHE:O     | 26:b:52:TYR:OH    | 2.28                     | 0.47              |
| 20:V:50:GLU:HA    | 20:V:60:ARG:HH21  | 1.79                     | 0.47              |
| 45:m:101:3PE:H381 | 45:m:101:3PE:H3B1 | 1.58                     | 0.47              |
| 3:C:142:ASN:HB2   | 20:V:126:GLN:NE2  | 2.29                     | 0.47              |
| 5:G:542:TYR:OH    | 5:G:563:GLN:OE1   | 2.33                     | 0.47              |
| 7:I:68:THR:HG23   | 7:I:72:LEU:HD12   | 1.95                     | 0.47              |
| 10:L:95:LEU:HD13  | 10:L:462:LEU:HG   | 1.95                     | 0.47              |
| 12:N:187:GLN:NE2  | 32:h:145:ARG:H    | 2.11                     | 0.47              |
| 18:T:86:SER:HB3   | 21:W:25:LEU:HD21  | 1.96                     | 0.47              |
| 3:C:63:VAL:HG12   | 27:c:75:HIS:NE2   | 2.30                     | 0.47              |
| 5:G:343:LEU:O     | 5:G:590:TYR:OH    | 2.32                     | 0.47              |
| 10:L:604:LEU:HD13 | 45:L:702:3PE:H352 | 1.97                     | 0.47              |
| 43:L:701:PLC:H63  | 33:i:19:TRP:CZ2   | 2.50                     | 0.47              |
| 12:N:346:MET:HE1  | 12:N:365:ASN:HB2  | 1.97                     | 0.47              |
| 16:R:51:ARG:HD3   | 16:R:70:ARG:NH1   | 2.30                     | 0.47              |
| 17:S:15:PHE:HE2   | 17:S:47:ILE:HG23  | 1.79                     | 0.47              |
| 5:G:649:ARG:NE    | 5:G:654:GLU:OE2   | 2.48                     | 0.47              |
| 6:H:141:TYR:HB2   | 6:H:227:THR:HG21  | 1.97                     | 0.47              |
| 8:J:99:GLU:OE1    | 25:a:112:ARG:HD3  | 2.14                     | 0.47              |
| 14:P:253:TYR:OH   | 14:P:337:SER:OG   | 2.32                     | 0.47              |
| 21:W:76:MET:HG2   | 21:W:80:MET:HE3   | 1.96                     | 0.47              |
| 46:q:203:CDL:H541 | 46:q:203:CDL:H511 | 1.70                     | 0.47              |
| 1:A:17:GLY:HA3    | 6:H:92:PHE:HZ     | 1.80                     | 0.47              |
| 2:B:61:LYS:HE2    | 2:B:65:ARG:HH22   | 1.78                     | 0.47              |
| 3:C:171:VAL:O     | 3:C:197:GLU:N     | 2.35                     | 0.47              |
| 8:J:98:ASN:OD1    | 25:a:106:ARG:NH2  | 2.46                     | 0.47              |
| 10:L:79:ASP:O     | 10:L:83:VAL:HG23  | 2.15                     | 0.47              |
| 10:L:246:LEU:O    | 10:L:251:CYS:HB2  | 2.14                     | 0.47              |
| 10:L:279:TRP:CG   | 43:L:709:PLC:H1'1 | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:L:347:ILE:HD13 | 10:L:355:GLN:HG2  | 1.97                     | 0.47              |
| 10:L:612:ILE:HD13 | 12:N:219:SER:HB2  | 1.96                     | 0.47              |
| 11:M:18:VAL:HG21  | 43:M:504:PLC:H1A2 | 1.96                     | 0.47              |
| 11:M:61:TRP:CD1   | 11:M:89:LEU:HD21  | 2.50                     | 0.47              |
| 13:O:110:SER:HB3  | 13:O:178:LYS:O    | 2.14                     | 0.47              |
| 20:V:77:ASN:OD1   | 20:V:86:LYS:NZ    | 2.32                     | 0.47              |
| 23:Y:88:PHE:HB2   | 23:Y:89:PRO:HD3   | 1.96                     | 0.47              |
| 31:g:179:GLU:OE2  | 40:p:6:ARG:NH2    | 2.48                     | 0.47              |
| 36:l:72:HIS:CD2   | 36:l:73:PRO:HD2   | 2.50                     | 0.47              |
| 39:o:73:GLU:HA    | 39:o:76:LYS:HE2   | 1.96                     | 0.47              |
| 40:p:13:ASP:OD1   | 40:p:13:ASP:N     | 2.47                     | 0.47              |
| 1:A:9:TYR:OH      | 6:H:95:LEU:O      | 2.31                     | 0.47              |
| 3:C:266:ASP:OD1   | 3:C:267:PHE:N     | 2.48                     | 0.47              |
| 5:G:110:GLY:O     | 5:G:114:MET:HG2   | 2.14                     | 0.47              |
| 10:L:527:GLU:OE1  | 35:k:23:ARG:NH2   | 2.48                     | 0.47              |
| 11:M:128:MET:SD   | 11:M:253:ILE:HG13 | 2.55                     | 0.47              |
| 14:P:324:LYS:HB3  | 14:P:328:ASP:CG   | 2.40                     | 0.47              |
| 23:Y:111:ALA:HB3  | 43:Y:302:PLC:H11  | 1.97                     | 0.47              |
| 43:Y:303:PLC:H8A2 | 37:m:47:PRO:HB3   | 1.96                     | 0.47              |
| 3:C:132:VAL:HB    | 3:C:184:PHE:HB3   | 1.97                     | 0.47              |
| 5:G:432:VAL:HG11  | 5:G:452:LEU:HD13  | 1.97                     | 0.47              |
| 8:J:96:ASP:OD2    | 30:f:51:LYS:NZ    | 2.48                     | 0.47              |
| 9:K:74:ARG:HE     | 18:T:133:ILE:HG22 | 1.80                     | 0.47              |
| 11:M:282:ILE:HD13 | 37:m:51:GLY:HA2   | 1.97                     | 0.47              |
| 19:U:88:LEU:HB3   | 38:n:49:ARG:HH12  | 1.80                     | 0.47              |
| 1:A:82:VAL:HA     | 1:A:85:MET:HE2    | 1.97                     | 0.47              |
| 5:G:641:ALA:HB2   | 5:G:648:LEU:HD11  | 1.97                     | 0.47              |
| 11:M:162:ASN:HB2  | 11:M:240:GLU:CD   | 2.40                     | 0.47              |
| 14:P:79:LEU:O     | 14:P:82:ASN:ND2   | 2.46                     | 0.47              |
| 14:P:326:PHE:HD1  | 14:P:331:MET:HE3  | 1.80                     | 0.47              |
| 31:g:172:GLU:HG2  | 40:p:36:ILE:HD11  | 1.97                     | 0.47              |
| 37:m:18:TYR:OH    | 37:m:22:ARG:NH1   | 2.48                     | 0.47              |
| 3:C:102:LEU:HD23  | 3:C:159:ILE:HG13  | 1.97                     | 0.46              |
| 4:D:166:ASN:O     | 4:D:169:VAL:HG12  | 2.15                     | 0.46              |
| 4:D:217:THR:OG1   | 6:H:310:ALA:O     | 2.20                     | 0.46              |
| 5:G:691:ASP:OD1   | 5:G:691:ASP:N     | 2.48                     | 0.46              |
| 7:I:138:ILE:HD13  | 7:I:157:ILE:HG12  | 1.97                     | 0.46              |
| 10:L:471:TYR:OH   | 45:j:101:3PE:O14  | 2.22                     | 0.46              |
| 13:O:18:ARG:NH2   | 13:O:100:GLU:OE2  | 2.47                     | 0.46              |
| 21:W:26:ASN:O     | 21:W:30:ARG:HG3   | 2.14                     | 0.46              |
| 21:W:60:GLU:HG2   | 21:W:63:ARG:HH21  | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:42:TYR:CG     | 4:D:92:LYS:HE3    | 2.50                     | 0.46              |
| 5:G:162:ILE:HG23  | 5:G:168:THR:HG21  | 1.98                     | 0.46              |
| 10:L:422:THR:O    | 10:L:426:SER:OG   | 2.20                     | 0.46              |
| 11:M:236:THR:O    | 11:M:240:GLU:HG2  | 2.15                     | 0.46              |
| 11:M:391:LEU:HD13 | 43:M:503:PLC:HE'3 | 1.96                     | 0.46              |
| 15:Q:37:LEU:HB3   | 21:W:70:LEU:HD11  | 1.96                     | 0.46              |
| 2:B:201:TYR:HA    | 14:P:122:LYS:HE2  | 1.97                     | 0.46              |
| 20:V:65:ALA:HB1   | 27:c:145:SER:HA   | 1.97                     | 0.46              |
| 22:X:38:GLU:HB3   | 25:a:89:VAL:HG13  | 1.97                     | 0.46              |
| 40:p:89:ASP:OD1   | 40:p:91:SER:OG    | 2.22                     | 0.46              |
| 1:A:24:ASN:HB2    | 6:H:232:SER:OG    | 2.16                     | 0.46              |
| 1:A:115:ILE:HD11  | 46:b:102:CDL:H561 | 1.96                     | 0.46              |
| 3:C:252:THR:HA    | 4:D:437:ARG:HH21  | 1.80                     | 0.46              |
| 5:G:218:ASN:O     | 5:G:222:LEU:HG    | 2.15                     | 0.46              |
| 10:L:93:SER:OG    | 10:L:121:THR:OG1  | 2.25                     | 0.46              |
| 10:L:574:ASN:OD1  | 11:M:298:GLN:NE2  | 2.49                     | 0.46              |
| 11:M:149:ALA:HB3  | 11:M:150:PRO:HD3  | 1.97                     | 0.46              |
| 15:Q:57:ILE:HG12  | 15:Q:77:ILE:HG12  | 1.97                     | 0.46              |
| 1:A:24:ASN:ND2    | 6:H:68:LEU:O      | 2.48                     | 0.46              |
| 3:C:76:GLU:HB3    | 27:c:150:PRO:HB3  | 1.97                     | 0.46              |
| 6:H:183:GLN:NE2   | 6:H:255:PHE:O     | 2.47                     | 0.46              |
| 10:L:243:VAL:HG13 | 10:L:247:LEU:HD13 | 1.98                     | 0.46              |
| 45:j:101:3PE:H31  | 45:j:101:3PE:H321 | 1.61                     | 0.46              |
| 40:p:84:GLY:O     | 40:p:88:ASN:ND2   | 2.45                     | 0.46              |
| 1:A:27:ILE:HG23   | 43:P:502:PLC:H5A2 | 1.96                     | 0.46              |
| 5:G:465:SER:O     | 5:G:500:ASN:ND2   | 2.48                     | 0.46              |
| 6:H:287:GLY:O     | 6:H:291:SER:OG    | 2.22                     | 0.46              |
| 7:I:75:GLU:OE1    | 7:I:75:GLU:N      | 2.38                     | 0.46              |
| 8:J:1:FME:HCN     | 8:J:1:FME:HB3     | 1.62                     | 0.46              |
| 10:L:564:ARG:NH1  | 36:l:77:ASP:O     | 2.29                     | 0.46              |
| 11:M:46:GLY:HA3   | 11:M:118:VAL:HG11 | 1.96                     | 0.46              |
| 17:S:26:PRO:O     | 17:S:29:SER:OG    | 2.28                     | 0.46              |
| 3:C:66:PRO:O      | 3:C:69:LYS:HG2    | 2.15                     | 0.46              |
| 5:G:278:ILE:HG23  | 5:G:391:ILE:HD12  | 1.98                     | 0.46              |
| 10:L:385:PRO:HA   | 10:L:390:PHE:CG   | 2.50                     | 0.46              |
| 21:W:49:SER:O     | 21:W:53:THR:OG1   | 2.30                     | 0.46              |
| 41:q:28:ASP:OD2   | 41:q:56:ARG:NH2   | 2.32                     | 0.46              |
| 2:B:59:LYS:NZ     | 2:B:192:MET:O     | 2.39                     | 0.46              |
| 2:B:73:THR:O      | 2:B:73:THR:OG1    | 2.24                     | 0.46              |
| 2:B:134:PRO:HD2   | 6:H:70:LYS:HD2    | 1.98                     | 0.46              |
| 3:C:84:ILE:O      | 3:C:88:LEU:N      | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:100:THR:OG1   | 4:D:119:GLU:OE1   | 2.25                     | 0.46              |
| 4:D:322:ARG:HD2   | 4:D:330:TYR:CE1   | 2.51                     | 0.46              |
| 4:D:379:ASP:HB3   | 4:D:382:VAL:HG22  | 1.97                     | 0.46              |
| 5:G:519:VAL:HG21  | 5:G:593:THR:HA    | 1.97                     | 0.46              |
| 12:N:194:ASP:OD1  | 12:N:194:ASP:N    | 2.44                     | 0.46              |
| 43:g:301:PLC:H4'2 | 32:h:74:TRP:CE3   | 2.50                     | 0.46              |
| 6:H:101:ILE:HG23  | 6:H:254:ILE:HD11  | 1.97                     | 0.46              |
| 7:I:145:ARG:NH1   | 7:I:151:ARG:HG3   | 2.31                     | 0.46              |
| 34:j:36:TRP:HB2   | 35:k:34:GLY:HA3   | 1.97                     | 0.46              |
| 4:D:185:ARG:HB3   | 4:D:374:PRO:O     | 2.16                     | 0.46              |
| 11:M:480:LEU:O    | 11:M:483:SER:OG   | 2.32                     | 0.46              |
| 13:O:8:ASP:CG     | 13:O:150:HIS:HD1  | 2.24                     | 0.46              |
| 14:P:301:SER:HB2  | 43:P:502:PLC:H11  | 1.97                     | 0.46              |
| 27:c:20:GLU:OE2   | 27:c:24:GLN:NE2   | 2.49                     | 0.46              |
| 41:q:77:TRP:CE2   | 41:q:89:PRO:HG2   | 2.51                     | 0.46              |
| 4:D:433:ASP:CG    | 4:D:439:TYR:HB2   | 2.41                     | 0.45              |
| 5:G:301:LYS:HD2   | 14:P:25:THR:HG21  | 1.98                     | 0.45              |
| 9:K:15:ILE:HD11   | 18:T:137:ILE:HG23 | 1.96                     | 0.45              |
| 10:L:623:ILE:HD13 | 12:N:203:CYS:SG   | 2.57                     | 0.45              |
| 11:M:36:ILE:HG23  | 31:g:98:GLU:HG2   | 1.99                     | 0.45              |
| 12:N:384:LYS:HD2  | 12:N:452:VAL:HG13 | 1.98                     | 0.45              |
| 14:P:155:TYR:HE2  | 47:P:501:NDP:H5N  | 1.80                     | 0.45              |
| 15:Q:53:ARG:NH2   | 15:Q:100:ASP:OD2  | 2.50                     | 0.45              |
| 19:U:128:ASP:OD1  | 19:U:128:ASP:N    | 2.34                     | 0.45              |
| 26:b:3:ILE:HG12   | 26:b:4:GLY:H      | 1.81                     | 0.45              |
| 1:A:125:ILE:O     | 1:A:126:THR:OG1   | 2.31                     | 0.45              |
| 13:O:55:MET:SD    | 13:O:56:PRO:HD2   | 2.57                     | 0.45              |
| 14:P:203:LEU:O    | 14:P:259:ARG:NH1  | 2.46                     | 0.45              |
| 18:T:59:VAL:O     | 18:T:63:ARG:N     | 2.40                     | 0.45              |
| 20:V:49:LEU:HD22  | 20:V:60:ARG:HG3   | 1.97                     | 0.45              |
| 9:K:42:ASP:OD2    | 12:N:178:TYR:OH   | 2.32                     | 0.45              |
| 46:O:201:CDL:HA31 | 46:O:201:CDL:H1   | 1.98                     | 0.45              |
| 14:P:139:LYS:HB2  | 14:P:179:ASN:HB3  | 1.98                     | 0.45              |
| 14:P:180:PHE:HE2  | 14:P:183:ASP:HB2  | 1.81                     | 0.45              |
| 16:R:17:LEU:O     | 16:R:50:PRO:HB3   | 2.16                     | 0.45              |
| 7:I:145:ARG:HG3   | 7:I:151:ARG:HB2   | 1.98                     | 0.45              |
| 45:L:706:3PE:H352 | 45:L:706:3PE:H382 | 1.60                     | 0.45              |
| 11:M:247:ILE:HG23 | 11:M:343:PRO:HB3  | 1.98                     | 0.45              |
| 13:O:180:LEU:O    | 13:O:184:GLN:HB2  | 2.16                     | 0.45              |
| 14:P:226:GLN:O    | 14:P:230:ALA:N    | 2.48                     | 0.45              |
| 27:c:26:LEU:HD13  | 46:q:203:CDL:H141 | 1.99                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:171:VAL:HG23  | 6:H:173:SER:H     | 1.81                     | 0.45              |
| 12:N:486:SER:OG   | 13:O:46:GLU:OE1   | 2.30                     | 0.45              |
| 14:P:341:TYR:CE2  | 14:P:359:VAL:HG13 | 2.51                     | 0.45              |
| 22:X:148:PRO:HD2  | 22:X:151:ARG:HD2  | 1.98                     | 0.45              |
| 1:A:86:LEU:HD23   | 1:A:89:ILE:HD12   | 1.98                     | 0.45              |
| 3:C:143:ARG:NH1   | 3:C:167:GLU:OE2   | 2.50                     | 0.45              |
| 4:D:231:GLU:OE1   | 4:D:235:ARG:NH2   | 2.42                     | 0.45              |
| 4:D:381:LYS:HE3   | 27:c:77:ARG:HH21  | 1.82                     | 0.45              |
| 6:H:191:PRO:HB3   | 24:Z:41:GLY:HA3   | 1.98                     | 0.45              |
| 10:L:127:LEU:HD12 | 10:L:136:LEU:HG   | 1.99                     | 0.45              |
| 11:M:462:ILE:HG12 | 45:M:501:3PE:H3H2 | 1.98                     | 0.45              |
| 24:Z:132:ALA:HB2  | 29:e:85:PHE:CD1   | 2.52                     | 0.45              |
| 31:g:136:GLU:HB2  | 31:g:138:TRP:CD1  | 2.52                     | 0.45              |
| 36:l:60:ASP:O     | 36:l:64:LYS:N     | 2.50                     | 0.45              |
| 3:C:217:ARG:HH12  | 15:Q:43:SER:HA    | 1.82                     | 0.45              |
| 4:D:161:VAL:HG11  | 4:D:204:MET:HG2   | 1.98                     | 0.45              |
| 43:D:501:PLC:H9'2 | 6:H:200:PHE:HD2   | 1.81                     | 0.45              |
| 11:M:402:ILE:HD13 | 11:M:417:ALA:HA   | 1.97                     | 0.45              |
| 11:M:410:PRO:O    | 11:M:414:SER:OG   | 2.34                     | 0.45              |
| 36:l:136:ASP:OD1  | 36:l:136:ASP:N    | 2.45                     | 0.45              |
| 5:G:434:GLU:HB2   | 5:G:681:LYS:HA    | 1.98                     | 0.45              |
| 5:G:476:SER:HB3   | 5:G:513:HIS:HA    | 1.97                     | 0.45              |
| 10:L:168:LEU:HD21 | 11:M:428:MET:HG3  | 1.98                     | 0.45              |
| 23:Y:211:ARG:NH1  | 37:m:58:GLU:OE2   | 2.50                     | 0.45              |
| 5:G:214:GLU:HG2   | 5:G:215:LEU:HG    | 1.99                     | 0.45              |
| 6:H:171:VAL:HG21  | 6:H:179:ILE:HG12  | 1.98                     | 0.45              |
| 12:N:89:ILE:HG13  | 12:N:90:THR:HG23  | 1.98                     | 0.45              |
| 3:C:85:MET:SD     | 27:c:90:VAL:HG21  | 2.57                     | 0.45              |
| 3:C:252:THR:HG22  | 4:D:437:ARG:CZ    | 2.47                     | 0.45              |
| 5:G:642:ASP:OD1   | 5:G:642:ASP:N     | 2.50                     | 0.45              |
| 10:L:26:ASN:O     | 10:L:30:TRP:HD1   | 2.00                     | 0.45              |
| 10:L:62:MET:HE1   | 45:M:501:3PE:H362 | 2.00                     | 0.45              |
| 12:N:481:ILE:HG21 | 28:d:26:PRO:HD2   | 1.99                     | 0.45              |
| 31:g:189:ASP:OD2  | 31:g:193:LYS:NZ   | 2.40                     | 0.45              |
| 43:g:301:PLC:H73  | 43:g:301:PLC:H42  | 1.83                     | 0.45              |
| 33:i:60:LYS:HB2   | 33:i:63:GLU:OE1   | 2.17                     | 0.45              |
| 1:A:49:PRO:HB2    | 6:H:140:LYS:HG3   | 2.00                     | 0.44              |
| 1:A:52:CYS:HA     | 4:D:106:GLN:HB3   | 1.99                     | 0.44              |
| 4:D:85:ASP:OD1    | 12:N:150:HIS:N    | 2.42                     | 0.44              |
| 6:H:122:SER:OG    | 30:f:3:TYR:OH     | 2.24                     | 0.44              |
| 43:L:701:PLC:H81  | 11:M:369:SER:O    | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:70:PHE:CE2   | 14:P:90:PHE:HB3   | 2.47                     | 0.44              |
| 15:Q:112:ARG:HE   | 15:Q:116:ILE:HD11 | 1.81                     | 0.44              |
| 29:e:20:PHE:HB2   | 29:e:45:TYR:CE1   | 2.52                     | 0.44              |
| 1:A:46:LYS:HA     | 2:B:130:GLN:HA    | 1.99                     | 0.44              |
| 10:L:423:SER:O    | 10:L:427:ILE:HG12 | 2.16                     | 0.44              |
| 11:M:183:LEU:HG   | 12:N:436:ILE:HD12 | 1.99                     | 0.44              |
| 5:G:366:THR:HG21  | 5:G:518:ARG:HD2   | 1.99                     | 0.44              |
| 5:G:471:LEU:HD23  | 5:G:471:LEU:HA    | 1.89                     | 0.44              |
| 6:H:163:VAL:HG11  | 6:H:199:PHE:HB2   | 1.98                     | 0.44              |
| 10:L:608:ASN:OD1  | 10:L:611:PHE:N    | 2.43                     | 0.44              |
| 43:L:709:PLC:H3A1 | 43:L:709:PLC:H6A1 | 1.75                     | 0.44              |
| 20:V:113:LYS:HA   | 20:V:115:TRP:CH2  | 2.51                     | 0.44              |
| 27:c:19:TRP:CE2   | 46:q:203:CDL:HB21 | 2.51                     | 0.44              |
| 45:m:101:3PE:H3H1 | 45:m:101:3PE:H3E1 | 1.78                     | 0.44              |
| 39:o:63:ASP:OD2   | 39:o:67:ARG:NH2   | 2.51                     | 0.44              |
| 2:B:63:TRP:HE1    | 43:q:202:PLC:P    | 2.40                     | 0.44              |
| 5:G:367:ASP:OD1   | 5:G:367:ASP:N     | 2.33                     | 0.44              |
| 12:N:108:ILE:HD13 | 12:N:108:ILE:HA   | 1.81                     | 0.44              |
| 20:V:113:LYS:HA   | 20:V:115:TRP:CZ3  | 2.52                     | 0.44              |
| 23:Y:213:ILE:O    | 23:Y:215:THR:N    | 2.50                     | 0.44              |
| 25:a:42:GLU:HG3   | 25:a:43:ILE:HG13  | 1.99                     | 0.44              |
| 33:i:68:ASN:OD1   | 33:i:68:ASN:N     | 2.51                     | 0.44              |
| 4:D:114:LEU:HD22  | 4:D:477:PHE:CZ    | 2.52                     | 0.44              |
| 4:D:197:THR:OG1   | 4:D:233:TYR:OH    | 2.34                     | 0.44              |
| 5:G:524:VAL:HG12  | 5:G:643:VAL:HG11  | 1.99                     | 0.44              |
| 7:I:180:THR:HG22  | 7:I:211:ILE:HD11  | 1.99                     | 0.44              |
| 10:L:170:ILE:HG12 | 45:L:706:3PE:H241 | 2.00                     | 0.44              |
| 20:V:65:ALA:HB3   | 27:c:146:PRO:HD3  | 1.99                     | 0.44              |
| 32:h:164:ASN:OD1  | 32:h:164:ASN:N    | 2.47                     | 0.44              |
| 38:n:23:LEU:HD13  | 38:n:71:THR:HG21  | 1.99                     | 0.44              |
| 38:n:34:TRP:CZ2   | 38:n:80:HIS:HA    | 2.52                     | 0.44              |
| 4:D:403:LEU:HD23  | 4:D:403:LEU:HA    | 1.73                     | 0.44              |
| 5:G:254:LEU:HD11  | 5:G:411:ALA:HB1   | 1.99                     | 0.44              |
| 6:H:322:LEU:O     | 6:H:326:TYR:HB2   | 2.17                     | 0.44              |
| 25:a:96:THR:O     | 25:a:96:THR:OG1   | 2.34                     | 0.44              |
| 6:H:139:SER:HB2   | 6:H:143:VAL:HG21  | 1.99                     | 0.44              |
| 7:I:207:TRP:CE3   | 41:q:75:PRO:HB3   | 2.53                     | 0.44              |
| 8:J:99:GLU:HG3    | 25:a:107:ARG:HD2  | 1.99                     | 0.44              |
| 11:M:136:ASP:N    | 11:M:136:ASP:OD1  | 2.50                     | 0.44              |
| 20:V:80:ILE:HG23  | 20:V:92:VAL:HG21  | 1.99                     | 0.44              |
| 21:W:76:MET:HE2   | 21:W:76:MET:HB3   | 1.90                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:86:VAL:HG21   | 2:B:180:LEU:HD23  | 1.99                     | 0.44              |
| 2:B:115:THR:OG1   | 2:B:143:CYS:SG    | 2.74                     | 0.44              |
| 5:G:176:CYS:SG    | 5:G:178:ARG:HB2   | 2.58                     | 0.44              |
| 13:O:78:THR:HG23  | 13:O:136:LEU:HD23 | 1.99                     | 0.44              |
| 17:S:14:ARG:HA    | 17:S:48:LEU:HB2   | 1.99                     | 0.44              |
| 43:Z:202:PLC:H4'2 | 46:Z:203:CDL:H722 | 2.00                     | 0.44              |
| 37:m:14:SER:OG    | 37:m:17:ARG:NH2   | 2.50                     | 0.44              |
| 1:A:44:ILE:HB     | 14:P:346:PRO:HB3  | 2.00                     | 0.44              |
| 5:G:650:HIS:O     | 5:G:652:VAL:HG23  | 2.18                     | 0.44              |
| 11:M:61:TRP:O     | 31:g:160:LYS:NZ   | 2.50                     | 0.44              |
| 16:R:50:PRO:HD3   | 41:q:125:ARG:HE   | 1.82                     | 0.44              |
| 20:V:58:VAL:HG11  | 27:c:139:LEU:HD23 | 2.00                     | 0.44              |
| 22:X:52:TYR:CD1   | 22:X:142:LYS:HE3  | 2.53                     | 0.44              |
| 24:Z:63:ARG:NH2   | 25:a:64:ASP:OD2   | 2.51                     | 0.44              |
| 25:a:72:VAL:O     | 25:a:76:ARG:HG3   | 2.17                     | 0.44              |
| 31:g:45:ASN:O     | 31:g:45:ASN:ND2   | 2.51                     | 0.44              |
| 31:g:229:LEU:HA   | 40:p:11:SER:HB3   | 2.00                     | 0.44              |
| 2:B:84:MET:HE1    | 4:D:204:MET:SD    | 2.58                     | 0.43              |
| 12:N:18:LYS:HZ1   | 12:N:103:ARG:HD2  | 1.82                     | 0.43              |
| 14:P:180:PHE:CE2  | 14:P:183:ASP:HB2  | 2.52                     | 0.43              |
| 19:U:79:PHE:O     | 19:U:85:LEU:HB2   | 2.18                     | 0.43              |
| 20:V:11:GLN:OE1   | 20:V:12:GLU:N     | 2.48                     | 0.43              |
| 24:Z:127:SER:HB2  | 24:Z:132:ALA:HA   | 2.00                     | 0.43              |
| 41:q:30:LYS:HB3   | 41:q:30:LYS:HE2   | 1.80                     | 0.43              |
| 2:B:60:MET:HE3    | 43:q:201:PLC:H7A1 | 2.00                     | 0.43              |
| 7:I:126:CYS:CB    | 7:I:128:LEU:H     | 2.28                     | 0.43              |
| 45:J:201:3PE:H282 | 45:J:201:3PE:H252 | 1.82                     | 0.43              |
| 10:L:559:ASN:ND2  | 36:l:84:ASP:O     | 2.32                     | 0.43              |
| 13:O:27:THR:HG21  | 13:O:75:TYR:HD1   | 1.83                     | 0.43              |
| 13:O:77:TYR:HE1   | 13:O:133:GLN:HE21 | 1.66                     | 0.43              |
| 23:Y:126:LEU:HD22 | 23:Y:130:ARG:HG3  | 2.00                     | 0.43              |
| 5:G:377:HIS:CD2   | 5:G:385:TYR:HB3   | 2.53                     | 0.43              |
| 10:L:63:ASN:OD1   | 10:L:64:TRP:N     | 2.50                     | 0.43              |
| 10:L:63:ASN:HD21  | 10:L:71:VAL:HG13  | 1.83                     | 0.43              |
| 11:M:299:THR:HG21 | 37:m:22:ARG:HG3   | 2.00                     | 0.43              |
| 46:O:201:CDL:HA22 | 46:O:201:CDL:H111 | 2.00                     | 0.43              |
| 21:W:26:ASN:OD1   | 21:W:29:ARG:NH2   | 2.51                     | 0.43              |
| 25:a:64:ASP:OD1   | 25:a:64:ASP:N     | 2.51                     | 0.43              |
| 5:G:335:GLU:HA    | 5:G:538:ALA:HA    | 2.00                     | 0.43              |
| 5:G:689:PHE:CE1   | 5:G:695:LYS:HA    | 2.53                     | 0.43              |
| 6:H:135:TRP:HZ2   | 8:J:67:LEU:HD23   | 1.82                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:J:139:LEU:HD22  | 12:N:130:ILE:HD12 | 2.01                     | 0.43              |
| 10:L:213:LEU:HD13 | 10:L:267:LEU:HA   | 2.00                     | 0.43              |
| 10:L:441:PRO:HD2  | 10:L:444:ILE:HD12 | 1.99                     | 0.43              |
| 45:M:501:3PE:H381 | 45:M:501:3PE:H3B2 | 1.72                     | 0.43              |
| 43:M:503:PLC:H3'2 | 43:g:301:PLC:H3A1 | 1.99                     | 0.43              |
| 23:Y:207:LEU:O    | 23:Y:211:ARG:NH2  | 2.32                     | 0.43              |
| 10:L:279:TRP:CE2  | 43:L:709:PLC:H2   | 2.53                     | 0.43              |
| 12:N:179:ASP:OD2  | 25:a:126:ARG:NH2  | 2.52                     | 0.43              |
| 12:N:506:GLN:HE21 | 43:d:101:PLC:H1'1 | 1.84                     | 0.43              |
| 19:U:85:LEU:HD22  | 19:U:89:ASP:HB3   | 1.98                     | 0.43              |
| 23:Y:65:GLY:O     | 23:Y:71:LEU:HD23  | 2.18                     | 0.43              |
| 34:j:42:ARG:NH1   | 45:j:101:3PE:O14  | 2.45                     | 0.43              |
| 43:B:302:PLC:H31  | 43:q:201:PLC:H1'2 | 2.00                     | 0.43              |
| 5:G:406:ASN:HB2   | 5:G:682:ASN:ND2   | 2.34                     | 0.43              |
| 7:I:107:PHE:HD2   | 7:I:181:PRO:HA    | 1.84                     | 0.43              |
| 8:J:50:LEU:HD23   | 8:J:50:LEU:HA     | 1.85                     | 0.43              |
| 13:O:5:GLU:OE2    | 13:O:161:ARG:NH2  | 2.51                     | 0.43              |
| 14:P:326:PHE:HB3  | 14:P:331:MET:O    | 2.19                     | 0.43              |
| 25:a:6:ALA:O      | 25:a:9:PRO:HD2    | 2.17                     | 0.43              |
| 25:a:40:ASN:O     | 25:a:44:LYS:HG3   | 2.19                     | 0.43              |
| 34:j:44:LYS:HD2   | 35:k:38:PHE:CE1   | 2.53                     | 0.43              |
| 37:m:79:PRO:O     | 39:o:78:ARG:NH1   | 2.51                     | 0.43              |
| 1:A:41:SER:HB2    | 14:P:347:HIS:HE1  | 1.82                     | 0.43              |
| 3:C:113:GLN:OE1   | 3:C:113:GLN:N     | 2.52                     | 0.43              |
| 10:L:93:SER:O     | 10:L:97:HIS:ND1   | 2.39                     | 0.43              |
| 10:L:132:ASN:OD1  | 10:L:135:ILE:HG12 | 2.19                     | 0.43              |
| 12:N:475:GLU:OE1  | 12:N:478:ASN:ND2  | 2.52                     | 0.43              |
| 14:P:113:ASN:HD22 | 14:P:137:ILE:HG21 | 1.84                     | 0.43              |
| 22:X:36:ASP:OD1   | 22:X:37:VAL:N     | 2.52                     | 0.43              |
| 36:l:25:LYS:HZ3   | 36:l:25:LYS:HB2   | 1.83                     | 0.43              |
| 40:p:73:MET:HB3   | 40:p:77:HIS:CE1   | 2.53                     | 0.43              |
| 4:D:80:ASN:O      | 12:N:287:ARG:NH2  | 2.39                     | 0.43              |
| 5:G:359:LEU:HD11  | 5:G:624:LEU:HD13  | 2.00                     | 0.43              |
| 10:L:167:ALA:O    | 10:L:171:ASN:ND2  | 2.52                     | 0.43              |
| 10:L:526:TYR:OH   | 43:L:708:PLC:H41  | 2.18                     | 0.43              |
| 11:M:140:PHE:O    | 11:M:144:PHE:HB2  | 2.19                     | 0.43              |
| 11:M:423:SER:HA   | 11:M:426:TYR:CE2  | 2.54                     | 0.43              |
| 23:Y:118:SER:HB2  | 23:Y:146:GLY:HA2  | 2.01                     | 0.43              |
| 1:A:34:ASP:OD2    | 2:B:133:TYR:HB2   | 2.18                     | 0.43              |
| 4:D:179:ASN:ND2   | 27:c:79:TYR:HA    | 2.34                     | 0.43              |
| 4:D:297:VAL:HG22  | 4:D:457:ILE:HG12  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:G:501:ILE:HG23  | 5:G:508:GLY:HA3   | 2.01                     | 0.43              |
| 6:H:170:ILE:HD11  | 6:H:339:ALA:HB1   | 2.01                     | 0.43              |
| 7:I:45:PRO:HB3    | 27:c:158:PHE:O    | 2.19                     | 0.43              |
| 8:J:128:ILE:HG23  | 9:K:47:ILE:HG12   | 2.01                     | 0.43              |
| 10:L:169:LEU:HB2  | 45:L:706:3PE:H231 | 2.01                     | 0.43              |
| 11:M:10:ASN:CG    | 11:M:126:ILE:HG13 | 2.44                     | 0.43              |
| 15:Q:92:LEU:HG    | 15:Q:93:MET:HG2   | 2.00                     | 0.43              |
| 17:S:14:ARG:NH1   | 17:S:68:GLU:OE2   | 2.52                     | 0.43              |
| 20:V:73:ILE:O     | 20:V:77:ASN:ND2   | 2.38                     | 0.43              |
| 31:g:32:LYS:HD2   | 31:g:32:LYS:HA    | 1.90                     | 0.43              |
| 45:h:201:3PE:H332 | 45:h:201:3PE:H362 | 1.84                     | 0.43              |
| 10:L:352:SER:HB3  | 10:L:444:ILE:HD11 | 2.01                     | 0.43              |
| 11:M:148:LEU:HD23 | 11:M:148:LEU:HA   | 1.76                     | 0.43              |
| 11:M:440:SER:O    | 38:n:102:ARG:NH2  | 2.51                     | 0.43              |
| 24:Z:132:ALA:O    | 24:Z:134:SER:N    | 2.51                     | 0.43              |
| 1:A:41:SER:HB2    | 14:P:347:HIS:CE1  | 2.54                     | 0.42              |
| 7:I:162:CYS:SG    | 7:I:164:TYR:N     | 2.73                     | 0.42              |
| 10:L:24:GLY:O     | 10:L:111:GLN:NE2  | 2.51                     | 0.42              |
| 11:M:238:HIS:NE2  | 11:M:250:ALA:HB2  | 2.34                     | 0.42              |
| 12:N:76:ILE:HD11  | 45:N:601:3PE:H321 | 2.01                     | 0.42              |
| 17:S:6:PHE:HB3    | 17:S:10:VAL:HG21  | 2.01                     | 0.42              |
| 31:g:184:ASP:OD2  | 31:g:217:ARG:NE   | 2.52                     | 0.42              |
| 36:l:128:TYR:HB2  | 36:l:132:GLY:HA2  | 2.00                     | 0.42              |
| 1:A:66:ILE:HG23   | 8:J:158:VAL:HG12  | 2.01                     | 0.42              |
| 3:C:140:ARG:HE    | 3:C:140:ARG:HB2   | 1.65                     | 0.42              |
| 4:D:71:LYS:HG3    | 4:D:72:ASP:OD1    | 2.19                     | 0.42              |
| 6:H:143:VAL:O     | 6:H:146:THR:HG22  | 2.19                     | 0.42              |
| 12:N:235:TYR:CE1  | 12:N:239:MET:HG3  | 2.54                     | 0.42              |
| 12:N:255:ILE:HG21 | 12:N:263:LEU:HD22 | 2.01                     | 0.42              |
| 16:R:76:ASP:O     | 16:R:80:LYS:HG3   | 2.19                     | 0.42              |
| 40:p:69:LYS:HZ2   | 40:p:73:MET:HE2   | 1.84                     | 0.42              |
| 2:B:177:SER:O     | 2:B:181:MET:HG3   | 2.19                     | 0.42              |
| 4:D:224:GLU:HG2   | 7:I:92:TYR:CZ     | 2.53                     | 0.42              |
| 5:G:377:HIS:HE1   | 5:G:479:THR:HG21  | 1.84                     | 0.42              |
| 5:G:377:HIS:HB3   | 5:G:488:TYR:CZ    | 2.54                     | 0.42              |
| 5:G:495:VAL:HG13  | 5:G:501:ILE:HG21  | 2.01                     | 0.42              |
| 7:I:49:ARG:NH1    | 20:V:93:GLU:OE2   | 2.40                     | 0.42              |
| 8:J:113:TYR:CD1   | 24:Z:78:VAL:HG22  | 2.54                     | 0.42              |
| 11:M:186:VAL:HG13 | 12:N:421:ILE:HG12 | 2.00                     | 0.42              |
| 12:N:510:ILE:HD11 | 43:d:101:PLC:H9'2 | 2.01                     | 0.42              |
| 25:a:86:ASP:OD1   | 25:a:86:ASP:N     | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:a:99:ILE:HD13  | 29:e:86:LEU:HD22  | 2.02                     | 0.42              |
| 3:C:91:PHE:HB3    | 3:C:110:ALA:HB1   | 2.01                     | 0.42              |
| 3:C:140:ARG:NH1   | 20:V:126:GLN:O    | 2.53                     | 0.42              |
| 5:G:162:ILE:HD11  | 5:G:166:ILE:HD12  | 2.02                     | 0.42              |
| 5:G:173:CYS:HA    | 5:G:227:ALA:HB2   | 2.02                     | 0.42              |
| 5:G:502:VAL:HG21  | 5:G:665:PHE:HE2   | 1.84                     | 0.42              |
| 10:L:21:ARG:NH2   | 33:i:13:LYS:HA    | 2.33                     | 0.42              |
| 10:L:494:LEU:HD23 | 36:l:126:ARG:NH1  | 2.34                     | 0.42              |
| 11:M:9:PHE:HE2    | 11:M:49:ILE:HG23  | 1.84                     | 0.42              |
| 11:M:156:GLY:HA3  | 12:N:455:PHE:CE1  | 2.54                     | 0.42              |
| 13:O:175:ASP:OD1  | 13:O:175:ASP:N    | 2.52                     | 0.42              |
| 25:a:22:GLY:O     | 25:a:26:SER:OG    | 2.22                     | 0.42              |
| 31:g:170:MET:HG2  | 31:g:200:GLY:HA2  | 2.01                     | 0.42              |
| 5:G:298:ARG:HD2   | 5:G:298:ARG:HA    | 1.85                     | 0.42              |
| 45:L:703:3PE:H2D1 | 45:L:703:3PE:H2G1 | 1.70                     | 0.42              |
| 14:P:43:THR:OG1   | 14:P:104:SER:O    | 2.36                     | 0.42              |
| 45:m:101:3PE:H341 | 45:m:101:3PE:H231 | 2.01                     | 0.42              |
| 4:D:50:ASP:OD1    | 4:D:50:ASP:N      | 2.42                     | 0.42              |
| 5:G:332:LYS:N     | 5:G:335:GLU:HB2   | 2.34                     | 0.42              |
| 5:G:341:GLY:HA2   | 5:G:367:ASP:OD2   | 2.20                     | 0.42              |
| 8:J:135:GLU:CD    | 12:N:58:ASN:HD21  | 2.28                     | 0.42              |
| 45:L:703:3PE:H3D1 | 45:L:703:3PE:H3G2 | 1.93                     | 0.42              |
| 11:M:342:SER:HB3  | 11:M:343:PRO:HD3  | 2.01                     | 0.42              |
| 13:O:160:VAL:HG11 | 13:O:165:GLU:HG3  | 2.01                     | 0.42              |
| 26:b:68:ARG:NH1   | 26:b:69:SER:O     | 2.51                     | 0.42              |
| 2:B:49:LEU:HD12   | 2:B:49:LEU:HA     | 1.91                     | 0.42              |
| 3:C:189:TYR:CZ    | 21:W:80:MET:HE1   | 2.55                     | 0.42              |
| 4:D:269:GLN:HE21  | 4:D:269:GLN:HB3   | 1.60                     | 0.42              |
| 5:G:129:GLY:HA2   | 42:G:802:SF4:S3   | 2.59                     | 0.42              |
| 5:G:580:GLY:O     | 5:G:610:ALA:HB1   | 2.18                     | 0.42              |
| 6:H:192:PHE:HD1   | 45:b:104:3PE:H3I1 | 1.85                     | 0.42              |
| 11:M:33:LEU:HD23  | 11:M:36:ILE:HD12  | 2.00                     | 0.42              |
| 11:M:446:THR:HB   | 37:m:8:LEU:HD13   | 2.02                     | 0.42              |
| 13:O:124:MET:HE3  | 13:O:124:MET:HB3  | 1.96                     | 0.42              |
| 21:W:82:PHE:CZ    | 21:W:86:VAL:HG21  | 2.55                     | 0.42              |
| 28:d:5:LEU:HD23   | 28:d:5:LEU:HA     | 1.86                     | 0.42              |
| 29:e:89:LYS:HD3   | 29:e:98:ASP:CG    | 2.45                     | 0.42              |
| 7:I:205:ASP:OD1   | 7:I:205:ASP:N     | 2.51                     | 0.42              |
| 8:J:149:MET:O     | 8:J:153:GLY:N     | 2.49                     | 0.42              |
| 11:M:214:PHE:CD2  | 11:M:265:LEU:HD22 | 2.55                     | 0.42              |
| 11:M:266:LEU:O    | 11:M:270:SER:OG   | 2.33                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:P:16:ASP:OD1   | 14:P:17:ILE:HG22  | 2.20                     | 0.42              |
| 15:Q:51:THR:OG1   | 15:Q:52:GLU:HG3   | 2.19                     | 0.42              |
| 27:c:156:MET:HA   | 27:c:180:GLN:HE22 | 1.85                     | 0.42              |
| 1:A:46:LYS:HE3    | 1:A:46:LYS:HB2    | 1.75                     | 0.42              |
| 3:C:202:LEU:O     | 21:W:80:MET:HE2   | 2.20                     | 0.42              |
| 4:D:133:GLY:H     | 4:D:481:ASP:CG    | 2.28                     | 0.42              |
| 5:G:432:VAL:HG11  | 5:G:452:LEU:HB2   | 2.02                     | 0.42              |
| 8:J:94:ASP:OD1    | 25:a:113:ARG:NH1  | 2.53                     | 0.42              |
| 8:J:109:TYR:OH    | 22:X:20:ASP:OD2   | 2.21                     | 0.42              |
| 11:M:84:ILE:HG12  | 11:M:133:ILE:HG22 | 2.02                     | 0.42              |
| 11:M:169:TYR:O    | 11:M:173:TYR:HB2  | 2.20                     | 0.42              |
| 12:N:387:PHE:CE1  | 12:N:454:SER:HB3  | 2.55                     | 0.42              |
| 14:P:262:ILE:O    | 14:P:266:ILE:HG12 | 2.19                     | 0.42              |
| 23:Y:60:MET:HE2   | 23:Y:60:MET:HB3   | 1.92                     | 0.42              |
| 34:j:47:TYR:CD2   | 34:j:48:PRO:HD3   | 2.55                     | 0.42              |
| 1:A:46:LYS:NZ     | 6:H:71:GLU:OE1    | 2.29                     | 0.42              |
| 6:H:266:THR:O     | 6:H:270:LEU:HG    | 2.20                     | 0.42              |
| 6:H:348:ALA:O     | 24:Z:49:ASN:ND2   | 2.49                     | 0.42              |
| 10:L:638:ILE:HG22 | 23:Y:145:MET:HE2  | 2.02                     | 0.42              |
| 11:M:99:GLY:HA2   | 11:M:125:VAL:HG21 | 2.01                     | 0.42              |
| 11:M:365:TYR:HA   | 11:M:443:LEU:HD11 | 2.01                     | 0.42              |
| 14:P:194:PHE:H    | 14:P:197:SER:HB2  | 1.85                     | 0.42              |
| 20:V:52:LYS:NZ    | 20:V:107:ASP:OD1  | 2.48                     | 0.42              |
| 31:g:211:ASP:OD1  | 31:g:211:ASP:N    | 2.52                     | 0.42              |
| 36:l:66:ASN:ND2   | 36:l:69:GLU:OE2   | 2.45                     | 0.42              |
| 2:B:78:CYS:HA     | 4:D:160:TYR:CG    | 2.55                     | 0.41              |
| 4:D:80:ASN:OD1    | 4:D:80:ASN:N      | 2.53                     | 0.41              |
| 4:D:381:LYS:HE2   | 27:c:70:TYR:CZ    | 2.54                     | 0.41              |
| 6:H:231:ALA:O     | 6:H:235:VAL:HG23  | 2.20                     | 0.41              |
| 6:H:311:ALA:HB3   | 7:I:80:LEU:HD23   | 2.02                     | 0.41              |
| 10:L:611:PHE:CZ   | 10:L:615:ILE:HD11 | 2.54                     | 0.41              |
| 19:U:95:LEU:HD23  | 19:U:95:LEU:HA    | 1.86                     | 0.41              |
| 36:l:90:GLN:HB2   | 36:l:93:ILE:HB    | 2.02                     | 0.41              |
| 43:q:201:PLC:H6A2 | 43:q:202:PLC:H7'2 | 2.01                     | 0.41              |
| 3:C:187:GLU:OE2   | 4:D:482:ARG:NH1   | 2.41                     | 0.41              |
| 3:C:246:GLN:OE1   | 7:I:161:LYS:NZ    | 2.53                     | 0.41              |
| 4:D:135:LEU:HD23  | 4:D:478:GLY:HA2   | 2.01                     | 0.41              |
| 5:G:292:ASP:OD2   | 5:G:699:THR:OG1   | 2.30                     | 0.41              |
| 6:H:173:SER:HB2   | 6:H:352:ILE:HG12  | 2.02                     | 0.41              |
| 10:L:81:LEU:HD23  | 10:L:262:ARG:HD2  | 2.01                     | 0.41              |
| 10:L:624:VAL:HG12 | 45:L:705:3PE:H332 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:M:272:ILE:HD12 | 11:M:272:ILE:HA   | 1.86                     | 0.41              |
| 14:P:84:ASP:CG    | 14:P:85:LEU:H     | 2.28                     | 0.41              |
| 23:Y:13:GLN:NE2   | 43:Y:303:PLC:H51  | 2.36                     | 0.41              |
| 34:j:41:TYR:OH    | 45:j:101:3PE:O12  | 2.26                     | 0.41              |
| 4:D:474:ASP:OD1   | 4:D:474:ASP:N     | 2.53                     | 0.41              |
| 5:G:433:GLY:O     | 5:G:447:SER:HA    | 2.20                     | 0.41              |
| 5:G:564:GLY:O     | 5:G:580:GLY:N     | 2.46                     | 0.41              |
| 10:L:475:ASP:OD2  | 39:o:53:ARG:NH2   | 2.52                     | 0.41              |
| 12:N:99:ASN:OD1   | 12:N:99:ASN:N     | 2.53                     | 0.41              |
| 14:P:310:LEU:O    | 14:P:313:SER:OG   | 2.38                     | 0.41              |
| 14:P:366:GLU:O    | 14:P:370:ASP:N    | 2.42                     | 0.41              |
| 23:Y:187:GLU:OE1  | 23:Y:187:GLU:N    | 2.39                     | 0.41              |
| 5:G:144:ASP:OD1   | 5:G:145:ARG:N     | 2.53                     | 0.41              |
| 5:G:529:GLN:HE22  | 17:S:46:PRO:HA    | 1.85                     | 0.41              |
| 8:J:51:TYR:O      | 8:J:55:TYR:HB2    | 2.21                     | 0.41              |
| 10:L:85:MET:HE2   | 10:L:258:PHE:HB2  | 2.03                     | 0.41              |
| 10:L:89:VAL:HG22  | 10:L:250:ALA:O    | 2.21                     | 0.41              |
| 10:L:415:ALA:O    | 10:L:419:ALA:N    | 2.50                     | 0.41              |
| 13:O:85:TRP:CH2   | 13:O:133:GLN:HB2  | 2.55                     | 0.41              |
| 16:R:90:ASN:HA    | 16:R:110:LEU:HD12 | 2.02                     | 0.41              |
| 19:U:50:LYS:HA    | 19:U:53:ILE:HB    | 2.01                     | 0.41              |
| 19:U:119:ALA:O    | 19:U:123:ILE:HG12 | 2.21                     | 0.41              |
| 38:n:14:GLU:OE1   | 38:n:17:LYS:NZ    | 2.47                     | 0.41              |
| 2:B:85:HIS:HE1    | 4:D:226:ARG:HE    | 1.68                     | 0.41              |
| 10:L:177:LEU:HD13 | 10:L:177:LEU:HA   | 1.91                     | 0.41              |
| 12:N:411:THR:HG23 | 12:N:500:ILE:HA   | 2.01                     | 0.41              |
| 3:C:155:HIS:HB3   | 27:c:149:ALA:HB3  | 2.03                     | 0.41              |
| 3:C:199:HIS:CD2   | 3:C:202:LEU:HD13  | 2.56                     | 0.41              |
| 5:G:285:ASP:OD1   | 5:G:285:ASP:N     | 2.53                     | 0.41              |
| 5:G:352:LEU:HD22  | 5:G:544:LEU:HD22  | 2.03                     | 0.41              |
| 10:L:124:MET:HE3  | 10:L:251:CYS:HA   | 2.02                     | 0.41              |
| 45:L:702:3PE:H362 | 45:L:702:3PE:H331 | 1.72                     | 0.41              |
| 5:G:175:HIS:O     | 5:G:176:CYS:CB    | 2.67                     | 0.41              |
| 5:G:585:GLU:OE1   | 5:G:607:PRO:HD3   | 2.21                     | 0.41              |
| 5:G:640:LEU:HD22  | 5:G:647:LEU:HD13  | 2.02                     | 0.41              |
| 7:I:116:TYR:CE2   | 7:I:122:ARG:HA    | 2.56                     | 0.41              |
| 10:L:13:SER:OG    | 10:L:119:MET:HB2  | 2.21                     | 0.41              |
| 10:L:406:PHE:HB2  | 36:l:118:TYR:CE1  | 2.55                     | 0.41              |
| 11:M:271:GLU:O    | 23:Y:207:LEU:HD21 | 2.20                     | 0.41              |
| 18:T:129:THR:O    | 18:T:131:GLN:NE2  | 2.53                     | 0.41              |
| 23:Y:211:ARG:H    | 23:Y:211:ARG:HE   | 1.67                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:g:192:ASP:OD1  | 31:g:192:ASP:N    | 2.53                     | 0.41              |
| 3:C:158:ARG:HG3   | 27:c:152:LEU:HD11 | 2.01                     | 0.41              |
| 6:H:230:SER:O     | 6:H:233:PRO:HD2   | 2.20                     | 0.41              |
| 45:J:201:3PE:H2C1 | 45:J:201:3PE:H291 | 1.84                     | 0.41              |
| 12:N:40:ILE:HD13  | 13:O:74:TYR:HB2   | 2.03                     | 0.41              |
| 15:Q:39:LYS:O     | 15:Q:42:VAL:HG22  | 2.21                     | 0.41              |
| 23:Y:122:SER:O    | 23:Y:126:LEU:N    | 2.38                     | 0.41              |
| 32:h:106:VAL:HG23 | 32:h:109:SER:H    | 1.85                     | 0.41              |
| 2:B:61:LYS:HE2    | 2:B:65:ARG:NH2    | 2.35                     | 0.41              |
| 2:B:99:ILE:HD11   | 6:H:37:ARG:CZ     | 2.51                     | 0.41              |
| 3:C:124:ALA:HB1   | 3:C:126:PHE:CE2   | 2.56                     | 0.41              |
| 5:G:173:CYS:SG    | 5:G:175:HIS:CG    | 3.14                     | 0.41              |
| 5:G:346:LEU:HD11  | 5:G:524:VAL:HG11  | 2.01                     | 0.41              |
| 5:G:550:VAL:HG13  | 5:G:569:LEU:HD21  | 2.02                     | 0.41              |
| 5:G:599:SER:OG    | 5:G:600:THR:N     | 2.54                     | 0.41              |
| 5:G:621:SER:OG    | 5:G:627:THR:HA    | 2.21                     | 0.41              |
| 6:H:278:HIS:CE1   | 25:a:53:PRO:HB2   | 2.56                     | 0.41              |
| 7:I:215:LEU:HD23  | 7:I:215:LEU:HA    | 1.90                     | 0.41              |
| 10:L:85:MET:HE1   | 10:L:329:LEU:HD21 | 2.03                     | 0.41              |
| 11:M:7:ILE:HG12   | 11:M:130:LEU:HD11 | 2.03                     | 0.41              |
| 11:M:97:ILE:O     | 11:M:100:PRO:HD2  | 2.21                     | 0.41              |
| 12:N:319:ILE:HD13 | 12:N:319:ILE:HA   | 1.98                     | 0.41              |
| 12:N:515:TYR:HB3  | 32:h:131:ILE:HD13 | 2.03                     | 0.41              |
| 14:P:16:ASP:OD1   | 14:P:17:ILE:N     | 2.53                     | 0.41              |
| 14:P:158:ASN:HB3  | 14:P:161:SER:HB2  | 2.03                     | 0.41              |
| 14:P:178:ASP:N    | 14:P:178:ASP:OD1  | 2.52                     | 0.41              |
| 27:c:38:LEU:HD23  | 27:c:38:LEU:HA    | 1.90                     | 0.41              |
| 31:g:172:GLU:OE1  | 40:p:4:HIS:NE2    | 2.32                     | 0.41              |
| 31:g:218:ILE:HD12 | 40:p:43:VAL:HG11  | 2.02                     | 0.41              |
| 34:j:48:PRO:HB2   | 34:j:54:LYS:HB3   | 2.01                     | 0.41              |
| 2:B:72:MET:HE3    | 2:B:110:MET:HG3   | 2.02                     | 0.41              |
| 3:C:88:LEU:HD22   | 3:C:91:PHE:HD2    | 1.86                     | 0.41              |
| 3:C:136:ASP:OD2   | 3:C:143:ARG:NH2   | 2.54                     | 0.41              |
| 12:N:218:TYR:CE1  | 12:N:277:ILE:HD13 | 2.56                     | 0.41              |
| 27:c:162:GLU:OE1  | 27:c:162:GLU:N    | 2.54                     | 0.41              |
| 1:A:65:PRO:HD2    | 1:A:68:PHE:HD2    | 1.85                     | 0.40              |
| 4:D:169:VAL:HG23  | 4:D:419:ILE:HG23  | 2.02                     | 0.40              |
| 5:G:298:ARG:HH21  | 5:G:582:ALA:HB2   | 1.85                     | 0.40              |
| 5:G:400:ILE:HG12  | 5:G:471:LEU:HB2   | 2.02                     | 0.40              |
| 11:M:98:LEU:HA    | 11:M:98:LEU:HD23  | 1.84                     | 0.40              |
| 1:A:135:ALA:HB1   | 20:V:16:LYS:O     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:D:158:LEU:HD22  | 4:D:482:ARG:HB2   | 2.03                     | 0.40              |
| 4:D:445:ALA:HB1   | 4:D:479:GLU:HG2   | 2.03                     | 0.40              |
| 5:G:253:ALA:HB1   | 5:G:593:THR:HB    | 2.03                     | 0.40              |
| 9:K:14:ASN:HD22   | 18:T:134:ASN:HB3  | 1.87                     | 0.40              |
| 11:M:291:SER:O    | 11:M:295:THR:OG1  | 2.39                     | 0.40              |
| 11:M:409:HIS:ND1  | 11:M:412:ILE:HG22 | 2.36                     | 0.40              |
| 12:N:458:LEU:O    | 12:N:461:LYS:HG2  | 2.21                     | 0.40              |
| 13:O:191:TYR:CE1  | 26:b:61:ASN:HB2   | 2.56                     | 0.40              |
| 49:U:201:EHZ:O1   | 38:n:55:ASN:OD1   | 2.39                     | 0.40              |
| 36:l:46:PRO:HG3   | 36:l:72:HIS:NE2   | 2.36                     | 0.40              |
| 41:q:5:GLN:O      | 41:q:9:ARG:HG3    | 2.20                     | 0.40              |
| 46:q:203:CDL:H571 | 46:q:203:CDL:H542 | 1.92                     | 0.40              |
| 1:A:101:ILE:HD11  | 45:b:103:3PE:H262 | 2.02                     | 0.40              |
| 4:D:200:LEU:HD23  | 4:D:226:ARG:HG2   | 2.02                     | 0.40              |
| 5:G:284:SER:HB3   | 5:G:412:ALA:HB3   | 2.03                     | 0.40              |
| 10:L:293:MET:HE1  | 43:L:708:PLC:H4A2 | 2.02                     | 0.40              |
| 43:L:708:PLC:H32  | 43:L:708:PLC:H1A2 | 1.80                     | 0.40              |
| 11:M:462:ILE:HD11 | 43:g:301:PLC:H2   | 2.03                     | 0.40              |
| 11:M:490:LEU:HD12 | 40:p:80:GLN:NE2   | 2.36                     | 0.40              |
| 14:P:258:LEU:HD23 | 14:P:261:MET:HE3  | 2.03                     | 0.40              |
| 14:P:361:SER:HB3  | 21:W:47:PRO:HG2   | 2.02                     | 0.40              |
| 19:U:79:PHE:HA    | 19:U:83:LEU:HD12  | 2.01                     | 0.40              |
| 22:X:81:LEU:HD23  | 22:X:81:LEU:HA    | 1.90                     | 0.40              |
| 29:e:9:ARG:HG3    | 29:e:10:HIS:CD2   | 2.57                     | 0.40              |
| 31:g:78:LEU:HD23  | 31:g:78:LEU:HA    | 1.87                     | 0.40              |
| 35:k:4:ASN:O      | 35:k:7:LYS:HG3    | 2.21                     | 0.40              |
| 38:n:27:SER:HA    | 38:n:75:LEU:HD21  | 2.04                     | 0.40              |
| 39:o:63:ASP:O     | 39:o:67:ARG:HG3   | 2.20                     | 0.40              |
| 3:C:84:ILE:HG22   | 3:C:92:VAL:HG21   | 2.04                     | 0.40              |
| 4:D:86:HIS:CE1    | 4:D:88:GLU:HB2    | 2.57                     | 0.40              |
| 4:D:149:MET:HE2   | 4:D:149:MET:HB3   | 1.86                     | 0.40              |
| 7:I:74:SER:HB3    | 43:Z:202:PLC:H1A2 | 2.04                     | 0.40              |
| 7:I:162:CYS:SG    | 7:I:163:ILE:N     | 2.94                     | 0.40              |
| 8:J:122:GLU:HB3   | 8:J:126:SER:OG    | 2.21                     | 0.40              |
| 8:J:141:LEU:HD13  | 46:O:201:CDL:H821 | 2.02                     | 0.40              |
| 10:L:134:LEU:HD23 | 10:L:134:LEU:HA   | 1.87                     | 0.40              |
| 10:L:504:PRO:HD2  | 10:L:507:LEU:HD12 | 2.02                     | 0.40              |
| 10:L:636:LEU:O    | 10:L:640:ILE:HG13 | 2.22                     | 0.40              |
| 11:M:41:LYS:HG3   | 31:g:83:TYR:CE1   | 2.57                     | 0.40              |
| 11:M:62:ILE:H     | 11:M:62:ILE:HG13  | 1.53                     | 0.40              |
| 11:M:206:SER:OG   | 23:Y:191:PHE:O    | 2.23                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:O:135:LEU:HD23 | 13:O:135:LEU:HA   | 1.93                     | 0.40              |
| 14:P:247:LEU:HB3  | 14:P:326:PHE:CE2  | 2.57                     | 0.40              |
| 24:Z:3:GLN:HG2    | 24:Z:4:ASP:H      | 1.86                     | 0.40              |
| 26:b:3:ILE:HG12   | 26:b:4:GLY:N      | 2.36                     | 0.40              |
| 36:l:121:LYS:HD2  | 37:m:77:TYR:CE1   | 2.57                     | 0.40              |
| 41:q:74:GLU:HG3   | 41:q:75:PRO:HD2   | 2.03                     | 0.40              |
| 1:A:76:LEU:HB3    | 1:A:77:PRO:HD3    | 2.04                     | 0.40              |
| 4:D:455:ASP:OD2   | 21:W:3:ASN:N      | 2.41                     | 0.40              |
| 5:G:123:CYS:HB2   | 5:G:124:PRO:HD3   | 2.04                     | 0.40              |
| 5:G:456:LEU:HD22  | 5:G:494:PHE:CG    | 2.57                     | 0.40              |
| 9:K:55:ILE:HD13   | 9:K:55:ILE:HA     | 1.86                     | 0.40              |
| 10:L:323:ASN:OD1  | 10:L:323:ASN:N    | 2.54                     | 0.40              |
| 45:L:705:3PE:H271 | 45:L:705:3PE:H242 | 1.80                     | 0.40              |
| 11:M:21:ASN:HD22  | 11:M:21:ASN:C     | 2.29                     | 0.40              |
| 11:M:249:LEU:O    | 11:M:254:LEU:HG   | 2.21                     | 0.40              |
| 18:T:110:ASN:HD21 | 21:W:22:THR:HG23  | 1.86                     | 0.40              |
| 23:Y:182:LYS:HA   | 23:Y:182:LYS:HD3  | 1.89                     | 0.40              |
| 24:Z:18:ARG:NH2   | 24:Z:20:LEU:HD13  | 2.37                     | 0.40              |
| 33:i:63:GLU:OE1   | 33:i:63:GLU:N     | 2.51                     | 0.40              |
| 40:p:30:LEU:HD23  | 40:p:82:PHE:HA    | 2.02                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 133/141 (94%) | 126 (95%) | 6 (4%)  | 1 (1%)   | 16          | 48  |
| 2   | B     | 173/204 (85%) | 166 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 3   | C     | 231/289 (80%) | 221 (96%) | 10 (4%) | 0        | 100         | 100 |
| 4   | D     | 435/482 (90%) | 406 (93%) | 29 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 5   | G     | 548/726 (76%)  | 515 (94%) | 33 (6%) | 0        | 100         | 100 |
| 6   | H     | 351/353 (99%)  | 323 (92%) | 27 (8%) | 1 (0%)   | 36          | 67  |
| 7   | I     | 190/222 (86%)  | 181 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 8   | J     | 151/161 (94%)  | 144 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 9   | K     | 78/82 (95%)    | 75 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 10  | L     | 640/642 (100%) | 622 (97%) | 17 (3%) | 1 (0%)   | 43          | 73  |
| 11  | M     | 489/491 (100%) | 470 (96%) | 19 (4%) | 0        | 100         | 100 |
| 12  | N     | 502/523 (96%)  | 492 (98%) | 10 (2%) | 0        | 100         | 100 |
| 13  | O     | 191/193 (99%)  | 185 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 14  | P     | 353/384 (92%)  | 342 (97%) | 11 (3%) | 0        | 100         | 100 |
| 15  | Q     | 84/159 (53%)   | 84 (100%) | 0       | 0        | 100         | 100 |
| 16  | R     | 122/139 (88%)  | 115 (94%) | 7 (6%)  | 0        | 100         | 100 |
| 17  | S     | 88/90 (98%)    | 83 (94%)  | 4 (4%)  | 1 (1%)   | 11          | 41  |
| 18  | T     | 91/138 (66%)   | 85 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 19  | U     | 86/130 (66%)   | 80 (93%)  | 6 (7%)  | 0        | 100         | 100 |
| 20  | V     | 124/134 (92%)  | 119 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 21  | W     | 111/122 (91%)  | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 22  | X     | 182/184 (99%)  | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 23  | Y     | 203/216 (94%)  | 190 (94%) | 13 (6%) | 0        | 100         | 100 |
| 24  | Z     | 140/147 (95%)  | 135 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 25  | a     | 147/150 (98%)  | 144 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 26  | b     | 76/79 (96%)    | 71 (93%)  | 5 (7%)  | 0        | 100         | 100 |
| 27  | c     | 140/182 (77%)  | 127 (91%) | 13 (9%) | 0        | 100         | 100 |
| 28  | d     | 73/78 (94%)    | 72 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 29  | e     | 103/106 (97%)  | 97 (94%)  | 6 (6%)  | 0        | 100         | 100 |
| 30  | f     | 76/86 (88%)    | 74 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 31  | g     | 152/239 (64%)  | 144 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 32  | h     | 129/182 (71%)  | 123 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 33  | i     | 67/74 (90%)    | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 34  | j     | 51/59 (86%)    | 51 (100%) | 0       | 0        | 100         | 100 |
| 35  | k     | 43/61 (70%)    | 41 (95%)  | 2 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 36  | l     | 130/156 (83%)   | 121 (93%)  | 8 (6%)   | 1 (1%)   | 16          | 48  |
| 37  | m     | 75/81 (93%)     | 71 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 38  | n     | 103/111 (93%)   | 101 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 39  | o     | 78/87 (90%)     | 75 (96%)   | 3 (4%)   | 0        | 100         | 100 |
| 40  | p     | 88/92 (96%)     | 83 (94%)   | 5 (6%)   | 0        | 100         | 100 |
| 41  | q     | 138/140 (99%)   | 133 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| All | All   | 7365/8315 (89%) | 7037 (96%) | 323 (4%) | 5 (0%)   | 49          | 79  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | l     | 145 | THR  |
| 6   | H     | 222 | VAL  |
| 17  | S     | 2   | SER  |
| 1   | A     | 2   | LEU  |
| 10  | 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   | A     | 124/128 (97%)  | 115 (93%) | 9 (7%)   | 13          | 39  |
| 2   | B     | 154/180 (86%)  | 149 (97%) | 5 (3%)   | 34          | 56  |
| 3   | C     | 208/254 (82%)  | 202 (97%) | 6 (3%)   | 37          | 58  |
| 4   | D     | 375/408 (92%)  | 359 (96%) | 16 (4%)  | 26          | 50  |
| 5   | G     | 469/610 (77%)  | 450 (96%) | 19 (4%)  | 27          | 51  |
| 6   | H     | 307/307 (100%) | 294 (96%) | 13 (4%)  | 26          | 50  |
| 7   | I     | 166/192 (86%)  | 158 (95%) | 8 (5%)   | 23          | 47  |
| 8   | J     | 143/149 (96%)  | 132 (92%) | 11 (8%)  | 12          | 37  |
| 9   | K     | 70/72 (97%)    | 70 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|-------------|-----|
| 10  | L     | 576/576 (100%) | 564 (98%) | 12 (2%)  | 47          | 64  |
| 11  | M     | 439/439 (100%) | 425 (97%) | 14 (3%)  | 34          | 56  |
| 12  | N     | 474/489 (97%)  | 455 (96%) | 19 (4%)  | 28          | 52  |
| 13  | O     | 169/169 (100%) | 165 (98%) | 4 (2%)   | 43          | 62  |
| 14  | P     | 309/332 (93%)  | 302 (98%) | 7 (2%)   | 44          | 63  |
| 15  | Q     | 76/135 (56%)   | 74 (97%)  | 2 (3%)   | 40          | 60  |
| 16  | R     | 104/118 (88%)  | 101 (97%) | 3 (3%)   | 37          | 58  |
| 17  | S     | 77/77 (100%)   | 72 (94%)  | 5 (6%)   | 15          | 42  |
| 18  | T     | 85/128 (66%)   | 78 (92%)  | 7 (8%)   | 10          | 35  |
| 19  | U     | 80/120 (67%)   | 73 (91%)  | 7 (9%)   | 9           | 33  |
| 20  | V     | 112/119 (94%)  | 107 (96%) | 5 (4%)   | 24          | 48  |
| 21  | W     | 107/114 (94%)  | 102 (95%) | 5 (5%)   | 23          | 48  |
| 22  | X     | 165/165 (100%) | 158 (96%) | 7 (4%)   | 26          | 50  |
| 23  | Y     | 163/173 (94%)  | 158 (97%) | 5 (3%)   | 35          | 57  |
| 24  | Z     | 123/128 (96%)  | 121 (98%) | 2 (2%)   | 55          | 68  |
| 25  | a     | 128/129 (99%)  | 127 (99%) | 1 (1%)   | 73          | 76  |
| 26  | b     | 66/67 (98%)    | 65 (98%)  | 1 (2%)   | 57          | 69  |
| 27  | c     | 128/159 (80%)  | 123 (96%) | 5 (4%)   | 28          | 52  |
| 28  | d     | 62/65 (95%)    | 62 (100%) | 0        | 100         | 100 |
| 29  | e     | 91/92 (99%)    | 90 (99%)  | 1 (1%)   | 65          | 73  |
| 30  | f     | 64/71 (90%)    | 63 (98%)  | 1 (2%)   | 55          | 68  |
| 31  | g     | 143/215 (66%)  | 135 (94%) | 8 (6%)   | 19          | 45  |
| 32  | h     | 118/167 (71%)  | 113 (96%) | 5 (4%)   | 26          | 50  |
| 33  | i     | 59/63 (94%)    | 57 (97%)  | 2 (3%)   | 32          | 55  |
| 34  | j     | 46/50 (92%)    | 44 (96%)  | 2 (4%)   | 26          | 50  |
| 35  | k     | 32/47 (68%)    | 30 (94%)  | 2 (6%)   | 16          | 42  |
| 36  | l     | 116/137 (85%)  | 107 (92%) | 9 (8%)   | 11          | 36  |
| 37  | m     | 64/66 (97%)    | 63 (98%)  | 1 (2%)   | 55          | 68  |
| 38  | n     | 95/100 (95%)   | 93 (98%)  | 2 (2%)   | 47          | 64  |
| 39  | o     | 74/79 (94%)    | 73 (99%)  | 1 (1%)   | 59          | 70  |
| 40  | p     | 83/85 (98%)    | 81 (98%)  | 2 (2%)   | 43          | 62  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 41  | q     | 125/125 (100%)  | 123 (98%)  | 2 (2%)   | 55 68       |
| All | All   | 6569/7299 (90%) | 6333 (96%) | 236 (4%) | 32 54       |

All (236) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | ILE  |
| 1   | A     | 69  | ILE  |
| 1   | A     | 76  | LEU  |
| 1   | A     | 90  | VAL  |
| 1   | A     | 118 | PHE  |
| 1   | A     | 128 | ILE  |
| 1   | A     | 131 | LYS  |
| 1   | A     | 134 | LYS  |
| 1   | A     | 137 | VAL  |
| 2   | B     | 73  | THR  |
| 2   | B     | 78  | CYS  |
| 2   | B     | 81  | VAL  |
| 2   | B     | 108 | ASP  |
| 2   | B     | 161 | ASP  |
| 3   | C     | 43  | GLU  |
| 3   | C     | 133 | THR  |
| 3   | C     | 143 | ARG  |
| 3   | C     | 223 | THR  |
| 3   | C     | 228 | VAL  |
| 3   | C     | 257 | VAL  |
| 4   | D     | 40  | ASP  |
| 4   | D     | 77  | GLU  |
| 4   | D     | 80  | ASN  |
| 4   | D     | 113 | VAL  |
| 4   | D     | 120 | LEU  |
| 4   | D     | 156 | ASP  |
| 4   | D     | 160 | TYR  |
| 4   | D     | 220 | LEU  |
| 4   | D     | 269 | GLN  |
| 4   | D     | 298 | THR  |
| 4   | D     | 332 | LYS  |
| 4   | D     | 355 | GLU  |
| 4   | D     | 406 | LYS  |
| 4   | D     | 433 | ASP  |
| 4   | D     | 459 | ARG  |
| 4   | D     | 482 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | G     | 126 | CYS  |
| 5   | G     | 128 | GLN  |
| 5   | G     | 139 | LEU  |
| 5   | G     | 176 | CYS  |
| 5   | G     | 245 | THR  |
| 5   | G     | 296 | THR  |
| 5   | G     | 298 | ARG  |
| 5   | G     | 348 | SER  |
| 5   | G     | 354 | ASP  |
| 5   | G     | 367 | ASP  |
| 5   | G     | 405 | THR  |
| 5   | G     | 414 | LEU  |
| 5   | G     | 418 | ILE  |
| 5   | G     | 442 | LEU  |
| 5   | G     | 473 | ILE  |
| 5   | G     | 513 | HIS  |
| 5   | G     | 577 | ILE  |
| 5   | G     | 593 | THR  |
| 5   | G     | 692 | VAL  |
| 6   | H     | 4   | ASN  |
| 6   | H     | 47  | LEU  |
| 6   | H     | 72  | ILE  |
| 6   | H     | 116 | ILE  |
| 6   | H     | 143 | VAL  |
| 6   | H     | 147 | VAL  |
| 6   | H     | 153 | LEU  |
| 6   | H     | 170 | ILE  |
| 6   | H     | 225 | HIS  |
| 6   | H     | 291 | SER  |
| 6   | H     | 299 | ASN  |
| 6   | H     | 329 | LEU  |
| 6   | H     | 333 | PHE  |
| 7   | I     | 40  | ILE  |
| 7   | I     | 124 | ILE  |
| 7   | I     | 128 | LEU  |
| 7   | I     | 145 | ARG  |
| 7   | I     | 152 | THR  |
| 7   | I     | 175 | ASP  |
| 7   | I     | 184 | GLU  |
| 7   | I     | 205 | ASP  |
| 8   | J     | 7   | ASP  |
| 8   | J     | 35  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | J     | 46  | LEU  |
| 8   | J     | 52  | THR  |
| 8   | J     | 59  | VAL  |
| 8   | J     | 61  | ILE  |
| 8   | J     | 69  | VAL  |
| 8   | J     | 72  | GLU  |
| 8   | J     | 124 | ASP  |
| 8   | J     | 130 | ASN  |
| 8   | J     | 135 | GLU  |
| 10  | L     | 2   | ILE  |
| 10  | L     | 119 | MET  |
| 10  | L     | 143 | ILE  |
| 10  | L     | 270 | THR  |
| 10  | L     | 348 | HIS  |
| 10  | L     | 394 | ASP  |
| 10  | L     | 432 | TYR  |
| 10  | L     | 485 | ASN  |
| 10  | L     | 486 | GLU  |
| 10  | L     | 509 | VAL  |
| 10  | L     | 536 | TYR  |
| 10  | L     | 607 | LEU  |
| 11  | M     | 21  | ASN  |
| 11  | M     | 23  | ASN  |
| 11  | M     | 28  | LEU  |
| 11  | M     | 30  | LYS  |
| 11  | M     | 62  | ILE  |
| 11  | M     | 94  | LEU  |
| 11  | M     | 108 | LYS  |
| 11  | M     | 111 | LYS  |
| 11  | M     | 192 | ILE  |
| 11  | M     | 238 | HIS  |
| 11  | M     | 301 | LEU  |
| 11  | M     | 317 | MET  |
| 11  | M     | 475 | THR  |
| 11  | M     | 489 | VAL  |
| 12  | N     | 15  | LEU  |
| 12  | N     | 18  | LYS  |
| 12  | N     | 48  | GLU  |
| 12  | N     | 67  | ASN  |
| 12  | N     | 99  | ASN  |
| 12  | N     | 108 | ILE  |
| 12  | N     | 222 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | N     | 258 | VAL  |
| 12  | N     | 261 | THR  |
| 12  | N     | 263 | LEU  |
| 12  | N     | 273 | ILE  |
| 12  | N     | 319 | ILE  |
| 12  | N     | 391 | ILE  |
| 12  | N     | 393 | ILE  |
| 12  | N     | 430 | LEU  |
| 12  | N     | 434 | VAL  |
| 12  | N     | 435 | LEU  |
| 12  | N     | 436 | ILE  |
| 12  | N     | 511 | VAL  |
| 13  | O     | 54  | LYS  |
| 13  | O     | 144 | VAL  |
| 13  | O     | 153 | ASP  |
| 13  | O     | 166 | ASN  |
| 14  | P     | 10  | THR  |
| 14  | P     | 17  | ILE  |
| 14  | P     | 119 | HIS  |
| 14  | P     | 127 | GLU  |
| 14  | P     | 130 | ASN  |
| 14  | P     | 178 | ASP  |
| 14  | P     | 316 | ASN  |
| 15  | Q     | 40  | GLU  |
| 15  | Q     | 106 | ILE  |
| 16  | R     | 97  | ASN  |
| 16  | R     | 109 | ASN  |
| 16  | R     | 118 | CYS  |
| 17  | S     | 1   | SER  |
| 17  | S     | 3   | LYS  |
| 17  | S     | 19  | GLN  |
| 17  | S     | 34  | THR  |
| 17  | S     | 84  | THR  |
| 18  | T     | 53  | ASP  |
| 18  | T     | 78  | PHE  |
| 18  | T     | 88  | ASP  |
| 18  | T     | 102 | VAL  |
| 18  | T     | 108 | THR  |
| 18  | T     | 130 | GLU  |
| 18  | T     | 137 | ILE  |
| 19  | U     | 45  | THR  |
| 19  | U     | 86  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | U     | 108 | ASN  |
| 19  | U     | 115 | THR  |
| 19  | U     | 121 | ASP  |
| 19  | U     | 128 | ASP  |
| 19  | U     | 130 | ILE  |
| 20  | V     | 41  | LEU  |
| 20  | V     | 45  | THR  |
| 20  | V     | 58  | VAL  |
| 20  | V     | 80  | ILE  |
| 20  | V     | 134 | LEU  |
| 21  | W     | 36  | ARG  |
| 21  | W     | 53  | THR  |
| 21  | W     | 65  | VAL  |
| 21  | W     | 91  | GLN  |
| 21  | W     | 114 | VAL  |
| 22  | X     | 7   | ASP  |
| 22  | X     | 18  | LEU  |
| 22  | X     | 134 | VAL  |
| 22  | X     | 139 | ASN  |
| 22  | X     | 150 | ASP  |
| 22  | X     | 160 | VAL  |
| 22  | X     | 183 | ILE  |
| 23  | Y     | 26  | THR  |
| 23  | Y     | 74  | TYR  |
| 23  | Y     | 96  | SER  |
| 23  | Y     | 175 | ASN  |
| 23  | Y     | 211 | ARG  |
| 24  | Z     | 8   | ILE  |
| 24  | Z     | 73  | GLU  |
| 25  | a     | 111 | LEU  |
| 26  | b     | 3   | ILE  |
| 27  | c     | 12  | THR  |
| 27  | c     | 86  | ASP  |
| 27  | c     | 88  | THR  |
| 27  | c     | 90  | VAL  |
| 27  | c     | 133 | LYS  |
| 29  | e     | 104 | GLU  |
| 30  | f     | 45  | ASP  |
| 31  | g     | 32  | LYS  |
| 31  | g     | 43  | LYS  |
| 31  | g     | 81  | THR  |
| 31  | g     | 96  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | g     | 161 | ASP  |
| 31  | g     | 177 | LEU  |
| 31  | g     | 192 | ASP  |
| 31  | g     | 207 | ILE  |
| 32  | h     | 104 | ILE  |
| 32  | h     | 148 | GLU  |
| 32  | h     | 156 | THR  |
| 32  | h     | 164 | ASN  |
| 32  | h     | 167 | ASP  |
| 33  | i     | 7   | HIS  |
| 33  | i     | 32  | LEU  |
| 34  | j     | 20  | VAL  |
| 34  | j     | 59  | HIS  |
| 35  | k     | 7   | LYS  |
| 35  | k     | 32  | PHE  |
| 36  | l     | 25  | LYS  |
| 36  | l     | 44  | LEU  |
| 36  | l     | 45  | LYS  |
| 36  | l     | 57  | LYS  |
| 36  | l     | 68  | ASN  |
| 36  | l     | 93  | ILE  |
| 36  | l     | 114 | ILE  |
| 36  | l     | 136 | ASP  |
| 36  | l     | 156 | ILE  |
| 37  | m     | 9   | LEU  |
| 38  | n     | 9   | VAL  |
| 38  | n     | 88  | CYS  |
| 39  | o     | 60  | GLN  |
| 40  | p     | 3   | ASP  |
| 40  | p     | 13  | ASP  |
| 41  | q     | 35  | VAL  |
| 41  | q     | 95  | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 197 | HIS  |
| 3   | C     | 199 | HIS  |
| 4   | D     | 150 | GLN  |
| 4   | D     | 399 | HIS  |
| 7   | I     | 44  | HIS  |
| 8   | J     | 118 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | K     | 14  | ASN  |
| 10  | L     | 171 | ASN  |
| 11  | M     | 22  | ASN  |
| 11  | M     | 23  | ASN  |
| 11  | M     | 298 | GLN  |
| 11  | M     | 358 | HIS  |
| 12  | N     | 123 | ASN  |
| 12  | N     | 185 | ASN  |
| 12  | N     | 187 | GLN  |
| 12  | N     | 310 | ASN  |
| 12  | N     | 365 | ASN  |
| 12  | N     | 477 | ASN  |
| 12  | N     | 506 | GLN  |
| 12  | N     | 521 | ASN  |
| 14  | P     | 62  | HIS  |
| 17  | S     | 19  | GLN  |
| 17  | S     | 67  | HIS  |
| 18  | T     | 131 | GLN  |
| 20  | V     | 98  | GLN  |
| 22  | X     | 154 | HIS  |
| 23  | Y     | 55  | HIS  |
| 23  | Y     | 109 | GLN  |
| 24  | Z     | 19  | ASN  |
| 24  | Z     | 136 | ASN  |
| 25  | a     | 25  | ASN  |
| 31  | g     | 181 | ASN  |
| 32  | h     | 92  | HIS  |
| 38  | n     | 55  | ASN  |
| 39  | o     | 36  | ASN  |
| 41  | q     | 42  | 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 |
| 6   | FME  | H     | 1   | 6    | 8,9,10       | 1.52 | 1 (12%)  | 8,9,11      | 1.45 | 2 (25%)  |
| 11  | FME  | M     | 1   | 11   | 8,9,10       | 1.51 | 1 (12%)  | 8,9,11      | 1.39 | 1 (12%)  |
| 8   | FME  | J     | 1   | 8    | 8,9,10       | 1.52 | 1 (12%)  | 8,9,11      | 1.37 | 1 (12%)  |
| 1   | FME  | A     | 1   | 1    | 8,9,10       | 1.50 | 1 (12%)  | 8,9,11      | 1.40 | 2 (25%)  |
| 12  | FME  | N     | 1   | 12   | 8,9,10       | 1.48 | 1 (12%)  | 8,9,11      | 1.50 | 2 (25%)  |
| 4   | 2MR  | D     | 137 | 4    | 10,12,13     | 2.45 | 2 (20%)  | 5,13,15     | 2.21 | 2 (40%)  |
| 10  | FME  | L     | 1   | 10   | 8,9,10       | 1.51 | 1 (12%)  | 8,9,11      | 1.51 | 2 (25%)  |
| 9   | FME  | K     | 1   | 9    | 8,9,10       | 1.54 | 1 (12%)  | 8,9,11      | 1.04 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 6   | FME  | H     | 1   | 6    | -       | 4/7/9/11   | -     |
| 11  | FME  | M     | 1   | 11   | -       | 4/7/9/11   | -     |
| 8   | FME  | J     | 1   | 8    | -       | 5/7/9/11   | -     |
| 1   | FME  | A     | 1   | 1    | -       | 2/7/9/11   | -     |
| 12  | FME  | N     | 1   | 12   | -       | 0/7/9/11   | -     |
| 4   | 2MR  | D     | 137 | 4    | -       | 4/10/13/15 | -     |
| 10  | FME  | L     | 1   | 10   | -       | 5/7/9/11   | -     |
| 9   | FME  | K     | 1   | 9    | -       | 5/7/9/11   | -     |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 4   | D     | 137 | 2MR  | CZ-NH2 | 5.34 | 1.44        | 1.33     |
| 4   | D     | 137 | 2MR  | CZ-NE  | 5.17 | 1.45        | 1.34     |
| 9   | K     | 1   | FME  | CN-N   | 3.88 | 1.46        | 1.33     |
| 6   | H     | 1   | FME  | CN-N   | 3.75 | 1.45        | 1.33     |
| 8   | J     | 1   | FME  | CN-N   | 3.75 | 1.45        | 1.33     |
| 11  | M     | 1   | FME  | CN-N   | 3.74 | 1.45        | 1.33     |
| 10  | L     | 1   | FME  | CN-N   | 3.73 | 1.45        | 1.33     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | A     | 1   | FME  | CN-N  | 3.65 | 1.45        | 1.33     |
| 12  | N     | 1   | FME  | CN-N  | 3.61 | 1.45        | 1.33     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 4   | D     | 137 | 2MR  | NE-CZ-NH2  | 3.66  | 122.83      | 119.48   |
| 4   | D     | 137 | 2MR  | CQ2-NH2-CZ | -2.61 | 118.03      | 123.65   |
| 12  | N     | 1   | FME  | O1-CN-N    | -2.32 | 119.32      | 125.32   |
| 10  | L     | 1   | FME  | O1-CN-N    | -2.30 | 119.38      | 125.32   |
| 12  | N     | 1   | FME  | CA-N-CN    | -2.26 | 119.35      | 122.82   |
| 1   | A     | 1   | FME  | O1-CN-N    | -2.19 | 119.66      | 125.32   |
| 6   | H     | 1   | FME  | CA-N-CN    | -2.17 | 119.49      | 122.82   |
| 10  | L     | 1   | FME  | CA-N-CN    | -2.16 | 119.50      | 122.82   |
| 6   | H     | 1   | FME  | O1-CN-N    | -2.07 | 119.97      | 125.32   |
| 1   | A     | 1   | FME  | O-C-CA     | -2.07 | 119.45      | 124.77   |
| 8   | J     | 1   | FME  | O1-CN-N    | -2.06 | 120.01      | 125.32   |
| 11  | M     | 1   | FME  | O1-CN-N    | -2.02 | 120.10      | 125.32   |

There are no chirality outliers.

All (29) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 1   | A     | 1   | FME  | O-C-CA-CB   |
| 6   | H     | 1   | FME  | N-CA-CB-CG  |
| 6   | H     | 1   | FME  | C-CA-CB-CG  |
| 8   | J     | 1   | FME  | O1-CN-N-CA  |
| 8   | J     | 1   | FME  | CB-CA-N-CN  |
| 8   | J     | 1   | FME  | N-CA-CB-CG  |
| 8   | J     | 1   | FME  | C-CA-CB-CG  |
| 9   | K     | 1   | FME  | CB-CA-N-CN  |
| 9   | K     | 1   | FME  | N-CA-CB-CG  |
| 10  | L     | 1   | FME  | N-CA-CB-CG  |
| 11  | M     | 1   | FME  | C-CA-CB-CG  |
| 11  | M     | 1   | FME  | O-C-CA-CB   |
| 9   | K     | 1   | FME  | CA-CB-CG-SD |
| 4   | D     | 137 | 2MR  | NE-CD-CG-CB |
| 11  | M     | 1   | FME  | CB-CG-SD-CE |
| 11  | M     | 1   | FME  | N-CA-CB-CG  |
| 8   | J     | 1   | FME  | CB-CG-SD-CE |
| 9   | K     | 1   | FME  | CB-CG-SD-CE |
| 10  | L     | 1   | FME  | CA-CB-CG-SD |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | H     | 1   | FME  | CB-CG-SD-CE |
| 10  | L     | 1   | FME  | CB-CG-SD-CE |
| 9   | K     | 1   | FME  | C-CA-CB-CG  |
| 10  | L     | 1   | FME  | C-CA-CB-CG  |
| 6   | H     | 1   | FME  | CB-CA-N-CN  |
| 4   | D     | 137 | 2MR  | CG-CD-NE-CZ |
| 4   | D     | 137 | 2MR  | N-CA-CB-CG  |
| 1   | A     | 1   | FME  | CA-CB-CG-SD |
| 10  | L     | 1   | FME  | CB-CA-N-CN  |
| 4   | D     | 137 | 2MR  | C-CA-CB-CG  |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 8   | J     | 1   | FME  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are monoatomic - leaving 50 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 | $\# Z  > 2$ |
| 42  | SF4  | I     | 302 | 7    | 0,12,12      | -    | -           | -           |      |             |
| 43  | PLC  | B     | 302 | -    | 30,30,41     | 0.59 | 0           | 36,38,49    | 0.54 | 0           |
| 45  | 3PE  | N     | 601 | -    | 39,39,50     | 0.98 | 4 (10%)     | 42,44,55    | 1.18 | 2 (4%)      |
| 45  | 3PE  | m     | 101 | -    | 45,45,50     | 0.91 | 4 (8%)      | 48,50,55    | 1.12 | 2 (4%)      |
| 45  | 3PE  | J     | 201 | -    | 50,50,50     | 0.87 | 4 (8%)      | 53,55,55    | 1.11 | 2 (3%)      |
| 45  | 3PE  | L     | 705 | -    | 50,50,50     | 0.87 | 4 (8%)      | 53,55,55    | 1.12 | 2 (3%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 42  | SF4  | G     | 801 | 5    | 0,12,12      | -    | -        | -           |      |          |
| 45  | 3PE  | L     | 706 | -    | 41,41,50     | 0.96 | 3 (7%)   | 44,46,55    | 1.16 | 2 (4%)   |
| 43  | PLC  | q     | 201 | -    | 41,41,41     | 0.51 | 0        | 47,49,49    | 0.57 | 0        |
| 43  | PLC  | q     | 202 | -    | 35,35,41     | 0.57 | 0        | 41,43,49    | 0.57 | 0        |
| 43  | PLC  | b     | 101 | -    | 38,38,41     | 0.55 | 0        | 44,46,49    | 0.58 | 0        |
| 43  | PLC  | d     | 102 | -    | 41,41,41     | 0.53 | 0        | 47,49,49    | 0.52 | 0        |
| 42  | SF4  | B     | 301 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 43  | PLC  | M     | 504 | -    | 41,41,41     | 0.50 | 0        | 47,49,49    | 0.57 | 0        |
| 43  | PLC  | Y     | 302 | -    | 35,35,41     | 0.53 | 0        | 41,43,49    | 0.63 | 0        |
| 45  | 3PE  | L     | 703 | -    | 50,50,50     | 0.87 | 3 (6%)   | 53,55,55    | 1.10 | 2 (3%)   |
| 45  | 3PE  | b     | 103 | -    | 30,30,50     | 1.10 | 4 (13%)  | 33,35,55    | 1.19 | 2 (6%)   |
| 43  | PLC  | a     | 201 | -    | 21,21,41     | 0.69 | 0        | 27,29,49    | 0.66 | 0        |
| 47  | NDP  | P     | 501 | -    | 51,52,52     | 3.99 | 27 (52%) | 71,80,80    | 2.02 | 15 (21%) |
| 43  | PLC  | P     | 502 | -    | 30,30,41     | 0.60 | 0        | 36,38,49    | 0.55 | 0        |
| 43  | PLC  | d     | 101 | -    | 41,41,41     | 0.54 | 0        | 47,49,49    | 0.51 | 0        |
| 45  | 3PE  | Y     | 301 | -    | 24,24,50     | 1.22 | 4 (16%)  | 27,29,55    | 1.40 | 2 (7%)   |
| 45  | 3PE  | L     | 702 | -    | 50,50,50     | 0.87 | 3 (6%)   | 53,55,55    | 1.14 | 2 (3%)   |
| 45  | 3PE  | h     | 201 | -    | 45,45,50     | 0.92 | 3 (6%)   | 48,50,55    | 1.10 | 2 (4%)   |
| 46  | CDL  | q     | 203 | -    | 59,59,99     | 1.13 | 8 (13%)  | 65,71,111   | 1.21 | 4 (6%)   |
| 45  | 3PE  | b     | 104 | -    | 39,39,50     | 0.97 | 4 (10%)  | 42,44,55    | 1.16 | 2 (4%)   |
| 45  | 3PE  | L     | 707 | -    | 28,28,50     | 1.15 | 3 (10%)  | 31,33,55    | 1.18 | 2 (6%)   |
| 49  | EHZ  | T     | 201 | -    | 31,36,37     | 1.56 | 5 (16%)  | 36,44,47    | 1.48 | 3 (8%)   |
| 42  | SF4  | I     | 301 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 43  | PLC  | Z     | 202 | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.59 | 1 (2%)   |
| 49  | EHZ  | U     | 201 | -    | 31,36,37     | 1.56 | 5 (16%)  | 36,44,47    | 1.53 | 6 (16%)  |
| 43  | PLC  | L     | 708 | -    | 34,34,41     | 0.57 | 0        | 40,42,49    | 0.61 | 0        |
| 46  | CDL  | b     | 102 | -    | 58,58,99     | 1.13 | 7 (12%)  | 64,70,111   | 1.24 | 4 (6%)   |
| 45  | 3PE  | L     | 704 | -    | 34,34,50     | 1.04 | 4 (11%)  | 37,39,55    | 1.15 | 2 (5%)   |
| 43  | PLC  | L     | 710 | -    | 41,41,41     | 0.54 | 0        | 47,49,49    | 0.51 | 0        |
| 45  | 3PE  | Z     | 201 | -    | 35,35,50     | 1.03 | 4 (11%)  | 38,40,55    | 1.16 | 2 (5%)   |
| 43  | PLC  | L     | 701 | -    | 41,41,41     | 0.50 | 0        | 47,49,49    | 0.73 | 2 (4%)   |
| 45  | 3PE  | M     | 502 | -    | 34,34,50     | 1.04 | 4 (11%)  | 37,39,55    | 1.17 | 2 (5%)   |
| 43  | PLC  | M     | 503 | -    | 41,41,41     | 0.53 | 0        | 47,49,49    | 0.57 | 1 (2%)   |
| 46  | CDL  | O     | 201 | -    | 74,74,99     | 1.01 | 7 (9%)   | 80,86,111   | 1.17 | 4 (5%)   |
| 45  | 3PE  | M     | 501 | -    | 50,50,50     | 0.87 | 4 (8%)   | 53,55,55    | 1.11 | 2 (3%)   |
| 43  | PLC  | L     | 709 | -    | 31,31,41     | 0.57 | 0        | 37,39,49    | 0.59 | 0        |
| 43  | PLC  | g     | 301 | -    | 38,38,41     | 0.56 | 0        | 44,46,49    | 0.49 | 0        |
| 42  | SF4  | G     | 802 | 5    | 0,12,12      | -    | -        | -           |      |          |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 46  | CDL  | Z     | 203 | -    | 48,48,99     | 1.24 | 8 (16%)  | 54,60,111   | 1.26 | 4 (7%)   |
| 43  | PLC  | D     | 501 | -    | 41,41,41     | 0.52 | 0        | 47,49,49    | 0.57 | 0        |
| 45  | 3PE  | j     | 101 | -    | 26,26,50     | 1.18 | 4 (15%)  | 29,31,55    | 1.18 | 2 (6%)   |
| 43  | PLC  | P     | 503 | -    | 30,30,41     | 0.59 | 0        | 36,38,49    | 0.63 | 0        |
| 43  | PLC  | Y     | 303 | -    | 35,35,41     | 0.55 | 0        | 41,43,49    | 0.56 | 0        |
| 43  | PLC  | H     | 401 | -    | 23,23,41     | 0.67 | 0        | 29,31,49    | 0.70 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 42  | SF4  | I     | 302 | 7    | -       | -           | 0/6/5/5 |
| 43  | PLC  | B     | 302 | -    | -       | 9/34/34/45  | -       |
| 45  | 3PE  | N     | 601 | -    | -       | 19/43/43/54 | -       |
| 45  | 3PE  | m     | 101 | -    | -       | 22/49/49/54 | -       |
| 45  | 3PE  | J     | 201 | -    | -       | 25/54/54/54 | -       |
| 45  | 3PE  | L     | 705 | -    | -       | 22/54/54/54 | -       |
| 42  | SF4  | G     | 801 | 5    | -       | -           | 0/6/5/5 |
| 45  | 3PE  | L     | 706 | -    | -       | 21/45/45/54 | -       |
| 43  | PLC  | q     | 201 | -    | -       | 25/45/45/45 | -       |
| 43  | PLC  | q     | 202 | -    | -       | 15/39/39/45 | -       |
| 43  | PLC  | b     | 101 | -    | -       | 7/42/42/45  | -       |
| 43  | PLC  | d     | 102 | -    | -       | 18/45/45/45 | -       |
| 43  | PLC  | M     | 504 | -    | -       | 18/45/45/45 | -       |
| 43  | PLC  | Y     | 302 | -    | -       | 14/39/39/45 | -       |
| 45  | 3PE  | L     | 703 | -    | -       | 26/54/54/54 | -       |
| 45  | 3PE  | b     | 103 | -    | -       | 18/34/34/54 | -       |
| 47  | NDP  | P     | 501 | -    | -       | 15/34/77/77 | 0/5/5/5 |
| 43  | PLC  | a     | 201 | -    | -       | 7/23/23/45  | -       |
| 42  | SF4  | B     | 301 | 2    | -       | -           | 0/6/5/5 |
| 43  | PLC  | P     | 502 | -    | -       | 14/34/34/45 | -       |
| 43  | PLC  | d     | 101 | -    | -       | 12/45/45/45 | -       |
| 45  | 3PE  | Y     | 301 | -    | -       | 15/27/27/54 | -       |
| 45  | 3PE  | L     | 702 | -    | -       | 18/54/54/54 | -       |
| 45  | 3PE  | h     | 201 | -    | -       | 16/49/49/54 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 46  | CDL  | q     | 203 | -    | -       | 26/70/70/110 | -       |
| 45  | 3PE  | b     | 104 | -    | -       | 23/43/43/54  | -       |
| 45  | 3PE  | L     | 707 | -    | -       | 5/32/32/54   | -       |
| 49  | EHZ  | T     | 201 | -    | -       | 22/42/44/45  | -       |
| 42  | SF4  | I     | 301 | 7    | -       | -            | 0/6/5/5 |
| 43  | PLC  | Z     | 202 | -    | -       | 22/45/45/45  | -       |
| 49  | EHZ  | U     | 201 | -    | -       | 14/42/44/45  | -       |
| 43  | PLC  | L     | 708 | -    | -       | 12/38/38/45  | -       |
| 46  | CDL  | b     | 102 | -    | -       | 23/69/69/110 | -       |
| 45  | 3PE  | L     | 704 | -    | -       | 15/38/38/54  | -       |
| 43  | PLC  | L     | 710 | -    | -       | 15/45/45/45  | -       |
| 45  | 3PE  | Z     | 201 | -    | -       | 13/39/39/54  | -       |
| 43  | PLC  | L     | 701 | -    | -       | 15/45/45/45  | -       |
| 45  | 3PE  | M     | 502 | -    | -       | 17/38/38/54  | -       |
| 43  | PLC  | M     | 503 | -    | -       | 14/45/45/45  | -       |
| 46  | CDL  | O     | 201 | -    | -       | 35/85/85/110 | -       |
| 45  | 3PE  | M     | 501 | -    | -       | 24/54/54/54  | -       |
| 43  | PLC  | L     | 709 | -    | -       | 10/35/35/45  | -       |
| 43  | PLC  | g     | 301 | -    | -       | 14/42/42/45  | -       |
| 42  | SF4  | G     | 802 | 5    | -       | -            | 0/6/5/5 |
| 46  | CDL  | Z     | 203 | -    | -       | 27/58/58/110 | -       |
| 43  | PLC  | D     | 501 | -    | -       | 10/45/45/45  | -       |
| 45  | 3PE  | j     | 101 | -    | -       | 14/30/30/54  | -       |
| 43  | PLC  | P     | 503 | -    | -       | 11/34/34/45  | -       |
| 43  | PLC  | Y     | 303 | -    | -       | 12/39/39/45  | -       |
| 43  | PLC  | H     | 401 | -    | -       | 5/26/26/45   | -       |

All (130) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | P     | 501 | NDP  | PA-O3   | 10.03 | 1.70        | 1.59     |
| 47  | P     | 501 | NDP  | C2B-C1B | -8.98 | 1.31        | 1.53     |
| 47  | P     | 501 | NDP  | O4B-C1B | 8.57  | 1.61        | 1.42     |
| 47  | P     | 501 | NDP  | O4D-C1D | 8.20  | 1.61        | 1.42     |
| 47  | P     | 501 | NDP  | C7N-N7N | 7.64  | 1.55        | 1.33     |
| 47  | P     | 501 | NDP  | C2D-C1D | -7.55 | 1.29        | 1.53     |
| 47  | P     | 501 | NDP  | C6N-C5N | 7.07  | 1.54        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | P     | 501 | NDP  | O4D-C4D | -6.44 | 1.30        | 1.45     |
| 47  | P     | 501 | NDP  | P2B-O2B | 5.81  | 1.69        | 1.59     |
| 47  | P     | 501 | NDP  | C6A-N6A | 5.46  | 1.48        | 1.34     |
| 47  | P     | 501 | NDP  | O4B-C4B | -5.24 | 1.33        | 1.45     |
| 49  | T     | 201 | EHZ  | C15-N2  | 5.06  | 1.45        | 1.33     |
| 49  | T     | 201 | EHZ  | C12-N1  | 5.06  | 1.45        | 1.33     |
| 49  | U     | 201 | EHZ  | C12-N1  | 4.98  | 1.45        | 1.33     |
| 49  | U     | 201 | EHZ  | C15-N2  | 4.95  | 1.45        | 1.33     |
| 47  | P     | 501 | NDP  | C2N-C3N | 4.76  | 1.48        | 1.35     |
| 47  | P     | 501 | NDP  | PN-O3   | 4.40  | 1.64        | 1.59     |
| 47  | P     | 501 | NDP  | C5A-C4A | -4.21 | 1.31        | 1.39     |
| 47  | P     | 501 | NDP  | O7N-C7N | -4.04 | 1.15        | 1.24     |
| 47  | P     | 501 | NDP  | C8A-N9A | -3.75 | 1.31        | 1.37     |
| 47  | P     | 501 | NDP  | O2D-C2D | 3.68  | 1.52        | 1.43     |
| 47  | P     | 501 | NDP  | C4N-C3N | 3.51  | 1.56        | 1.50     |
| 46  | O     | 201 | CDL  | OB6-CB4 | -2.93 | 1.39        | 1.46     |
| 45  | L     | 706 | 3PE  | O21-C2  | -2.92 | 1.39        | 1.46     |
| 47  | P     | 501 | NDP  | C4N-C5N | 2.87  | 1.56        | 1.49     |
| 46  | b     | 102 | CDL  | OB6-CB4 | -2.84 | 1.39        | 1.46     |
| 45  | h     | 201 | 3PE  | O21-C2  | -2.83 | 1.39        | 1.46     |
| 45  | L     | 707 | 3PE  | O21-C2  | -2.82 | 1.40        | 1.46     |
| 45  | L     | 703 | 3PE  | O21-C2  | -2.82 | 1.40        | 1.46     |
| 45  | L     | 705 | 3PE  | O21-C2  | -2.81 | 1.40        | 1.46     |
| 45  | L     | 702 | 3PE  | O21-C2  | -2.80 | 1.40        | 1.46     |
| 46  | q     | 203 | CDL  | OB6-CB4 | -2.78 | 1.40        | 1.46     |
| 45  | j     | 101 | 3PE  | O21-C2  | -2.72 | 1.40        | 1.46     |
| 45  | L     | 704 | 3PE  | O21-C2  | -2.72 | 1.40        | 1.46     |
| 45  | b     | 104 | 3PE  | O21-C2  | -2.71 | 1.40        | 1.46     |
| 45  | M     | 501 | 3PE  | O21-C2  | -2.71 | 1.40        | 1.46     |
| 46  | b     | 102 | CDL  | OA6-CA4 | -2.69 | 1.40        | 1.46     |
| 46  | Z     | 203 | CDL  | OB6-CB4 | -2.68 | 1.40        | 1.46     |
| 45  | J     | 201 | 3PE  | O21-C2  | -2.67 | 1.40        | 1.46     |
| 45  | b     | 103 | 3PE  | O21-C2  | -2.65 | 1.40        | 1.46     |
| 45  | N     | 601 | 3PE  | O21-C2  | -2.63 | 1.40        | 1.46     |
| 45  | Z     | 201 | 3PE  | O21-C2  | -2.60 | 1.40        | 1.46     |
| 46  | Z     | 203 | CDL  | OA6-CA5 | 2.58  | 1.40        | 1.35     |
| 45  | M     | 502 | 3PE  | O21-C2  | -2.57 | 1.40        | 1.46     |
| 47  | P     | 501 | NDP  | C5A-N7A | -2.57 | 1.34        | 1.39     |
| 47  | P     | 501 | NDP  | C7N-C3N | 2.56  | 1.54        | 1.48     |
| 47  | P     | 501 | NDP  | O3B-C3B | -2.52 | 1.36        | 1.43     |
| 45  | Y     | 301 | 3PE  | O21-C21 | 2.50  | 1.40        | 1.35     |
| 46  | b     | 102 | CDL  | OB8-CB7 | 2.47  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | P     | 501 | NDP  | O3D-C3D | -2.45 | 1.36        | 1.43     |
| 46  | q     | 203 | CDL  | OA6-CA4 | -2.45 | 1.40        | 1.46     |
| 45  | j     | 101 | 3PE  | O31-C31 | 2.44  | 1.40        | 1.33     |
| 46  | O     | 201 | CDL  | OA8-CA7 | 2.44  | 1.40        | 1.33     |
| 46  | O     | 201 | CDL  | OA6-CA5 | 2.42  | 1.41        | 1.34     |
| 45  | b     | 103 | 3PE  | O31-C3  | -2.42 | 1.39        | 1.45     |
| 45  | L     | 705 | 3PE  | O31-C3  | -2.42 | 1.39        | 1.45     |
| 46  | Z     | 203 | CDL  | OA6-CA4 | -2.41 | 1.40        | 1.46     |
| 49  | U     | 201 | EHZ  | O3-C12  | -2.41 | 1.18        | 1.23     |
| 45  | Y     | 301 | 3PE  | O31-C31 | 2.40  | 1.40        | 1.33     |
| 45  | Z     | 201 | 3PE  | O31-C31 | 2.39  | 1.40        | 1.33     |
| 45  | L     | 706 | 3PE  | O31-C31 | 2.38  | 1.40        | 1.33     |
| 46  | q     | 203 | CDL  | OB8-CB7 | 2.38  | 1.40        | 1.33     |
| 46  | b     | 102 | CDL  | OA8-CA7 | 2.38  | 1.40        | 1.33     |
| 49  | T     | 201 | EHZ  | O4-C15  | -2.38 | 1.18        | 1.23     |
| 49  | U     | 201 | EHZ  | O4-C15  | -2.38 | 1.18        | 1.23     |
| 45  | b     | 104 | 3PE  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 45  | L     | 707 | 3PE  | O31-C31 | 2.37  | 1.40        | 1.33     |
| 45  | m     | 101 | 3PE  | O31-C3  | -2.36 | 1.39        | 1.45     |
| 46  | O     | 201 | CDL  | OB8-CB6 | -2.36 | 1.39        | 1.45     |
| 45  | J     | 201 | 3PE  | O31-C3  | -2.36 | 1.39        | 1.45     |
| 46  | q     | 203 | CDL  | OA8-CA7 | 2.36  | 1.40        | 1.33     |
| 45  | m     | 101 | 3PE  | O21-C21 | 2.35  | 1.40        | 1.34     |
| 47  | P     | 501 | NDP  | P2B-O1X | 2.35  | 1.57        | 1.50     |
| 45  | Y     | 301 | 3PE  | O21-C2  | -2.34 | 1.41        | 1.46     |
| 47  | P     | 501 | NDP  | C6N-N1N | 2.33  | 1.42        | 1.37     |
| 45  | M     | 502 | 3PE  | O31-C31 | 2.33  | 1.40        | 1.33     |
| 46  | Z     | 203 | CDL  | OA8-CA6 | -2.32 | 1.40        | 1.45     |
| 46  | Z     | 203 | CDL  | OB8-CB7 | 2.32  | 1.40        | 1.33     |
| 46  | Z     | 203 | CDL  | OA8-CA7 | 2.31  | 1.40        | 1.33     |
| 45  | h     | 201 | 3PE  | O31-C31 | 2.31  | 1.40        | 1.33     |
| 49  | T     | 201 | EHZ  | C9-S1   | 2.31  | 1.81        | 1.76     |
| 45  | L     | 703 | 3PE  | O31-C31 | 2.31  | 1.40        | 1.33     |
| 45  | N     | 601 | 3PE  | O31-C31 | 2.31  | 1.40        | 1.33     |
| 46  | O     | 201 | CDL  | OB8-CB7 | 2.30  | 1.40        | 1.33     |
| 45  | L     | 703 | 3PE  | O31-C3  | -2.30 | 1.40        | 1.45     |
| 45  | L     | 704 | 3PE  | O31-C31 | 2.30  | 1.40        | 1.33     |
| 49  | U     | 201 | EHZ  | C9-S1   | 2.30  | 1.81        | 1.76     |
| 46  | q     | 203 | CDL  | OA6-CA5 | 2.29  | 1.40        | 1.34     |
| 46  | q     | 203 | CDL  | OA8-CA6 | -2.29 | 1.40        | 1.45     |
| 45  | L     | 702 | 3PE  | O31-C31 | 2.29  | 1.40        | 1.33     |
| 45  | M     | 501 | 3PE  | O31-C31 | 2.28  | 1.40        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 45  | M     | 501 | 3PE  | O31-C3  | -2.28 | 1.40        | 1.45     |
| 45  | J     | 201 | 3PE  | O31-C31 | 2.27  | 1.40        | 1.33     |
| 45  | L     | 702 | 3PE  | O31-C3  | -2.27 | 1.40        | 1.45     |
| 45  | m     | 101 | 3PE  | O21-C2  | -2.26 | 1.41        | 1.46     |
| 47  | P     | 501 | NDP  | PA-O5B  | 2.25  | 1.68        | 1.59     |
| 45  | L     | 704 | 3PE  | O31-C3  | -2.24 | 1.40        | 1.45     |
| 46  | b     | 102 | CDL  | OA8-CA6 | -2.24 | 1.40        | 1.45     |
| 46  | q     | 203 | CDL  | OB8-CB6 | -2.23 | 1.40        | 1.45     |
| 45  | m     | 101 | 3PE  | O31-C31 | 2.23  | 1.39        | 1.33     |
| 45  | b     | 104 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 45  | L     | 707 | 3PE  | O31-C3  | -2.22 | 1.40        | 1.45     |
| 45  | M     | 502 | 3PE  | O31-C3  | -2.21 | 1.40        | 1.45     |
| 45  | b     | 103 | 3PE  | O31-C31 | 2.21  | 1.39        | 1.33     |
| 45  | b     | 103 | 3PE  | O21-C21 | 2.21  | 1.40        | 1.34     |
| 45  | L     | 706 | 3PE  | O31-C3  | -2.20 | 1.40        | 1.45     |
| 45  | N     | 601 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 46  | b     | 102 | CDL  | OB8-CB6 | -2.19 | 1.40        | 1.45     |
| 45  | h     | 201 | 3PE  | O31-C3  | -2.19 | 1.40        | 1.45     |
| 46  | O     | 201 | CDL  | OA6-CA4 | -2.18 | 1.41        | 1.46     |
| 45  | Z     | 201 | 3PE  | O31-C3  | -2.18 | 1.40        | 1.45     |
| 45  | M     | 502 | 3PE  | O21-C21 | 2.18  | 1.40        | 1.34     |
| 49  | T     | 201 | EHZ  | O3-C12  | -2.17 | 1.19        | 1.23     |
| 46  | Z     | 203 | CDL  | OB6-CB5 | 2.17  | 1.40        | 1.34     |
| 46  | Z     | 203 | CDL  | OB8-CB6 | -2.16 | 1.40        | 1.45     |
| 45  | L     | 705 | 3PE  | O31-C31 | 2.15  | 1.39        | 1.33     |
| 45  | Y     | 301 | 3PE  | O31-C3  | -2.13 | 1.40        | 1.45     |
| 46  | q     | 203 | CDL  | OB6-CB5 | 2.12  | 1.40        | 1.34     |
| 45  | Z     | 201 | 3PE  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 45  | j     | 101 | 3PE  | O31-C3  | -2.12 | 1.40        | 1.45     |
| 45  | N     | 601 | 3PE  | O21-C21 | 2.12  | 1.40        | 1.34     |
| 46  | O     | 201 | CDL  | OA8-CA6 | -2.11 | 1.40        | 1.45     |
| 46  | b     | 102 | CDL  | OA6-CA5 | 2.10  | 1.40        | 1.34     |
| 47  | P     | 501 | NDP  | C5B-C4B | 2.05  | 1.57        | 1.51     |
| 45  | L     | 704 | 3PE  | O21-C21 | 2.04  | 1.40        | 1.34     |
| 45  | j     | 101 | 3PE  | O21-C21 | 2.04  | 1.40        | 1.34     |
| 45  | b     | 104 | 3PE  | O21-C21 | 2.04  | 1.40        | 1.34     |
| 45  | M     | 501 | 3PE  | O21-C21 | 2.03  | 1.40        | 1.34     |
| 45  | L     | 705 | 3PE  | O21-C21 | 2.02  | 1.40        | 1.34     |
| 45  | J     | 201 | 3PE  | O21-C21 | 2.01  | 1.40        | 1.34     |

All (78) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 47  | P     | 501 | NDP  | C4A-N9A-C1B | -5.94 | 112.74      | 126.63   |
| 47  | P     | 501 | NDP  | N6A-C6A-N1A | -5.67 | 105.75      | 118.38   |
| 47  | P     | 501 | NDP  | N3A-C2A-N1A | -5.67 | 120.00      | 128.58   |
| 47  | P     | 501 | NDP  | C1B-N9A-C8A | 5.35  | 138.97      | 127.09   |
| 45  | Y     | 301 | 3PE  | O21-C21-C22 | 5.17  | 120.32      | 111.09   |
| 49  | T     | 201 | EHZ  | C8-C9-S1    | 4.84  | 119.67      | 113.56   |
| 46  | Z     | 203 | CDL  | OA6-CA5-C11 | 4.80  | 119.64      | 111.09   |
| 47  | P     | 501 | NDP  | C5A-C4A-N3A | -4.74 | 120.19      | 126.72   |
| 49  | U     | 201 | EHZ  | C8-C9-S1    | 4.69  | 119.47      | 113.56   |
| 45  | N     | 601 | 3PE  | O21-C21-C22 | 4.44  | 121.08      | 111.48   |
| 46  | q     | 203 | CDL  | OA6-CA5-C11 | 4.31  | 120.80      | 111.48   |
| 47  | P     | 501 | NDP  | N9A-C8A-N7A | -4.24 | 107.92      | 113.94   |
| 47  | P     | 501 | NDP  | C5A-C6A-N6A | 4.22  | 133.74      | 123.29   |
| 45  | L     | 705 | 3PE  | O21-C21-C22 | 4.17  | 120.51      | 111.48   |
| 45  | m     | 101 | 3PE  | O21-C21-C22 | 4.17  | 120.51      | 111.48   |
| 46  | b     | 102 | CDL  | OA6-CA5-C11 | 4.16  | 120.47      | 111.48   |
| 45  | Z     | 201 | 3PE  | O21-C21-C22 | 4.14  | 120.44      | 111.48   |
| 46  | O     | 201 | CDL  | OB6-CB5-C51 | 4.09  | 120.32      | 111.48   |
| 45  | M     | 501 | 3PE  | O21-C21-C22 | 4.06  | 120.26      | 111.48   |
| 46  | b     | 102 | CDL  | OB6-CB5-C51 | 4.05  | 120.25      | 111.48   |
| 45  | L     | 702 | 3PE  | O21-C21-C22 | 4.00  | 120.14      | 111.48   |
| 45  | b     | 104 | 3PE  | O21-C21-C22 | 4.00  | 120.13      | 111.48   |
| 45  | J     | 201 | 3PE  | O21-C21-C22 | 3.99  | 120.11      | 111.48   |
| 45  | L     | 707 | 3PE  | O21-C21-C22 | 3.98  | 120.09      | 111.48   |
| 46  | O     | 201 | CDL  | OA6-CA5-C11 | 3.98  | 120.09      | 111.48   |
| 45  | M     | 502 | 3PE  | O21-C21-C22 | 3.98  | 120.08      | 111.48   |
| 45  | L     | 706 | 3PE  | O21-C21-C22 | 3.95  | 120.03      | 111.48   |
| 45  | h     | 201 | 3PE  | O21-C21-C22 | 3.92  | 119.97      | 111.48   |
| 46  | q     | 203 | CDL  | OB6-CB5-C51 | 3.91  | 119.93      | 111.48   |
| 45  | b     | 103 | 3PE  | O21-C21-C22 | 3.89  | 119.89      | 111.48   |
| 45  | j     | 101 | 3PE  | O21-C21-C22 | 3.88  | 119.88      | 111.48   |
| 45  | L     | 704 | 3PE  | O21-C21-C22 | 3.85  | 119.80      | 111.48   |
| 46  | Z     | 203 | CDL  | OB6-CB5-C51 | 3.84  | 119.79      | 111.48   |
| 45  | L     | 703 | 3PE  | O21-C21-C22 | 3.80  | 119.71      | 111.48   |
| 47  | P     | 501 | NDP  | C3N-C2N-N1N | -3.55 | 117.99      | 123.20   |
| 47  | P     | 501 | NDP  | C2A-N3A-C4A | 3.43  | 120.20      | 111.83   |
| 46  | b     | 102 | CDL  | OB8-CB7-C71 | 3.04  | 120.39      | 111.15   |
| 45  | L     | 706 | 3PE  | O31-C31-C32 | 2.95  | 120.84      | 111.83   |
| 45  | Y     | 301 | 3PE  | O31-C31-C32 | 2.91  | 120.70      | 111.83   |
| 45  | M     | 502 | 3PE  | O31-C31-C32 | 2.86  | 120.54      | 111.83   |
| 47  | P     | 501 | NDP  | C5A-N7A-C8A | 2.82  | 107.88      | 103.45   |
| 45  | L     | 702 | 3PE  | O31-C31-C32 | 2.81  | 120.40      | 111.83   |
| 45  | b     | 104 | 3PE  | O31-C31-C32 | 2.81  | 120.39      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 45  | N     | 601 | 3PE  | O31-C31-C32 | 2.81  | 120.39      | 111.83   |
| 47  | P     | 501 | NDP  | N3A-C4A-N9A | 2.80  | 131.92      | 127.17   |
| 46  | O     | 201 | CDL  | OB8-CB7-C71 | 2.79  | 120.33      | 111.83   |
| 45  | m     | 101 | 3PE  | O31-C31-C32 | 2.78  | 120.33      | 111.83   |
| 46  | Z     | 203 | CDL  | OB8-CB7-C71 | 2.77  | 120.29      | 111.83   |
| 46  | q     | 203 | CDL  | OA8-CA7-C31 | 2.77  | 120.29      | 111.83   |
| 45  | Z     | 201 | 3PE  | O31-C31-C32 | 2.75  | 120.23      | 111.83   |
| 46  | O     | 201 | CDL  | OA8-CA7-C31 | 2.75  | 120.22      | 111.83   |
| 45  | h     | 201 | 3PE  | O31-C31-C32 | 2.75  | 120.21      | 111.83   |
| 46  | q     | 203 | CDL  | OB8-CB7-C71 | 2.74  | 120.19      | 111.83   |
| 45  | j     | 101 | 3PE  | O31-C31-C32 | 2.72  | 120.13      | 111.83   |
| 45  | b     | 103 | 3PE  | O31-C31-C32 | 2.71  | 120.11      | 111.83   |
| 45  | M     | 501 | 3PE  | O31-C31-C32 | 2.71  | 120.10      | 111.83   |
| 46  | b     | 102 | CDL  | OA8-CA7-C31 | 2.71  | 120.08      | 111.83   |
| 46  | Z     | 203 | CDL  | OA8-CA7-C31 | 2.70  | 120.07      | 111.83   |
| 45  | L     | 707 | 3PE  | O31-C31-C32 | 2.70  | 120.06      | 111.83   |
| 49  | U     | 201 | EHZ  | C10-S1-C9   | 2.69  | 109.79      | 101.84   |
| 49  | U     | 201 | EHZ  | C11-N1-C12  | -2.67 | 117.85      | 122.82   |
| 45  | L     | 703 | 3PE  | O31-C31-C32 | 2.67  | 119.97      | 111.83   |
| 45  | L     | 704 | 3PE  | O31-C31-C32 | 2.65  | 119.92      | 111.83   |
| 47  | P     | 501 | NDP  | C2B-C1B-N9A | -2.57 | 109.53      | 113.75   |
| 43  | L     | 701 | PLC  | C3-C2-C1    | 2.51  | 117.64      | 111.78   |
| 45  | L     | 705 | 3PE  | O31-C31-C32 | 2.51  | 119.48      | 111.83   |
| 45  | J     | 201 | 3PE  | O31-C31-C32 | 2.49  | 119.42      | 111.83   |
| 43  | L     | 701 | PLC  | C2-O2-C'    | 2.45  | 123.65      | 117.80   |
| 47  | P     | 501 | NDP  | C4A-N9A-C8A | 2.43  | 108.29      | 105.74   |
| 49  | T     | 201 | EHZ  | O2-C9-S1    | -2.33 | 119.72      | 122.68   |
| 49  | U     | 201 | EHZ  | C14-C13-C12 | -2.31 | 108.55      | 112.39   |
| 49  | U     | 201 | EHZ  | O2-C9-S1    | -2.30 | 119.76      | 122.68   |
| 49  | U     | 201 | EHZ  | C13-C12-N1  | 2.28  | 120.50      | 116.34   |
| 49  | T     | 201 | EHZ  | C10-S1-C9   | 2.26  | 108.52      | 101.84   |
| 47  | P     | 501 | NDP  | C4A-C5A-N7A | -2.24 | 108.02      | 110.58   |
| 43  | Z     | 202 | PLC  | C3-C2-C1    | 2.07  | 116.61      | 111.78   |
| 47  | P     | 501 | NDP  | C5B-C4B-C3B | -2.01 | 107.97      | 115.21   |
| 43  | M     | 503 | PLC  | C3-C2-C1    | 2.01  | 116.47      | 111.78   |

There are no chirality outliers.

All (754) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 43  | B     | 302 | PLC  | C4-O4P-P-O1P |
| 43  | D     | 501 | PLC  | C1'-C'-O2-C2 |

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| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 43  | D     | 501 | PLC  | O'-C'-O2-C2  |
| 43  | D     | 501 | PLC  | C1-O3P-P-O2P |
| 43  | H     | 401 | PLC  | C1'-C'-O2-C2 |
| 43  | H     | 401 | PLC  | C4-O4P-P-O1P |
| 43  | L     | 701 | PLC  | C2-C1-O3P-P  |
| 43  | L     | 701 | PLC  | C1-O3P-P-O4P |
| 43  | L     | 701 | PLC  | C4-O4P-P-O3P |
| 43  | L     | 709 | PLC  | C1'-C'-O2-C2 |
| 43  | L     | 709 | PLC  | C4-O4P-P-O1P |
| 43  | L     | 710 | PLC  | C1-O3P-P-O1P |
| 43  | L     | 710 | PLC  | C1-O3P-P-O2P |
| 43  | L     | 710 | PLC  | C1-O3P-P-O4P |
| 43  | M     | 503 | PLC  | C1'-C'-O2-C2 |
| 43  | M     | 503 | PLC  | O'-C'-O2-C2  |
| 43  | M     | 504 | PLC  | C1'-C'-O2-C2 |
| 43  | M     | 504 | PLC  | C1-O3P-P-O1P |
| 43  | M     | 504 | PLC  | C1-O3P-P-O2P |
| 43  | M     | 504 | PLC  | C1-O3P-P-O4P |
| 43  | P     | 502 | PLC  | O4P-C4-C5-N  |
| 43  | P     | 502 | PLC  | C1'-C'-O2-C2 |
| 43  | P     | 502 | PLC  | C4-O4P-P-O3P |
| 43  | P     | 503 | PLC  | O3P-C1-C2-O2 |
| 43  | P     | 503 | PLC  | C4-O4P-P-O1P |
| 43  | Y     | 302 | PLC  | C5-C4-O4P-P  |
| 43  | Y     | 302 | PLC  | C1'-C'-O2-C2 |
| 43  | Y     | 302 | PLC  | O'-C'-O2-C2  |
| 43  | Y     | 302 | PLC  | C1-O3P-P-O1P |
| 43  | Y     | 302 | PLC  | C1-O3P-P-O2P |
| 43  | Y     | 302 | PLC  | C1-O3P-P-O4P |
| 43  | Y     | 303 | PLC  | C1'-C'-O2-C2 |
| 43  | Z     | 202 | PLC  | C1-O3P-P-O2P |
| 43  | Z     | 202 | PLC  | C1-O3P-P-O4P |
| 43  | a     | 201 | PLC  | C1-O3P-P-O1P |
| 43  | a     | 201 | PLC  | C1-O3P-P-O2P |
| 43  | a     | 201 | PLC  | C1-O3P-P-O4P |
| 43  | a     | 201 | PLC  | C4-O4P-P-O1P |
| 43  | b     | 101 | PLC  | C1-O3P-P-O2P |
| 43  | d     | 101 | PLC  | C1-O3P-P-O2P |
| 43  | d     | 102 | PLC  | C1-O3P-P-O4P |
| 43  | d     | 102 | PLC  | C4-O4P-P-O2P |
| 43  | g     | 301 | PLC  | O4P-C4-C5-N  |
| 43  | g     | 301 | PLC  | O'-C'-O2-C2  |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 43  | g     | 301 | PLC  | C4-O4P-P-O3P   |
| 43  | q     | 201 | PLC  | O3P-C1-C2-O2   |
| 43  | q     | 201 | PLC  | C1-O3P-P-O2P   |
| 43  | q     | 201 | PLC  | C1-O3P-P-O4P   |
| 43  | q     | 201 | PLC  | C4-O4P-P-O3P   |
| 43  | q     | 202 | PLC  | O4P-C4-C5-N    |
| 43  | q     | 202 | PLC  | C1'-C'-O2-C2   |
| 43  | q     | 202 | PLC  | C1-O3P-P-O2P   |
| 43  | q     | 202 | PLC  | C4-O4P-P-O1P   |
| 43  | q     | 202 | PLC  | C4-O4P-P-O3P   |
| 45  | J     | 201 | 3PE  | C1-O11-P-O13   |
| 45  | J     | 201 | 3PE  | C1-O11-P-O14   |
| 45  | J     | 201 | 3PE  | C12-C11-O13-P  |
| 45  | J     | 201 | 3PE  | O22-C21-O21-C2 |
| 45  | L     | 702 | 3PE  | C22-C21-O21-C2 |
| 45  | L     | 703 | 3PE  | C1-O11-P-O12   |
| 45  | L     | 703 | 3PE  | C1-O11-P-O13   |
| 45  | L     | 703 | 3PE  | C1-O11-P-O14   |
| 45  | L     | 705 | 3PE  | C11-O13-P-O11  |
| 45  | L     | 705 | 3PE  | C11-O13-P-O14  |
| 45  | L     | 705 | 3PE  | C22-C21-O21-C2 |
| 45  | L     | 706 | 3PE  | C1-O11-P-O12   |
| 45  | L     | 706 | 3PE  | C1-O11-P-O13   |
| 45  | L     | 706 | 3PE  | C1-O11-P-O14   |
| 45  | M     | 501 | 3PE  | C22-C21-O21-C2 |
| 45  | M     | 502 | 3PE  | C11-O13-P-O11  |
| 45  | M     | 502 | 3PE  | C11-O13-P-O12  |
| 45  | M     | 502 | 3PE  | C11-O13-P-O14  |
| 45  | M     | 502 | 3PE  | O13-C11-C12-N  |
| 45  | N     | 601 | 3PE  | C1-O11-P-O13   |
| 45  | N     | 601 | 3PE  | C1-O11-P-O14   |
| 45  | N     | 601 | 3PE  | C11-O13-P-O14  |
| 45  | N     | 601 | 3PE  | O13-C11-C12-N  |
| 45  | N     | 601 | 3PE  | C22-C21-O21-C2 |
| 45  | Y     | 301 | 3PE  | C1-O11-P-O12   |
| 45  | Y     | 301 | 3PE  | C1-O11-P-O13   |
| 45  | Y     | 301 | 3PE  | C1-O11-P-O14   |
| 45  | Y     | 301 | 3PE  | O13-C11-C12-N  |
| 45  | Y     | 301 | 3PE  | C22-C21-O21-C2 |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O12   |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O13   |
| 45  | b     | 103 | 3PE  | C11-O13-P-O11  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | b     | 103 | 3PE  | C11-O13-P-O12   |
| 45  | b     | 103 | 3PE  | O22-C21-O21-C2  |
| 45  | b     | 104 | 3PE  | C1-O11-P-O14    |
| 45  | b     | 104 | 3PE  | C11-O13-P-O11   |
| 45  | b     | 104 | 3PE  | C11-O13-P-O12   |
| 45  | b     | 104 | 3PE  | C22-C21-O21-C2  |
| 45  | h     | 201 | 3PE  | C11-O13-P-O11   |
| 45  | h     | 201 | 3PE  | C11-O13-P-O12   |
| 45  | h     | 201 | 3PE  | O13-C11-C12-N   |
| 45  | j     | 101 | 3PE  | O13-C11-C12-N   |
| 45  | j     | 101 | 3PE  | O32-C31-O31-C3  |
| 45  | j     | 101 | 3PE  | C32-C31-O31-C3  |
| 45  | m     | 101 | 3PE  | O32-C31-O31-C3  |
| 45  | m     | 101 | 3PE  | O22-C21-O21-C2  |
| 46  | O     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 46  | O     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 46  | O     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 46  | O     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 46  | O     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 46  | Z     | 203 | CDL  | CB3-OB5-PB2-OB2 |
| 46  | Z     | 203 | CDL  | CB3-OB5-PB2-OB3 |
| 46  | Z     | 203 | CDL  | CB3-OB5-PB2-OB4 |
| 46  | b     | 102 | CDL  | CB2-OB2-PB2-OB3 |
| 46  | b     | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 46  | b     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 46  | q     | 203 | CDL  | CB3-OB5-PB2-OB2 |
| 46  | q     | 203 | CDL  | CB3-OB5-PB2-OB3 |
| 46  | q     | 203 | CDL  | CB3-OB5-PB2-OB4 |
| 46  | q     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 47  | P     | 501 | NDP  | C5B-O5B-PA-O2A  |
| 47  | P     | 501 | NDP  | C5B-O5B-PA-O3   |
| 47  | P     | 501 | NDP  | C5D-O5D-PN-O1N  |
| 47  | P     | 501 | NDP  | O4D-C1D-N1N-C6N |
| 47  | P     | 501 | NDP  | C2N-C3N-C7N-N7N |
| 49  | T     | 201 | EHZ  | C5-C6-C7-C8     |
| 49  | T     | 201 | EHZ  | S1-C10-C11-N1   |
| 49  | T     | 201 | EHZ  | C15-C16-C17-C19 |
| 49  | T     | 201 | EHZ  | C15-C16-C17-C20 |
| 49  | T     | 201 | EHZ  | O5-C16-C17-C19  |
| 49  | T     | 201 | EHZ  | O5-C16-C17-C20  |
| 49  | T     | 201 | EHZ  | C16-C17-C20-O6  |
| 49  | T     | 201 | EHZ  | C18-C17-C20-O6  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | T     | 201 | EHZ  | C19-C17-C20-O6  |
| 49  | T     | 201 | EHZ  | O2-C9-S1-C10    |
| 49  | T     | 201 | EHZ  | C8-C9-S1-C10    |
| 49  | U     | 201 | EHZ  | C4-C5-C6-C7     |
| 49  | U     | 201 | EHZ  | C6-C7-C8-C9     |
| 49  | U     | 201 | EHZ  | C16-C17-C20-O6  |
| 49  | U     | 201 | EHZ  | C18-C17-C20-O6  |
| 49  | U     | 201 | EHZ  | C19-C17-C20-O6  |
| 49  | U     | 201 | EHZ  | O2-C9-S1-C10    |
| 49  | U     | 201 | EHZ  | C8-C9-S1-C10    |
| 45  | Y     | 301 | 3PE  | O22-C21-O21-C2  |
| 46  | Z     | 203 | CDL  | C11-CA5-OA6-CA4 |
| 43  | H     | 401 | PLC  | O'-C'-O2-C2     |
| 45  | L     | 703 | 3PE  | O32-C31-O31-C3  |
| 45  | L     | 705 | 3PE  | O32-C31-O31-C3  |
| 46  | O     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 46  | b     | 102 | CDL  | OB9-CB7-OB8-CB6 |
| 46  | b     | 102 | CDL  | C71-CB7-OB8-CB6 |
| 43  | L     | 708 | PLC  | OB-CB-O3-C3     |
| 45  | L     | 706 | 3PE  | O32-C31-O31-C3  |
| 45  | Z     | 201 | 3PE  | O32-C31-O31-C3  |
| 46  | Z     | 203 | CDL  | OA9-CA7-OA8-CA6 |
| 46  | q     | 203 | CDL  | OB9-CB7-OB8-CB6 |
| 46  | Z     | 203 | CDL  | OA7-CA5-OA6-CA4 |
| 43  | L     | 709 | PLC  | O'-C'-O2-C2     |
| 43  | M     | 504 | PLC  | O'-C'-O2-C2     |
| 43  | P     | 502 | PLC  | O'-C'-O2-C2     |
| 43  | Y     | 303 | PLC  | O'-C'-O2-C2     |
| 43  | q     | 202 | PLC  | O'-C'-O2-C2     |
| 45  | L     | 702 | 3PE  | O22-C21-O21-C2  |
| 45  | L     | 705 | 3PE  | O22-C21-O21-C2  |
| 45  | M     | 501 | 3PE  | O22-C21-O21-C2  |
| 45  | N     | 601 | 3PE  | O22-C21-O21-C2  |
| 45  | b     | 104 | 3PE  | O22-C21-O21-C2  |
| 46  | O     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 46  | O     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 46  | q     | 203 | CDL  | OA7-CA5-OA6-CA4 |
| 46  | q     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | L     | 703 | 3PE  | C32-C31-O31-C3  |
| 45  | L     | 705 | 3PE  | C32-C31-O31-C3  |
| 45  | L     | 706 | 3PE  | C32-C31-O31-C3  |
| 45  | m     | 101 | 3PE  | C32-C31-O31-C3  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | g     | 301 | PLC  | C1'-C'-O2-C2    |
| 45  | J     | 201 | 3PE  | C22-C21-O21-C2  |
| 45  | b     | 103 | 3PE  | C22-C21-O21-C2  |
| 45  | m     | 101 | 3PE  | C22-C21-O21-C2  |
| 46  | q     | 203 | CDL  | C11-CA5-OA6-CA4 |
| 45  | b     | 103 | 3PE  | O32-C31-O31-C3  |
| 45  | b     | 104 | 3PE  | O32-C31-O31-C3  |
| 46  | q     | 203 | CDL  | OA9-CA7-OA8-CA6 |
| 43  | L     | 708 | PLC  | C1B-CB-O3-C3    |
| 45  | Z     | 201 | 3PE  | C32-C31-O31-C3  |
| 45  | b     | 104 | 3PE  | C32-C31-O31-C3  |
| 46  | Z     | 203 | CDL  | C31-CA7-OA8-CA6 |
| 46  | q     | 203 | CDL  | C71-CB7-OB8-CB6 |
| 45  | N     | 601 | 3PE  | O32-C31-O31-C3  |
| 45  | N     | 601 | 3PE  | C32-C31-O31-C3  |
| 45  | L     | 704 | 3PE  | C22-C21-O21-C2  |
| 45  | b     | 103 | 3PE  | C32-C31-O31-C3  |
| 46  | q     | 203 | CDL  | C31-CA7-OA8-CA6 |
| 45  | L     | 704 | 3PE  | O22-C21-O21-C2  |
| 43  | L     | 710 | PLC  | C1B-CB-O3-C3    |
| 43  | g     | 301 | PLC  | C7'-C8'-C9'-CA' |
| 43  | Z     | 202 | PLC  | C'-C1'-C2'-C3'  |
| 49  | T     | 201 | EHZ  | C5-C6-C7-O1     |
| 43  | L     | 710 | PLC  | OB-CB-O3-C3     |
| 43  | P     | 503 | PLC  | C1'-C'-O2-C2    |
| 45  | L     | 702 | 3PE  | C32-C31-O31-C3  |
| 43  | d     | 101 | PLC  | C'-C1'-C2'-C3'  |
| 47  | P     | 501 | NDP  | O4B-C4B-C5B-O5B |
| 47  | P     | 501 | NDP  | O4D-C4D-C5D-O5D |
| 47  | P     | 501 | NDP  | C3D-C4D-C5D-O5D |
| 43  | L     | 708 | PLC  | CB-C1B-C2B-C3B  |
| 43  | Y     | 302 | PLC  | C'-C1'-C2'-C3'  |
| 45  | L     | 703 | 3PE  | C21-C22-C23-C24 |
| 46  | O     | 201 | CDL  | CA5-C11-C12-C13 |
| 43  | P     | 503 | PLC  | O'-C'-O2-C2     |
| 45  | L     | 702 | 3PE  | O32-C31-O31-C3  |
| 43  | d     | 102 | PLC  | C'-C1'-C2'-C3'  |
| 45  | L     | 706 | 3PE  | C21-C22-C23-C24 |
| 43  | M     | 504 | PLC  | C3'-C4'-C5'-C6' |
| 47  | P     | 501 | NDP  | C3B-C2B-O2B-P2B |
| 47  | P     | 501 | NDP  | C3B-C4B-C5B-O5B |
| 43  | Z     | 202 | PLC  | C1'-C'-O2-C2    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | Z     | 202 | PLC  | O'-C'-O2-C2     |
| 45  | Z     | 201 | 3PE  | C21-C22-C23-C24 |
| 43  | L     | 708 | PLC  | C4'-C5'-C6'-C7' |
| 43  | q     | 201 | PLC  | C1'-C'-O2-C2    |
| 45  | L     | 706 | 3PE  | C22-C21-O21-C2  |
| 46  | b     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 43  | P     | 503 | PLC  | C1'-C2'-C3'-C4' |
| 45  | h     | 201 | 3PE  | C34-C35-C36-C37 |
| 45  | L     | 702 | 3PE  | C32-C33-C34-C35 |
| 45  | L     | 703 | 3PE  | C33-C34-C35-C36 |
| 45  | M     | 501 | 3PE  | C33-C34-C35-C36 |
| 45  | j     | 101 | 3PE  | C33-C34-C35-C36 |
| 46  | O     | 201 | CDL  | C76-C77-C78-C79 |
| 43  | Z     | 202 | PLC  | C1B-C2B-C3B-C4B |
| 45  | M     | 501 | 3PE  | C34-C35-C36-C37 |
| 45  | M     | 501 | 3PE  | C3A-C3B-C3C-C3D |
| 43  | q     | 201 | PLC  | O'-C'-O2-C2     |
| 46  | b     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 45  | L     | 705 | 3PE  | C2A-C2B-C2C-C2D |
| 46  | Z     | 203 | CDL  | C72-C73-C74-C75 |
| 43  | L     | 701 | PLC  | C'-C1'-C2'-C3'  |
| 45  | J     | 201 | 3PE  | C3A-C3B-C3C-C3D |
| 45  | Y     | 301 | 3PE  | C33-C34-C35-C36 |
| 46  | q     | 203 | CDL  | C14-C15-C16-C17 |
| 45  | Z     | 201 | 3PE  | C22-C21-O21-C2  |
| 43  | d     | 102 | PLC  | C3B-C4B-C5B-C6B |
| 47  | P     | 501 | NDP  | C1B-C2B-O2B-P2B |
| 43  | L     | 710 | PLC  | C3B-C4B-C5B-C6B |
| 45  | J     | 201 | 3PE  | C33-C34-C35-C36 |
| 45  | b     | 104 | 3PE  | C36-C37-C38-C39 |
| 43  | L     | 701 | PLC  | C1B-CB-O3-C3    |
| 46  | q     | 203 | CDL  | CB3-CB4-CB6-OB8 |
| 43  | d     | 101 | PLC  | C7'-C8'-C9'-CA' |
| 45  | L     | 703 | 3PE  | C35-C36-C37-C38 |
| 45  | h     | 201 | 3PE  | C2E-C2F-C2G-C2H |
| 43  | L     | 701 | PLC  | C3B-C4B-C5B-C6B |
| 43  | M     | 504 | PLC  | C5'-C6'-C7'-C8' |
| 43  | d     | 101 | PLC  | C3'-C4'-C5'-C6' |
| 46  | O     | 201 | CDL  | C31-C32-C33-C34 |
| 46  | O     | 201 | CDL  | C72-C73-C74-C75 |
| 43  | Y     | 303 | PLC  | C1'-C2'-C3'-C4' |
| 45  | L     | 703 | 3PE  | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | L     | 703 | 3PE  | C23-C24-C25-C26 |
| 43  | Y     | 302 | PLC  | C1'-C2'-C3'-C4' |
| 45  | L     | 706 | 3PE  | C33-C34-C35-C36 |
| 45  | M     | 501 | 3PE  | C35-C36-C37-C38 |
| 45  | M     | 501 | 3PE  | C3E-C3F-C3G-C3H |
| 45  | M     | 501 | 3PE  | C24-C25-C26-C27 |
| 45  | m     | 101 | 3PE  | C31-C32-C33-C34 |
| 43  | b     | 101 | PLC  | C1'-C'-O2-C2    |
| 43  | P     | 502 | PLC  | C1B-C2B-C3B-C4B |
| 45  | L     | 704 | 3PE  | C25-C26-C27-C28 |
| 46  | O     | 201 | CDL  | C74-C75-C76-C77 |
| 43  | d     | 102 | PLC  | C4'-C5'-C6'-C7' |
| 45  | M     | 502 | 3PE  | C23-C24-C25-C26 |
| 45  | L     | 705 | 3PE  | C21-C22-C23-C24 |
| 45  | b     | 103 | 3PE  | C22-C23-C24-C25 |
| 45  | L     | 706 | 3PE  | C37-C38-C39-C3A |
| 45  | L     | 706 | 3PE  | O22-C21-O21-C2  |
| 45  | J     | 201 | 3PE  | C36-C37-C38-C39 |
| 43  | P     | 503 | PLC  | C1B-CB-O3-C3    |
| 43  | q     | 202 | PLC  | C1'-C2'-C3'-C4' |
| 45  | J     | 201 | 3PE  | C34-C35-C36-C37 |
| 45  | L     | 702 | 3PE  | C2A-C2B-C2C-C2D |
| 45  | M     | 502 | 3PE  | C22-C23-C24-C25 |
| 45  | m     | 101 | 3PE  | C24-C25-C26-C27 |
| 45  | Z     | 201 | 3PE  | C33-C34-C35-C36 |
| 43  | d     | 102 | PLC  | C1'-C2'-C3'-C4' |
| 45  | L     | 703 | 3PE  | C37-C38-C39-C3A |
| 49  | U     | 201 | EHZ  | C3-C4-C5-C6     |
| 45  | M     | 501 | 3PE  | C36-C37-C38-C39 |
| 46  | O     | 201 | CDL  | C78-C79-C80-C81 |
| 43  | L     | 708 | PLC  | C1'-C'-O2-C2    |
| 45  | h     | 201 | 3PE  | C22-C21-O21-C2  |
| 46  | Z     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 46  | b     | 102 | CDL  | C51-CB5-OB6-CB4 |
| 43  | L     | 701 | PLC  | OB-CB-O3-C3     |
| 45  | m     | 101 | 3PE  | C3D-C3E-C3F-C3G |
| 45  | h     | 201 | 3PE  | O22-C21-O21-C2  |
| 46  | Z     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 46  | b     | 102 | CDL  | OB7-CB5-OB6-CB4 |
| 45  | L     | 705 | 3PE  | C26-C27-C28-C29 |
| 45  | L     | 705 | 3PE  | C2E-C2F-C2G-C2H |
| 43  | L     | 710 | PLC  | C4-C5-N-C8      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | L     | 702 | 3PE  | C38-C39-C3A-C3B |
| 43  | M     | 503 | PLC  | C5'-C6'-C7'-C8' |
| 46  | q     | 203 | CDL  | C53-C54-C55-C56 |
| 45  | L     | 702 | 3PE  | C21-C22-C23-C24 |
| 45  | Z     | 201 | 3PE  | O22-C21-O21-C2  |
| 45  | M     | 501 | 3PE  | C25-C26-C27-C28 |
| 45  | b     | 104 | 3PE  | C33-C34-C35-C36 |
| 43  | B     | 302 | PLC  | CB-C1B-C2B-C3B  |
| 45  | b     | 103 | 3PE  | C31-C32-C33-C34 |
| 46  | O     | 201 | CDL  | C71-C72-C73-C74 |
| 45  | L     | 707 | 3PE  | O21-C2-C3-O31   |
| 46  | q     | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 43  | Z     | 202 | PLC  | C2B-C3B-C4B-C5B |
| 43  | M     | 503 | PLC  | C6B-C7B-C8B-C9B |
| 43  | d     | 101 | PLC  | C5'-C6'-C7'-C8' |
| 43  | Z     | 202 | PLC  | C1'-C2'-C3'-C4' |
| 46  | O     | 201 | CDL  | C52-C53-C54-C55 |
| 45  | M     | 502 | 3PE  | C26-C27-C28-C29 |
| 43  | Y     | 302 | PLC  | C2B-C3B-C4B-C5B |
| 45  | L     | 705 | 3PE  | C23-C24-C25-C26 |
| 43  | L     | 710 | PLC  | C4-C5-N-C7      |
| 45  | L     | 702 | 3PE  | C36-C37-C38-C39 |
| 43  | d     | 102 | PLC  | C4B-C5B-C6B-C7B |
| 43  | q     | 201 | PLC  | O3P-C1-C2-C3    |
| 45  | Y     | 301 | 3PE  | O11-C1-C2-C3    |
| 45  | b     | 104 | 3PE  | O11-C1-C2-C3    |
| 45  | h     | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | j     | 101 | 3PE  | O11-C1-C2-C3    |
| 46  | Z     | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 45  | M     | 501 | 3PE  | C32-C33-C34-C35 |
| 43  | P     | 503 | PLC  | OB-CB-O3-C3     |
| 45  | N     | 601 | 3PE  | C27-C28-C29-C2A |
| 45  | b     | 103 | 3PE  | C24-C25-C26-C27 |
| 45  | J     | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 43  | b     | 101 | PLC  | O'-C'-O2-C2     |
| 43  | L     | 709 | PLC  | C1-C2-C3-O3     |
| 43  | d     | 102 | PLC  | C1-C2-C3-O3     |
| 45  | J     | 201 | 3PE  | C1-C2-C3-O31    |
| 45  | L     | 707 | 3PE  | C1-C2-C3-O31    |
| 45  | N     | 601 | 3PE  | C1-C2-C3-O31    |
| 45  | h     | 201 | 3PE  | C1-C2-C3-O31    |
| 46  | O     | 201 | CDL  | CB3-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | q     | 203 | CDL  | CA3-CA4-CA6-OA8 |
| 43  | d     | 101 | PLC  | C5B-C6B-C7B-C8B |
| 45  | J     | 201 | 3PE  | C35-C36-C37-C38 |
| 43  | Z     | 202 | PLC  | C3B-C4B-C5B-C6B |
| 45  | M     | 502 | 3PE  | C32-C31-O31-C3  |
| 46  | O     | 201 | CDL  | C11-C12-C13-C14 |
| 45  | M     | 501 | 3PE  | C2E-C2F-C2G-C2H |
| 45  | h     | 201 | 3PE  | C26-C27-C28-C29 |
| 43  | M     | 503 | PLC  | C1'-C2'-C3'-C4' |
| 45  | Z     | 201 | 3PE  | C22-C23-C24-C25 |
| 43  | D     | 501 | PLC  | C3-C2-O2-C'     |
| 45  | m     | 101 | 3PE  | C3-C2-O21-C21   |
| 46  | Z     | 203 | CDL  | CA6-CA4-OA6-CA5 |
| 45  | L     | 702 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | L     | 705 | 3PE  | C3D-C3E-C3F-C3G |
| 45  | h     | 201 | 3PE  | C22-C23-C24-C25 |
| 45  | L     | 706 | 3PE  | C31-C32-C33-C34 |
| 43  | Z     | 202 | PLC  | C2'-C3'-C4'-C5' |
| 43  | Y     | 303 | PLC  | O3P-C1-C2-O2    |
| 43  | M     | 504 | PLC  | C1B-CB-O3-C3    |
| 45  | Y     | 301 | 3PE  | C32-C31-O31-C3  |
| 45  | L     | 706 | 3PE  | C36-C37-C38-C39 |
| 45  | h     | 201 | 3PE  | C27-C28-C29-C2A |
| 43  | Z     | 202 | PLC  | C7'-C8'-C9'-CA' |
| 45  | L     | 703 | 3PE  | O21-C2-C3-O31   |
| 46  | O     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 45  | b     | 103 | 3PE  | C28-C29-C2A-C2B |
| 45  | L     | 704 | 3PE  | C32-C31-O31-C3  |
| 45  | h     | 201 | 3PE  | C2C-C2D-C2E-C2F |
| 49  | T     | 201 | EHZ  | O5-C16-C17-C18  |
| 45  | L     | 705 | 3PE  | C2F-C2G-C2H-C2I |
| 45  | Z     | 201 | 3PE  | C34-C35-C36-C37 |
| 43  | q     | 202 | PLC  | C'-C1'-C2'-C3'  |
| 43  | d     | 102 | PLC  | C2B-C3B-C4B-C5B |
| 43  | M     | 503 | PLC  | C1B-CB-O3-C3    |
| 45  | M     | 501 | 3PE  | C31-C32-C33-C34 |
| 45  | b     | 104 | 3PE  | C31-C32-C33-C34 |
| 45  | L     | 703 | 3PE  | C36-C37-C38-C39 |
| 43  | q     | 201 | PLC  | C1B-CB-O3-C3    |
| 45  | L     | 706 | 3PE  | C24-C25-C26-C27 |
| 43  | L     | 708 | PLC  | C1B-C2B-C3B-C4B |
| 43  | L     | 708 | PLC  | O'-C'-O2-C2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | q     | 202 | PLC  | C2-C1-O3P-P     |
| 43  | Z     | 202 | PLC  | C8'-C9'-CA'-CB' |
| 45  | j     | 101 | 3PE  | C34-C35-C36-C37 |
| 45  | L     | 705 | 3PE  | C36-C37-C38-C39 |
| 43  | Y     | 303 | PLC  | O3P-C1-C2-C3    |
| 43  | L     | 710 | PLC  | C1'-C'-O2-C2    |
| 43  | L     | 710 | PLC  | C4-C5-N-C6      |
| 45  | m     | 101 | 3PE  | C36-C37-C38-C39 |
| 45  | M     | 502 | 3PE  | O32-C31-O31-C3  |
| 43  | Z     | 202 | PLC  | C6'-C7'-C8'-C9' |
| 45  | m     | 101 | 3PE  | C23-C24-C25-C26 |
| 43  | M     | 504 | PLC  | C1-C2-C3-O3     |
| 45  | L     | 702 | 3PE  | C1-C2-C3-O31    |
| 46  | b     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 46  | b     | 102 | CDL  | CB3-CB4-CB6-OB8 |
| 45  | L     | 703 | 3PE  | C38-C39-C3A-C3B |
| 45  | M     | 501 | 3PE  | C3F-C3G-C3H-C3I |
| 43  | M     | 503 | PLC  | O3P-C1-C2-O2    |
| 43  | P     | 502 | PLC  | O3P-C1-C2-O2    |
| 43  | d     | 101 | PLC  | O3P-C1-C2-O2    |
| 43  | q     | 202 | PLC  | O3P-C1-C2-O2    |
| 45  | h     | 201 | 3PE  | O11-C1-C2-O21   |
| 46  | Z     | 203 | CDL  | OB5-CB3-CB4-OB6 |
| 46  | b     | 102 | CDL  | OB5-CB3-CB4-OB6 |
| 43  | L     | 709 | PLC  | C2B-C3B-C4B-C5B |
| 45  | L     | 702 | 3PE  | C23-C24-C25-C26 |
| 46  | q     | 203 | CDL  | C1-CB2-OB2-PB2  |
| 49  | T     | 201 | EHZ  | O1-C7-C8-C9     |
| 49  | U     | 201 | EHZ  | O1-C7-C8-C9     |
| 45  | b     | 103 | 3PE  | C23-C24-C25-C26 |
| 45  | L     | 702 | 3PE  | C34-C35-C36-C37 |
| 45  | b     | 104 | 3PE  | C3B-C3C-C3D-C3E |
| 43  | B     | 302 | PLC  | O2-C2-C3-O3     |
| 43  | M     | 504 | PLC  | O2-C2-C3-O3     |
| 45  | L     | 705 | 3PE  | O21-C2-C3-O31   |
| 46  | Z     | 203 | CDL  | OA6-CA4-CA6-OA8 |
| 46  | Z     | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 46  | b     | 102 | CDL  | OB6-CB4-CB6-OB8 |
| 43  | d     | 102 | PLC  | C7B-C8B-C9B-CAA |
| 45  | L     | 703 | 3PE  | C2A-C2B-C2C-C2D |
| 43  | b     | 101 | PLC  | C7'-C8'-C9'-CA' |
| 45  | L     | 705 | 3PE  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | N     | 601 | 3PE  | C29-C2A-C2B-C2C |
| 45  | b     | 104 | 3PE  | C35-C36-C37-C38 |
| 43  | D     | 501 | PLC  | C5'-C6'-C7'-C8' |
| 43  | L     | 701 | PLC  | C6B-C7B-C8B-C9B |
| 49  | U     | 201 | EHZ  | C1-C2-C3-C4     |
| 43  | M     | 504 | PLC  | OB-CB-O3-C3     |
| 43  | M     | 503 | PLC  | C1B-C2B-C3B-C4B |
| 46  | b     | 102 | CDL  | C58-C59-C60-C61 |
| 47  | P     | 501 | NDP  | PN-O3-PA-O5B    |
| 43  | L     | 708 | PLC  | C5'-C6'-C7'-C8' |
| 45  | m     | 101 | 3PE  | C29-C2A-C2B-C2C |
| 43  | P     | 502 | PLC  | C2B-C3B-C4B-C5B |
| 49  | T     | 201 | EHZ  | C6-C7-C8-C9     |
| 49  | T     | 201 | EHZ  | C3-C4-C5-C6     |
| 43  | d     | 102 | PLC  | C6B-C7B-C8B-C9B |
| 45  | j     | 101 | 3PE  | C22-C23-C24-C25 |
| 45  | M     | 501 | 3PE  | C2D-C2E-C2F-C2G |
| 43  | q     | 201 | PLC  | OB-CB-O3-C3     |
| 43  | q     | 201 | PLC  | C1'-C2'-C3'-C4' |
| 43  | P     | 503 | PLC  | O3P-C1-C2-C3    |
| 45  | L     | 704 | 3PE  | O11-C1-C2-C3    |
| 45  | M     | 502 | 3PE  | O11-C1-C2-C3    |
| 46  | Z     | 203 | CDL  | OB5-CB3-CB4-CB6 |
| 46  | b     | 102 | CDL  | OB5-CB3-CB4-CB6 |
| 46  | q     | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 49  | U     | 201 | EHZ  | C2-C1-C21-C22   |
| 45  | L     | 703 | 3PE  | C34-C35-C36-C37 |
| 43  | M     | 503 | PLC  | OB-CB-O3-C3     |
| 45  | L     | 704 | 3PE  | O32-C31-O31-C3  |
| 45  | Y     | 301 | 3PE  | O32-C31-O31-C3  |
| 43  | M     | 503 | PLC  | C6'-C7'-C8'-C9' |
| 45  | J     | 201 | 3PE  | C31-C32-C33-C34 |
| 46  | b     | 102 | CDL  | C16-C17-C18-C19 |
| 43  | L     | 709 | PLC  | C3B-C4B-C5B-C6B |
| 43  | q     | 201 | PLC  | C3-C2-O2-C'     |
| 45  | Y     | 301 | 3PE  | C3-C2-O21-C21   |
| 45  | L     | 706 | 3PE  | C3A-C3B-C3C-C3D |
| 45  | L     | 703 | 3PE  | C22-C23-C24-C25 |
| 43  | g     | 301 | PLC  | O3P-C1-C2-O2    |
| 46  | q     | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 45  | Z     | 201 | 3PE  | C32-C33-C34-C35 |
| 46  | O     | 201 | CDL  | C73-C74-C75-C76 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | Z     | 202 | PLC  | C1-C2-C3-O3     |
| 46  | Z     | 203 | CDL  | CB3-CB4-CB6-OB8 |
| 43  | B     | 302 | PLC  | C1B-C2B-C3B-C4B |
| 43  | d     | 101 | PLC  | C1'-C2'-C3'-C4' |
| 43  | d     | 102 | PLC  | C5-C4-O4P-P     |
| 43  | g     | 301 | PLC  | C5-C4-O4P-P     |
| 43  | q     | 202 | PLC  | C5-C4-O4P-P     |
| 45  | b     | 104 | 3PE  | C12-C11-O13-P   |
| 49  | T     | 201 | EHZ  | C15-C16-C17-C18 |
| 45  | m     | 101 | 3PE  | C35-C36-C37-C38 |
| 43  | L     | 701 | PLC  | C4B-C5B-C6B-C7B |
| 43  | L     | 709 | PLC  | O2-C2-C3-O3     |
| 45  | J     | 201 | 3PE  | O21-C2-C3-O31   |
| 45  | L     | 702 | 3PE  | O21-C2-C3-O31   |
| 45  | L     | 704 | 3PE  | O21-C2-C3-O31   |
| 45  | N     | 601 | 3PE  | O21-C2-C3-O31   |
| 45  | h     | 201 | 3PE  | O21-C2-C3-O31   |
| 46  | b     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 46  | q     | 203 | CDL  | OA6-CA4-CA6-OA8 |
| 46  | Z     | 203 | CDL  | C31-C32-C33-C34 |
| 45  | J     | 201 | 3PE  | C38-C39-C3A-C3B |
| 49  | T     | 201 | EHZ  | C2-C3-C4-C5     |
| 43  | D     | 501 | PLC  | C4-C5-N-C7      |
| 43  | d     | 102 | PLC  | C1B-C2B-C3B-C4B |
| 45  | L     | 704 | 3PE  | C24-C25-C26-C27 |
| 45  | L     | 704 | 3PE  | C26-C27-C28-C29 |
| 43  | M     | 503 | PLC  | C5B-C6B-C7B-C8B |
| 45  | Y     | 301 | 3PE  | C35-C36-C37-C38 |
| 43  | B     | 302 | PLC  | O4P-C4-C5-N     |
| 43  | D     | 501 | PLC  | O4P-C4-C5-N     |
| 43  | H     | 401 | PLC  | O4P-C4-C5-N     |
| 43  | L     | 709 | PLC  | O4P-C4-C5-N     |
| 43  | L     | 710 | PLC  | O4P-C4-C5-N     |
| 43  | M     | 504 | PLC  | O4P-C4-C5-N     |
| 43  | Y     | 303 | PLC  | O4P-C4-C5-N     |
| 43  | d     | 101 | PLC  | O4P-C4-C5-N     |
| 43  | d     | 102 | PLC  | O4P-C4-C5-N     |
| 45  | L     | 704 | 3PE  | O21-C21-C22-C23 |
| 45  | M     | 501 | 3PE  | C32-C31-O31-C3  |
| 45  | Y     | 301 | 3PE  | C31-C32-C33-C34 |
| 46  | O     | 201 | CDL  | C75-C76-C77-C78 |
| 43  | b     | 101 | PLC  | C8'-C9'-CA'-CB' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | q     | 203 | CDL  | C58-C59-C60-C61 |
| 43  | D     | 501 | PLC  | C4-C5-N-C6      |
| 43  | q     | 201 | PLC  | C4-C5-N-C6      |
| 43  | Z     | 202 | PLC  | C5'-C6'-C7'-C8' |
| 46  | O     | 201 | CDL  | C33-C34-C35-C36 |
| 45  | L     | 704 | 3PE  | C22-C23-C24-C25 |
| 43  | L     | 708 | PLC  | O3P-C1-C2-C3    |
| 43  | L     | 710 | PLC  | O3P-C1-C2-C3    |
| 43  | P     | 502 | PLC  | O3P-C1-C2-C3    |
| 43  | d     | 101 | PLC  | O3P-C1-C2-C3    |
| 43  | g     | 301 | PLC  | O3P-C1-C2-C3    |
| 43  | q     | 202 | PLC  | O3P-C1-C2-C3    |
| 43  | L     | 710 | PLC  | O'-C'-O2-C2     |
| 45  | L     | 706 | 3PE  | C38-C39-C3A-C3B |
| 49  | U     | 201 | EHZ  | C15-C16-C17-C20 |
| 43  | B     | 302 | PLC  | C2-C1-O3P-P     |
| 43  | L     | 708 | PLC  | C2-C1-O3P-P     |
| 43  | M     | 503 | PLC  | C2-C1-O3P-P     |
| 49  | T     | 201 | EHZ  | C11-C10-S1-C9   |
| 43  | L     | 708 | PLC  | O3P-C1-C2-O2    |
| 43  | L     | 710 | PLC  | O3P-C1-C2-O2    |
| 45  | L     | 704 | 3PE  | O11-C1-C2-O21   |
| 45  | M     | 502 | 3PE  | O11-C1-C2-O21   |
| 45  | Y     | 301 | 3PE  | O11-C1-C2-O21   |
| 45  | b     | 104 | 3PE  | O11-C1-C2-O21   |
| 45  | j     | 101 | 3PE  | O11-C1-C2-O21   |
| 46  | Z     | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 43  | D     | 501 | PLC  | C4-C5-N-C8      |
| 43  | P     | 502 | PLC  | C4-C5-N-C8      |
| 43  | g     | 301 | PLC  | C1'-C2'-C3'-C4' |
| 46  | O     | 201 | CDL  | C36-C37-C38-C39 |
| 45  | N     | 601 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | L     | 706 | 3PE  | C1-C2-C3-O31    |
| 46  | Z     | 203 | CDL  | CA3-CA4-CA6-OA8 |
| 46  | Z     | 203 | CDL  | C72-C71-CB7-OB8 |
| 45  | M     | 501 | 3PE  | O32-C31-O31-C3  |
| 45  | M     | 501 | 3PE  | C3D-C3E-C3F-C3G |
| 43  | H     | 401 | PLC  | C4-O4P-P-O3P    |
| 43  | L     | 701 | PLC  | C1-O3P-P-O1P    |
| 43  | P     | 502 | PLC  | C4-O4P-P-O1P    |
| 43  | Y     | 302 | PLC  | C4-O4P-P-O2P    |
| 43  | Y     | 303 | PLC  | C4-O4P-P-O1P    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | d     | 102 | PLC  | C1-O3P-P-O1P    |
| 43  | d     | 102 | PLC  | C4-O4P-P-O3P    |
| 43  | g     | 301 | PLC  | C4-O4P-P-O1P    |
| 43  | q     | 201 | PLC  | C4-O4P-P-O1P    |
| 45  | J     | 201 | 3PE  | C1-O11-P-O12    |
| 45  | L     | 705 | 3PE  | C1-O11-P-O14    |
| 45  | M     | 501 | 3PE  | O13-C11-C12-N   |
| 45  | M     | 502 | 3PE  | C1-O11-P-O14    |
| 45  | N     | 601 | 3PE  | C11-O13-P-O11   |
| 45  | Z     | 201 | 3PE  | C1-O11-P-O14    |
| 45  | b     | 103 | 3PE  | C1-O11-P-O12    |
| 45  | b     | 103 | 3PE  | C1-O11-P-O13    |
| 45  | b     | 103 | 3PE  | C1-O11-P-O14    |
| 45  | b     | 104 | 3PE  | C11-O13-P-O14   |
| 45  | j     | 101 | 3PE  | C1-O11-P-O13    |
| 45  | j     | 101 | 3PE  | C1-O11-P-O14    |
| 46  | O     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 46  | O     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 46  | O     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 46  | O     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 46  | O     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 46  | Z     | 203 | CDL  | CA3-OA5-PA1-OA3 |
| 46  | b     | 102 | CDL  | CB3-OB5-PB2-OB2 |
| 46  | b     | 102 | CDL  | CB3-OB5-PB2-OB3 |
| 45  | b     | 104 | 3PE  | C34-C35-C36-C37 |
| 45  | L     | 702 | 3PE  | C3B-C3C-C3D-C3E |
| 45  | m     | 101 | 3PE  | C39-C3A-C3B-C3C |
| 43  | Y     | 303 | PLC  | C2-C1-O3P-P     |
| 45  | M     | 501 | 3PE  | C2-C1-O11-P     |
| 46  | O     | 201 | CDL  | C13-C14-C15-C16 |
| 43  | P     | 503 | PLC  | C3-C2-O2-C'     |
| 46  | O     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 46  | q     | 203 | CDL  | CA6-CA4-OA6-CA5 |
| 43  | B     | 302 | PLC  | C3B-C4B-C5B-C6B |
| 45  | m     | 101 | 3PE  | C34-C35-C36-C37 |
| 43  | Y     | 303 | PLC  | C8B-C9B-CAA-CBA |
| 43  | q     | 201 | PLC  | C6B-C7B-C8B-C9B |
| 43  | M     | 504 | PLC  | C2B-C3B-C4B-C5B |
| 43  | Y     | 303 | PLC  | C3B-C4B-C5B-C6B |
| 45  | L     | 706 | 3PE  | C28-C29-C2A-C2B |
| 45  | L     | 702 | 3PE  | C31-C32-C33-C34 |
| 45  | L     | 707 | 3PE  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | L     | 706 | 3PE  | O21-C2-C3-O31   |
| 45  | m     | 101 | 3PE  | C21-C22-C23-C24 |
| 45  | m     | 101 | 3PE  | O21-C21-C22-C23 |
| 45  | J     | 201 | 3PE  | O31-C31-C32-C33 |
| 46  | q     | 203 | CDL  | C12-C13-C14-C15 |
| 45  | b     | 103 | 3PE  | C21-C22-C23-C24 |
| 45  | m     | 101 | 3PE  | C33-C34-C35-C36 |
| 43  | q     | 201 | PLC  | C'-C1'-C2'-C3'  |
| 43  | Z     | 202 | PLC  | C4-C5-N-C8      |
| 45  | L     | 703 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | L     | 706 | 3PE  | C34-C35-C36-C37 |
| 43  | q     | 201 | PLC  | C2-C1-O3P-P     |
| 45  | M     | 502 | 3PE  | C2-C1-O11-P     |
| 43  | q     | 201 | PLC  | C3'-C4'-C5'-C6' |
| 45  | L     | 705 | 3PE  | C38-C39-C3A-C3B |
| 43  | L     | 701 | PLC  | O3P-C1-C2-O2    |
| 45  | N     | 601 | 3PE  | O11-C1-C2-O21   |
| 46  | b     | 102 | CDL  | C11-C12-C13-C14 |
| 45  | J     | 201 | 3PE  | C3C-C3D-C3E-C3F |
| 45  | L     | 703 | 3PE  | C3E-C3F-C3G-C3H |
| 46  | Z     | 203 | CDL  | C71-CB7-OB8-CB6 |
| 45  | M     | 501 | 3PE  | C38-C39-C3A-C3B |
| 43  | d     | 102 | PLC  | O2-C2-C3-O3     |
| 45  | b     | 104 | 3PE  | O21-C2-C3-O31   |
| 45  | L     | 706 | 3PE  | C35-C36-C37-C38 |
| 45  | N     | 601 | 3PE  | C25-C26-C27-C28 |
| 46  | q     | 203 | CDL  | CB5-C51-C52-C53 |
| 45  | M     | 502 | 3PE  | C32-C33-C34-C35 |
| 46  | b     | 102 | CDL  | C51-C52-C53-C54 |
| 43  | Y     | 303 | PLC  | C6B-C7B-C8B-C9B |
| 45  | Y     | 301 | 3PE  | C34-C35-C36-C37 |
| 43  | d     | 102 | PLC  | C8B-C9B-CAA-CBA |
| 45  | L     | 702 | 3PE  | C33-C34-C35-C36 |
| 45  | m     | 101 | 3PE  | C38-C39-C3A-C3B |
| 45  | L     | 703 | 3PE  | C1-C2-C3-O31    |
| 49  | U     | 201 | EHZ  | C10-C11-N1-C12  |
| 45  | b     | 104 | 3PE  | C39-C3A-C3B-C3C |
| 43  | M     | 504 | PLC  | C2'-C3'-C4'-C5' |
| 43  | L     | 701 | PLC  | C1-C2-O2-C'     |
| 45  | J     | 201 | 3PE  | C26-C27-C28-C29 |
| 43  | q     | 201 | PLC  | C4-C5-N-C7      |
| 43  | q     | 201 | PLC  | C4-C5-N-C8      |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | q     | 201 | PLC  | C5B-C6B-C7B-C8B |
| 45  | L     | 703 | 3PE  | C26-C27-C28-C29 |
| 46  | O     | 201 | CDL  | CB4-CB3-OB5-PB2 |
| 46  | O     | 201 | CDL  | C51-C52-C53-C54 |
| 43  | B     | 302 | PLC  | C1'-C2'-C3'-C4' |
| 45  | J     | 201 | 3PE  | C37-C38-C39-C3A |
| 43  | g     | 301 | PLC  | C1B-CB-O3-C3    |
| 45  | M     | 502 | 3PE  | C21-C22-C23-C24 |
| 43  | L     | 701 | PLC  | C1B-C2B-C3B-C4B |
| 43  | q     | 201 | PLC  | C2'-C3'-C4'-C5' |
| 45  | L     | 705 | 3PE  | C22-C23-C24-C25 |
| 45  | b     | 104 | 3PE  | C22-C23-C24-C25 |
| 46  | Z     | 203 | CDL  | C1-CA2-OA2-PA1  |
| 43  | g     | 301 | PLC  | C5B-C6B-C7B-C8B |
| 43  | g     | 301 | PLC  | OB-CB-O3-C3     |
| 46  | Z     | 203 | CDL  | OB9-CB7-OB8-CB6 |
| 43  | B     | 302 | PLC  | C1-C2-C3-O3     |
| 43  | P     | 503 | PLC  | C3'-C4'-C5'-C6' |
| 45  | m     | 101 | 3PE  | C32-C33-C34-C35 |
| 43  | Y     | 302 | PLC  | C5'-C6'-C7'-C8' |
| 45  | L     | 703 | 3PE  | O11-C1-C2-O21   |
| 45  | b     | 104 | 3PE  | C32-C33-C34-C35 |
| 43  | q     | 201 | PLC  | C5'-C6'-C7'-C8' |
| 45  | b     | 104 | 3PE  | C3F-C3G-C3H-C3I |
| 43  | Y     | 302 | PLC  | C4-C5-N-C7      |
| 43  | a     | 201 | PLC  | C4-C5-N-C7      |
| 43  | L     | 708 | PLC  | C3B-C4B-C5B-C6B |
| 45  | m     | 101 | 3PE  | C25-C26-C27-C28 |
| 43  | M     | 503 | PLC  | O3P-C1-C2-C3    |
| 46  | Z     | 203 | CDL  | CB7-C71-C72-C73 |
| 43  | a     | 201 | PLC  | C1B-CB-O3-C3    |
| 43  | Z     | 202 | PLC  | C7B-C8B-C9B-CAA |
| 45  | M     | 502 | 3PE  | C33-C34-C35-C36 |
| 43  | L     | 710 | PLC  | C5B-C6B-C7B-C8B |
| 43  | Y     | 303 | PLC  | C'-C1'-C2'-C3'  |
| 45  | N     | 601 | 3PE  | C34-C35-C36-C37 |
| 46  | O     | 201 | CDL  | C34-C35-C36-C37 |
| 43  | L     | 709 | PLC  | C1'-C2'-C3'-C4' |
| 46  | O     | 201 | CDL  | C82-C83-C84-C85 |
| 49  | T     | 201 | EHZ  | O3-C12-C13-C14  |
| 43  | L     | 701 | PLC  | C2B-C3B-C4B-C5B |
| 45  | L     | 703 | 3PE  | C2D-C2E-C2F-C2G |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | M     | 504 | PLC  | C8'-C9'-CA'-CB' |
| 43  | P     | 502 | PLC  | C4-C5-N-C6      |
| 45  | L     | 704 | 3PE  | C1-C2-C3-O31    |
| 45  | L     | 705 | 3PE  | C1-C2-C3-O31    |
| 45  | b     | 104 | 3PE  | C1-C2-C3-O31    |
| 45  | Z     | 201 | 3PE  | O21-C21-C22-C23 |
| 43  | M     | 503 | PLC  | C7B-C8B-C9B-CAA |
| 43  | P     | 503 | PLC  | C5-C4-O4P-P     |
| 45  | M     | 502 | 3PE  | C12-C11-O13-P   |
| 45  | j     | 101 | 3PE  | C12-C11-O13-P   |
| 49  | U     | 201 | EHZ  | C15-C16-C17-C19 |
| 45  | L     | 703 | 3PE  | C3A-C3B-C3C-C3D |
| 46  | b     | 102 | CDL  | C56-C57-C58-C59 |
| 43  | q     | 202 | PLC  | O2-C2-C3-O3     |
| 45  | L     | 704 | 3PE  | C21-C22-C23-C24 |
| 46  | O     | 201 | CDL  | C77-C78-C79-C80 |
| 45  | M     | 501 | 3PE  | O31-C31-C32-C33 |
| 45  | L     | 705 | 3PE  | O11-C1-C2-C3    |
| 45  | N     | 601 | 3PE  | O11-C1-C2-C3    |
| 43  | q     | 201 | PLC  | C8'-C9'-CA'-CB' |
| 45  | h     | 201 | 3PE  | C35-C36-C37-C38 |
| 45  | L     | 706 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | j     | 101 | 3PE  | C32-C33-C34-C35 |
| 43  | Y     | 302 | PLC  | O4P-C4-C5-N     |
| 45  | b     | 103 | 3PE  | O31-C31-C32-C33 |
| 43  | L     | 709 | PLC  | C2B-C1B-CB-O3   |
| 43  | M     | 504 | PLC  | C1'-C2'-C3'-C4' |
| 43  | a     | 201 | PLC  | C4-C5-N-C6      |
| 43  | Z     | 202 | PLC  | C2B-C1B-CB-O3   |
| 45  | J     | 201 | 3PE  | O11-C1-C2-O21   |
| 45  | L     | 707 | 3PE  | O21-C21-C22-C23 |
| 43  | Z     | 202 | PLC  | C4'-C5'-C6'-C7' |
| 45  | N     | 601 | 3PE  | C28-C29-C2A-C2B |
| 43  | q     | 201 | PLC  | C2B-C3B-C4B-C5B |
| 43  | P     | 502 | PLC  | C4-C5-N-C7      |
| 43  | Y     | 302 | PLC  | C4-C5-N-C6      |
| 45  | J     | 201 | 3PE  | O21-C21-C22-C23 |
| 45  | j     | 101 | 3PE  | O21-C21-C22-C23 |
| 43  | q     | 202 | PLC  | O2-C'-C1'-C2'   |
| 43  | q     | 201 | PLC  | C7B-C8B-C9B-CAA |
| 45  | L     | 703 | 3PE  | C2F-C2G-C2H-C2I |
| 43  | L     | 701 | PLC  | C7'-C8'-C9'-CA' |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 43  | M     | 504 | PLC  | C3-C2-O2-C'     |
| 46  | q     | 203 | CDL  | C31-C32-C33-C34 |
| 45  | L     | 705 | 3PE  | C2C-C2D-C2E-C2F |
| 45  | m     | 101 | 3PE  | C37-C38-C39-C3A |
| 49  | T     | 201 | EHZ  | N1-C12-C13-C14  |
| 43  | D     | 501 | PLC  | C8'-C9'-CA'-CB' |
| 43  | P     | 502 | PLC  | CB-C1B-C2B-C3B  |
| 45  | L     | 703 | 3PE  | C2-C1-O11-P     |
| 46  | b     | 102 | CDL  | C1-CA2-OA2-PA1  |
| 47  | P     | 501 | NDP  | C2B-O2B-P2B-O1X |
| 49  | T     | 201 | EHZ  | C1-C2-C3-C4     |
| 45  | L     | 704 | 3PE  | O22-C21-C22-C23 |
| 43  | M     | 504 | PLC  | C7B-C8B-C9B-CAA |
| 43  | d     | 101 | PLC  | C2'-C3'-C4'-C5' |
| 45  | b     | 103 | 3PE  | O32-C31-C32-C33 |
| 46  | q     | 203 | CDL  | C51-C52-C53-C54 |
| 43  | d     | 101 | PLC  | C6'-C7'-C8'-C9' |
| 43  | b     | 101 | PLC  | C4-C5-N-C7      |
| 43  | b     | 101 | PLC  | C4-C5-N-C8      |
| 45  | j     | 101 | 3PE  | O22-C21-C22-C23 |
| 47  | P     | 501 | NDP  | C2N-C3N-C7N-O7N |
| 45  | J     | 201 | 3PE  | O22-C21-C22-C23 |
| 45  | M     | 501 | 3PE  | O32-C31-C32-C33 |
| 43  | Z     | 202 | PLC  | C5B-C6B-C7B-C8B |
| 45  | M     | 501 | 3PE  | C37-C38-C39-C3A |
| 43  | q     | 202 | PLC  | O'-C'-C1'-C2'   |
| 45  | L     | 707 | 3PE  | O22-C21-C22-C23 |
| 43  | P     | 502 | PLC  | C2-C1-O3P-P     |
| 46  | Z     | 203 | CDL  | C32-C31-CA7-OA8 |
| 43  | Z     | 202 | PLC  | C4-C5-N-C7      |
| 43  | Z     | 202 | PLC  | C2B-C1B-CB-OB   |
| 45  | J     | 201 | 3PE  | C2B-C2C-C2D-C2E |
| 45  | L     | 702 | 3PE  | C25-C26-C27-C28 |
| 45  | m     | 101 | 3PE  | O31-C31-C32-C33 |
| 47  | P     | 501 | NDP  | PN-O3-PA-O1A    |
| 45  | J     | 201 | 3PE  | C39-C3A-C3B-C3C |
| 43  | g     | 301 | PLC  | C3B-C4B-C5B-C6B |
| 45  | b     | 103 | 3PE  | O21-C21-C22-C23 |

There are no ring outliers.

44 monomers are involved in 113 short contacts:

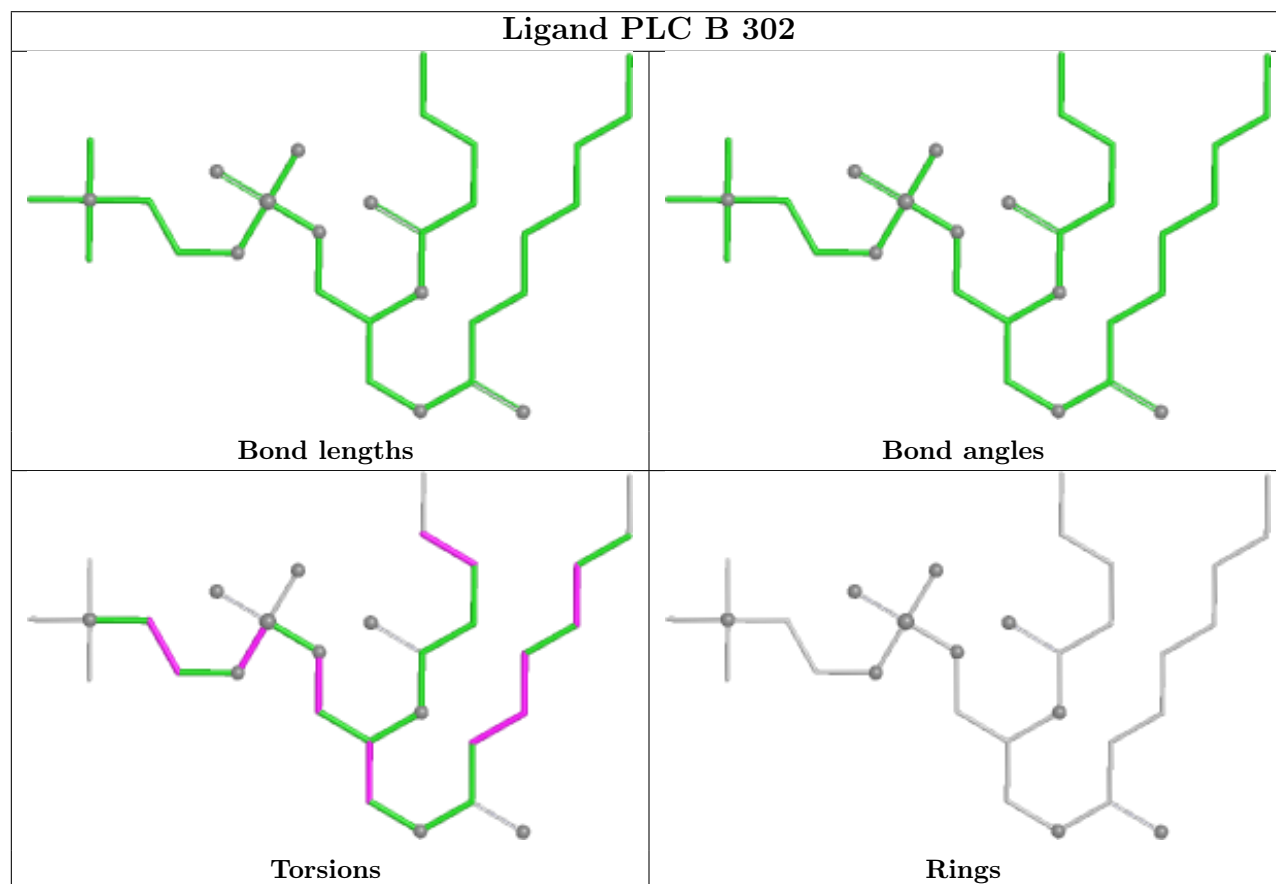
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 42  | I     | 302 | SF4  | 2       | 0            |
| 43  | B     | 302 | PLC  | 3       | 0            |
| 45  | N     | 601 | 3PE  | 1       | 0            |
| 45  | m     | 101 | 3PE  | 4       | 0            |
| 45  | J     | 201 | 3PE  | 4       | 0            |
| 45  | L     | 705 | 3PE  | 4       | 0            |
| 42  | G     | 801 | SF4  | 4       | 0            |
| 45  | L     | 706 | 3PE  | 5       | 0            |
| 43  | q     | 201 | PLC  | 4       | 0            |
| 43  | q     | 202 | PLC  | 2       | 0            |
| 43  | d     | 102 | PLC  | 1       | 0            |
| 42  | B     | 301 | SF4  | 1       | 0            |
| 43  | M     | 504 | PLC  | 2       | 0            |
| 43  | Y     | 302 | PLC  | 2       | 0            |
| 45  | L     | 703 | 3PE  | 3       | 0            |
| 45  | b     | 103 | 3PE  | 2       | 0            |
| 47  | P     | 501 | NDP  | 2       | 0            |
| 43  | P     | 502 | PLC  | 2       | 0            |
| 43  | d     | 101 | PLC  | 2       | 0            |
| 45  | Y     | 301 | 3PE  | 1       | 0            |
| 45  | L     | 702 | 3PE  | 6       | 0            |
| 45  | h     | 201 | 3PE  | 5       | 0            |
| 46  | q     | 203 | CDL  | 5       | 0            |
| 45  | b     | 104 | 3PE  | 1       | 0            |
| 42  | I     | 301 | SF4  | 1       | 0            |
| 43  | Z     | 202 | PLC  | 3       | 0            |
| 49  | U     | 201 | EHZ  | 2       | 0            |
| 43  | L     | 708 | PLC  | 4       | 0            |
| 46  | b     | 102 | CDL  | 3       | 0            |
| 45  | L     | 704 | 3PE  | 2       | 0            |
| 45  | Z     | 201 | 3PE  | 1       | 0            |
| 43  | L     | 701 | PLC  | 6       | 0            |
| 45  | M     | 502 | 3PE  | 1       | 0            |
| 43  | M     | 503 | PLC  | 2       | 0            |
| 46  | O     | 201 | CDL  | 3       | 0            |
| 45  | M     | 501 | 3PE  | 5       | 0            |
| 43  | L     | 709 | PLC  | 3       | 0            |
| 43  | g     | 301 | PLC  | 5       | 0            |
| 42  | G     | 802 | SF4  | 2       | 0            |
| 46  | Z     | 203 | CDL  | 1       | 0            |
| 43  | D     | 501 | PLC  | 3       | 0            |
| 45  | j     | 101 | 3PE  | 4       | 0            |
| 43  | P     | 503 | PLC  | 1       | 0            |

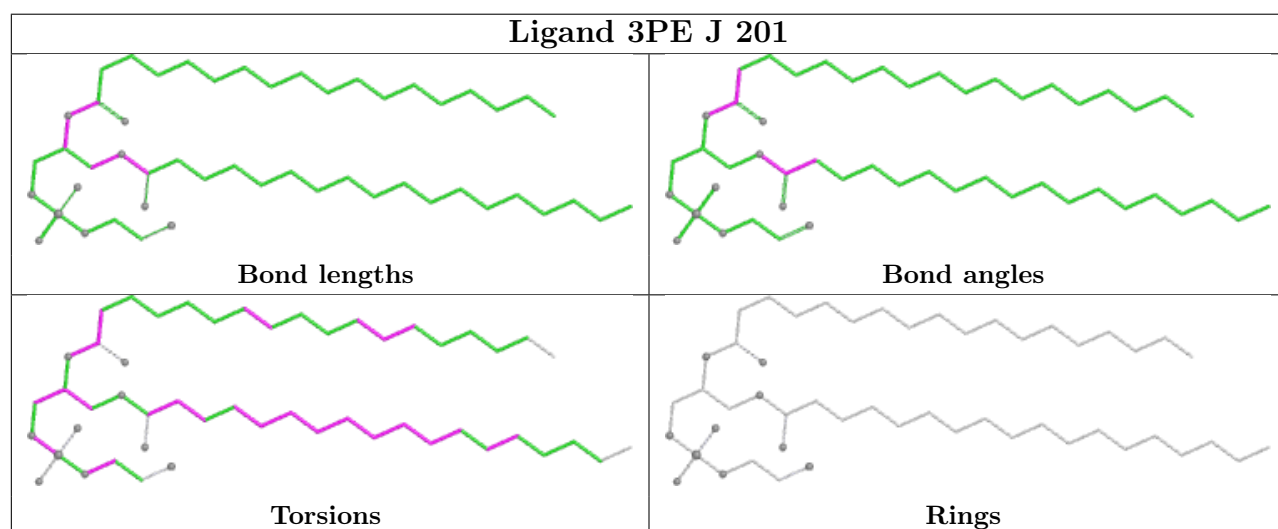
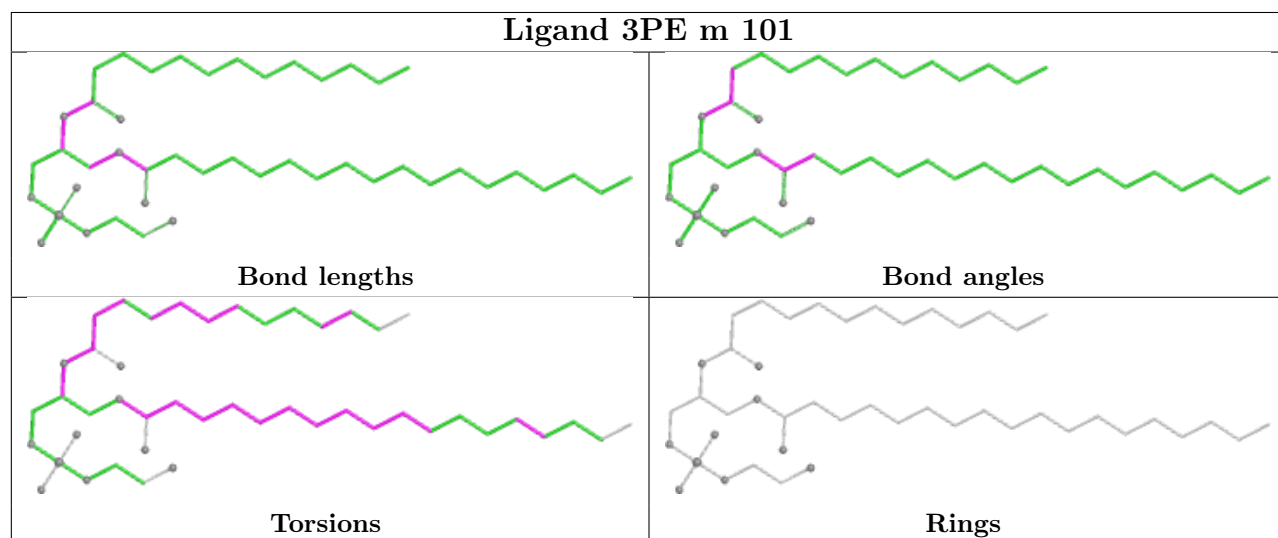
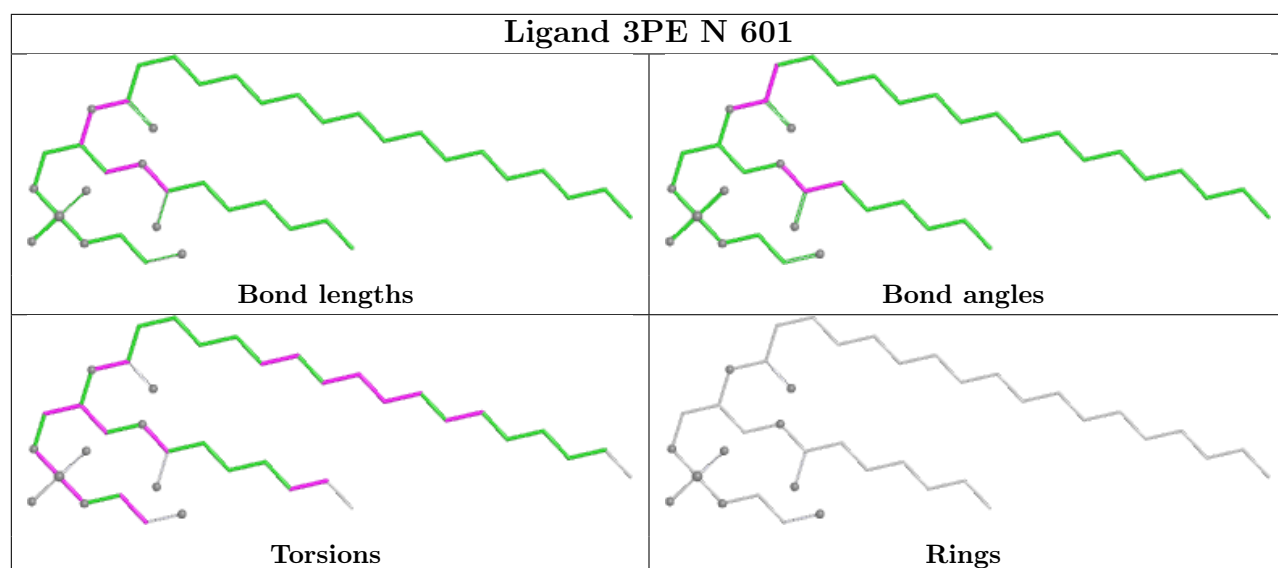
*Continued on next page...*

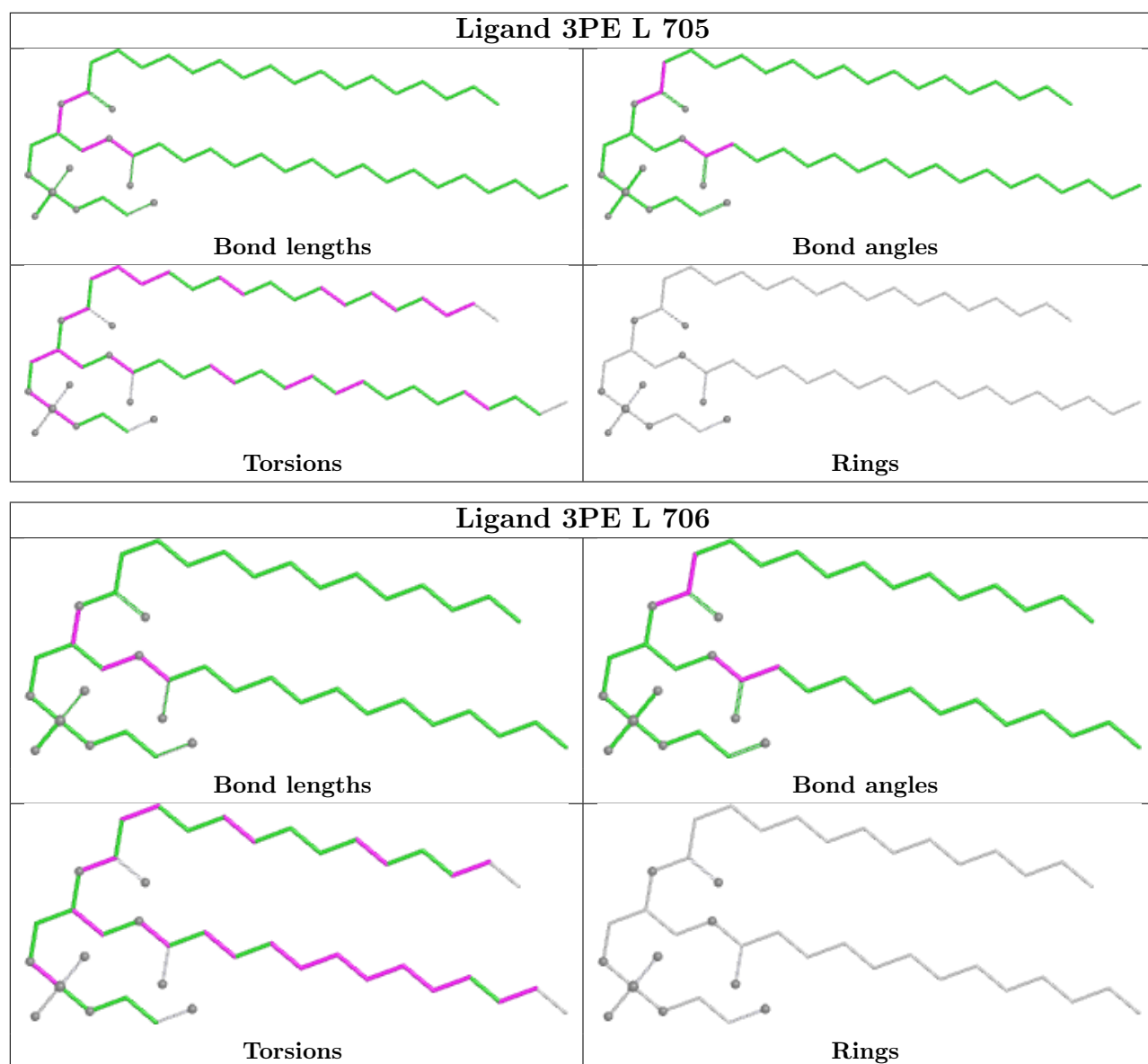
*Continued from previous page...*

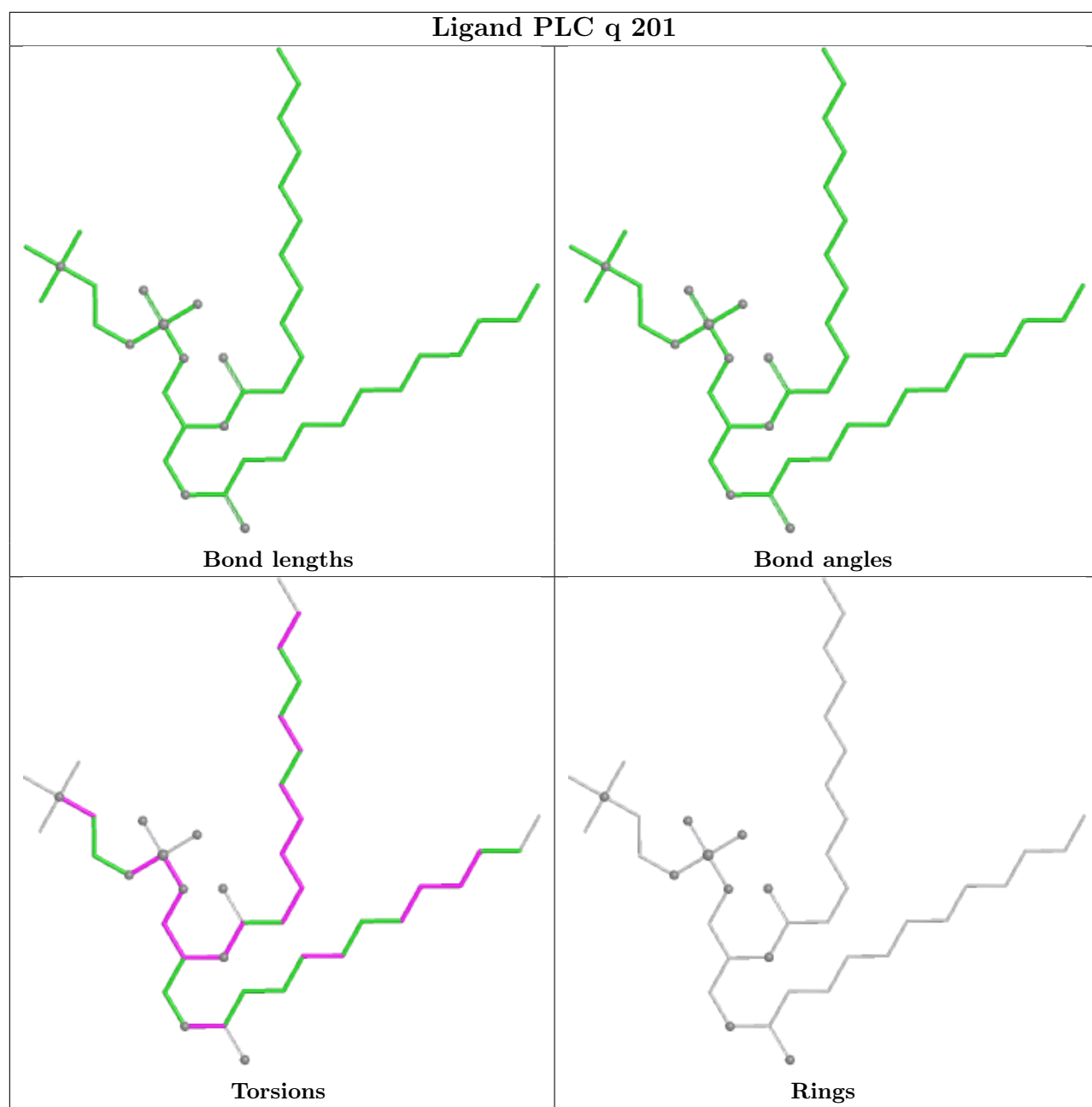
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 43  | Y     | 303 | PLC  | 2       | 0            |

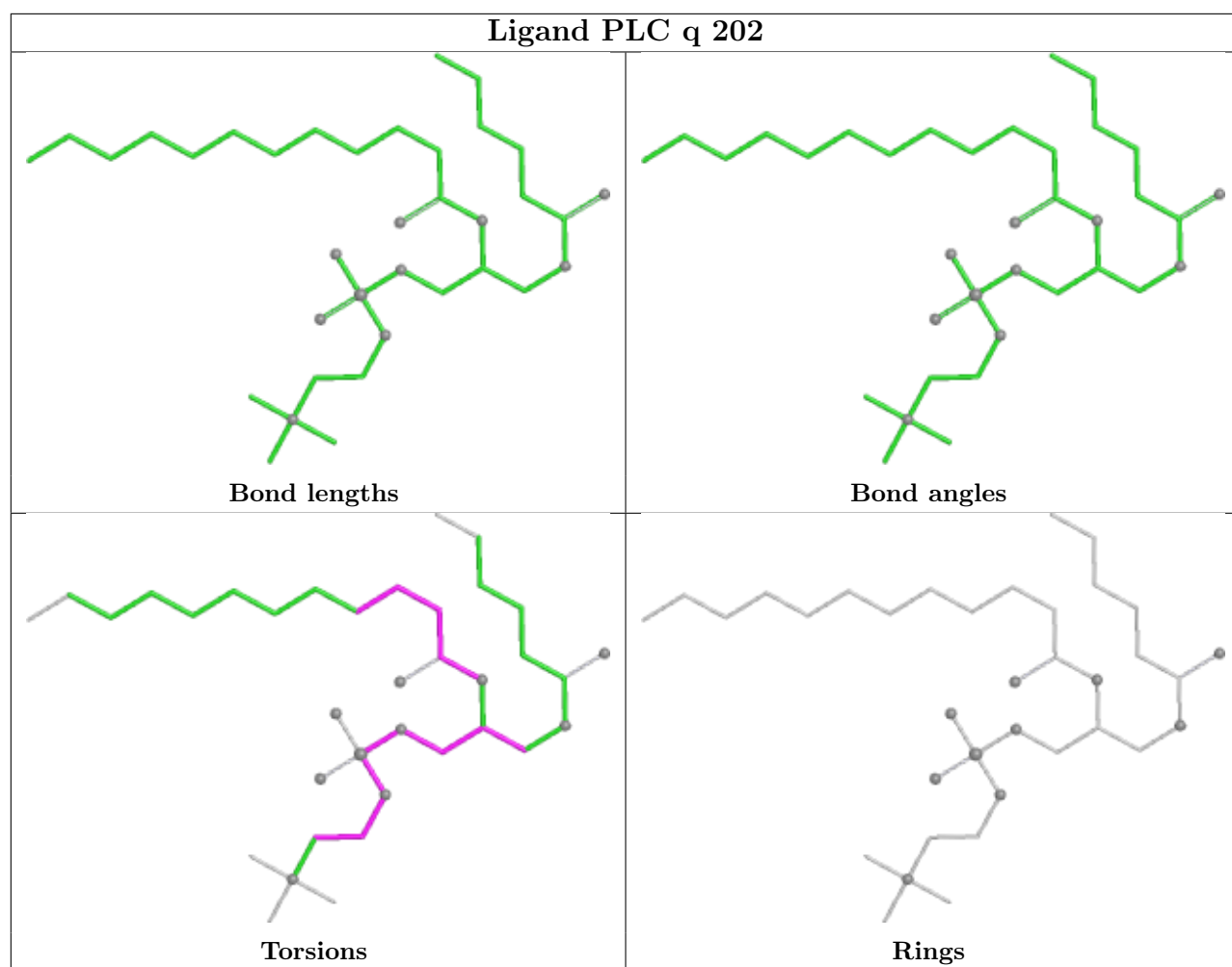
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

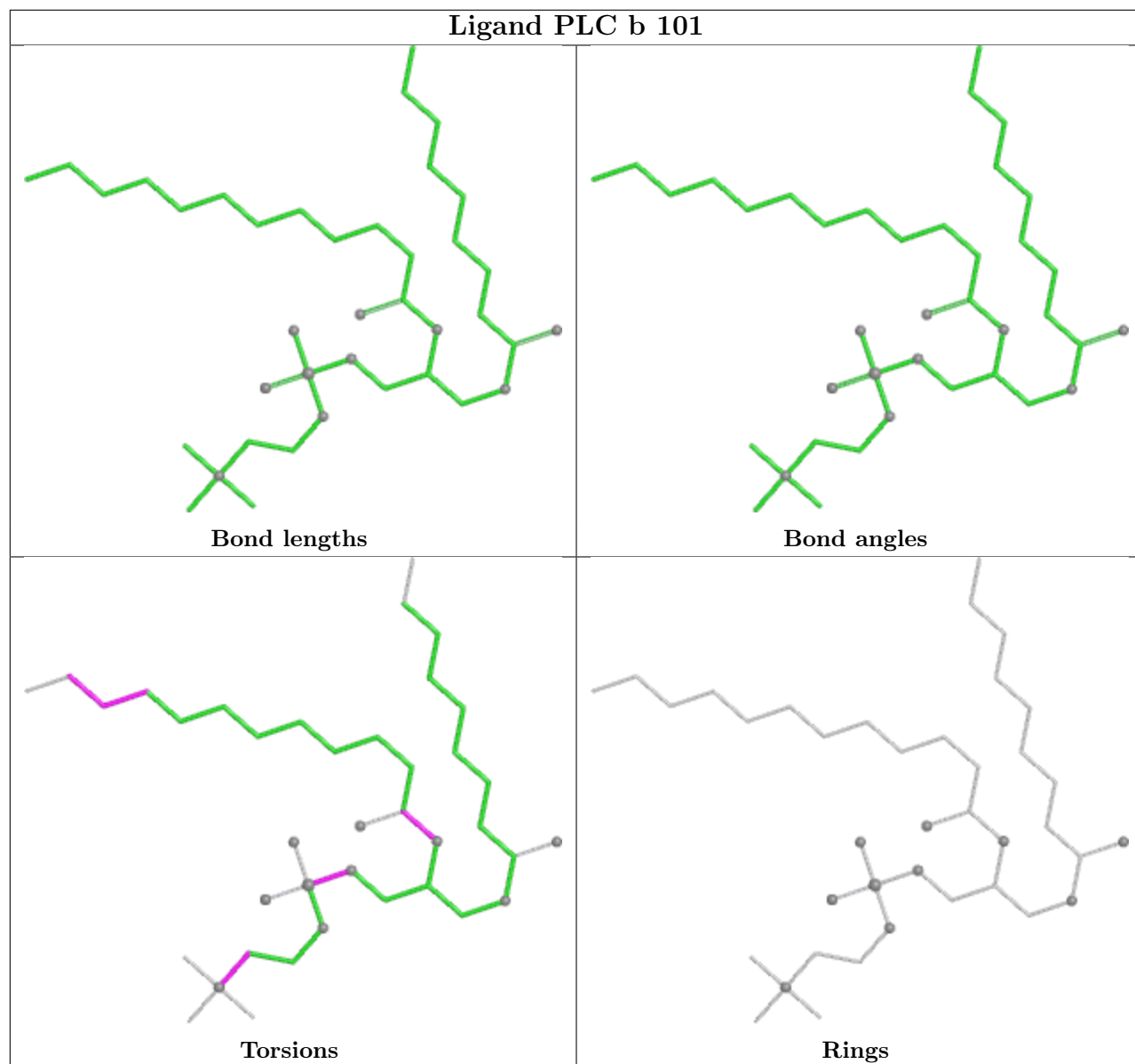


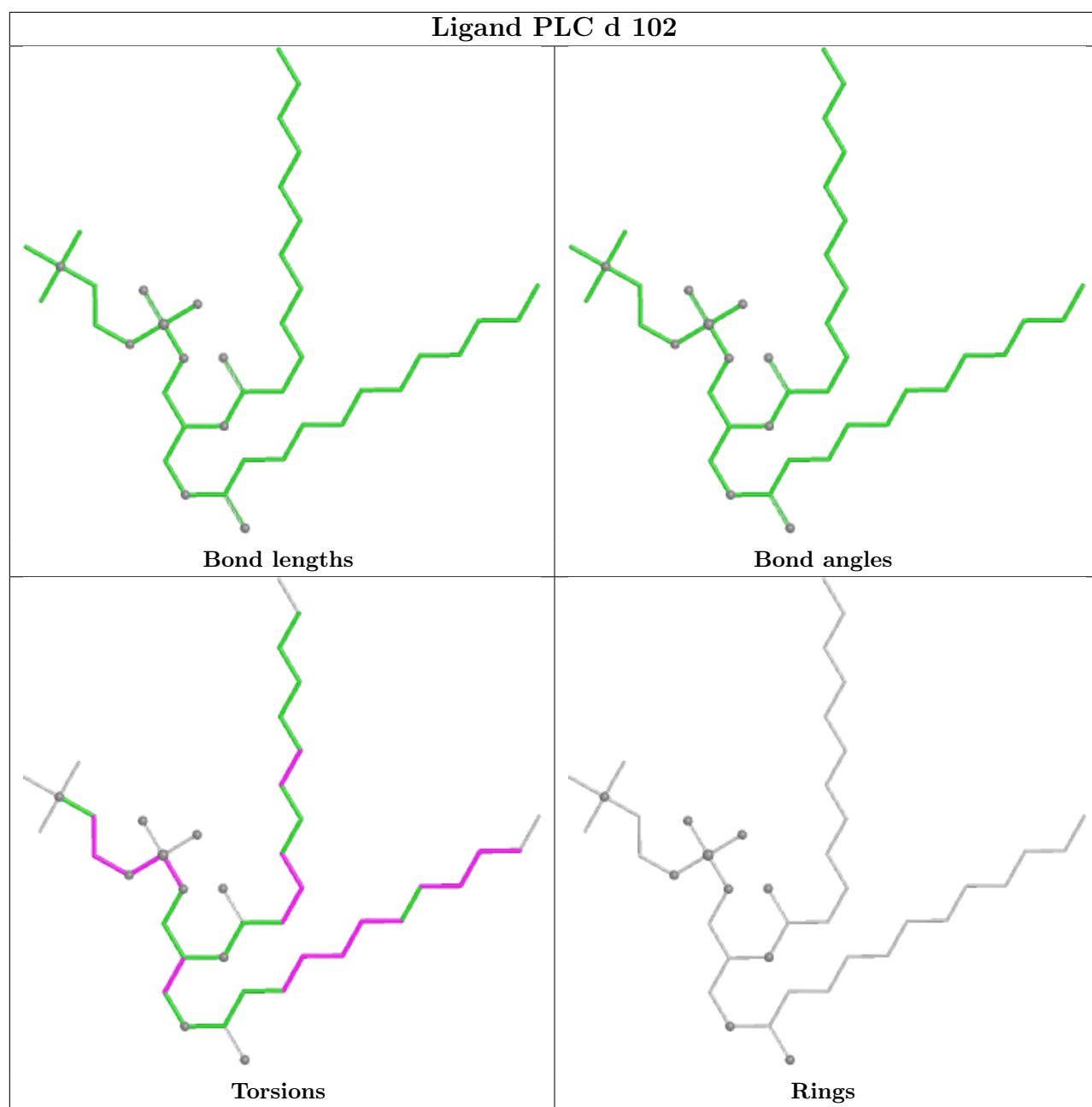


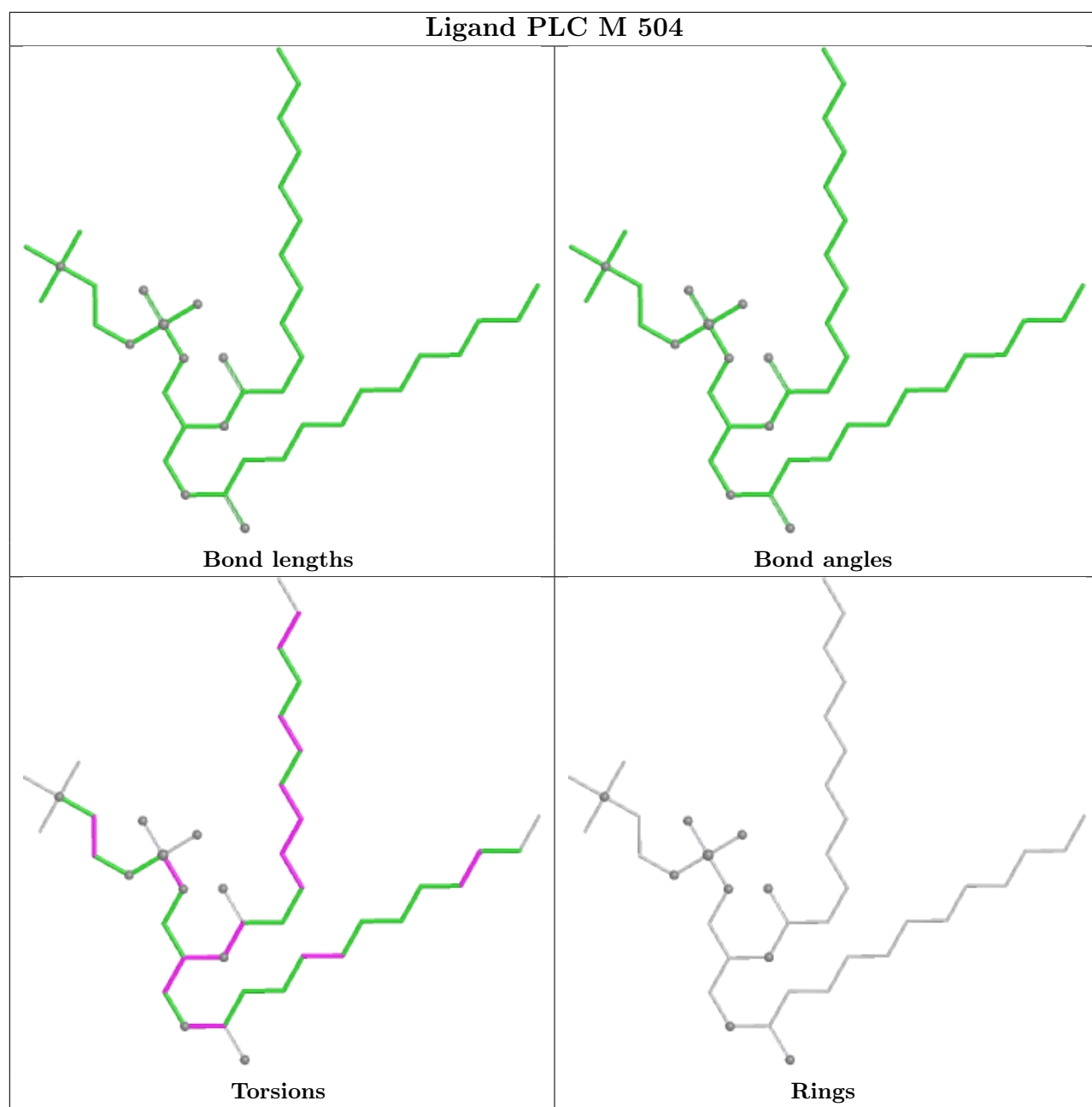


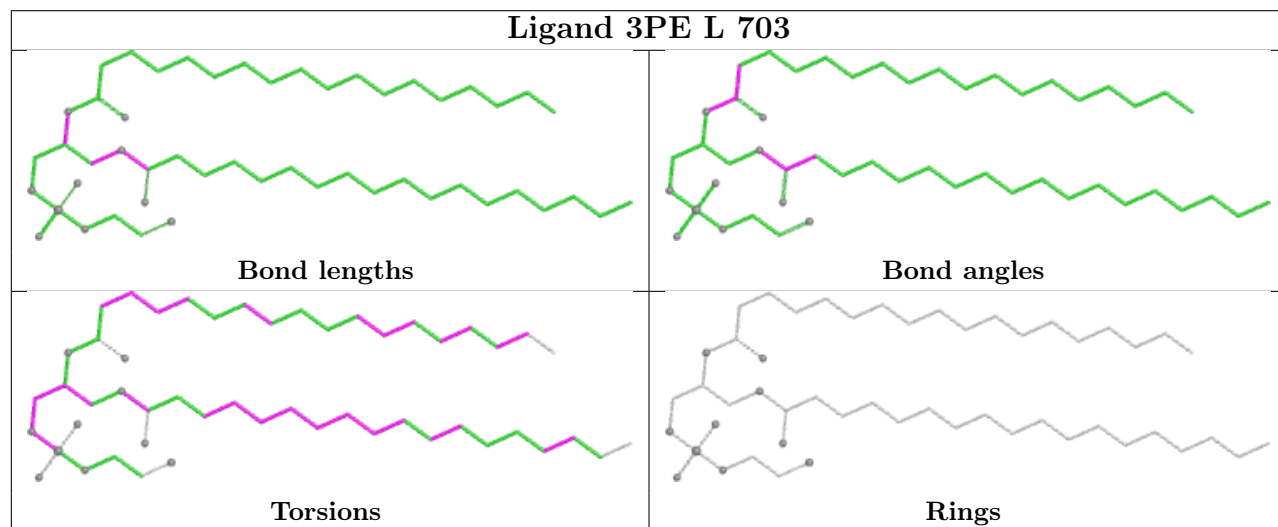
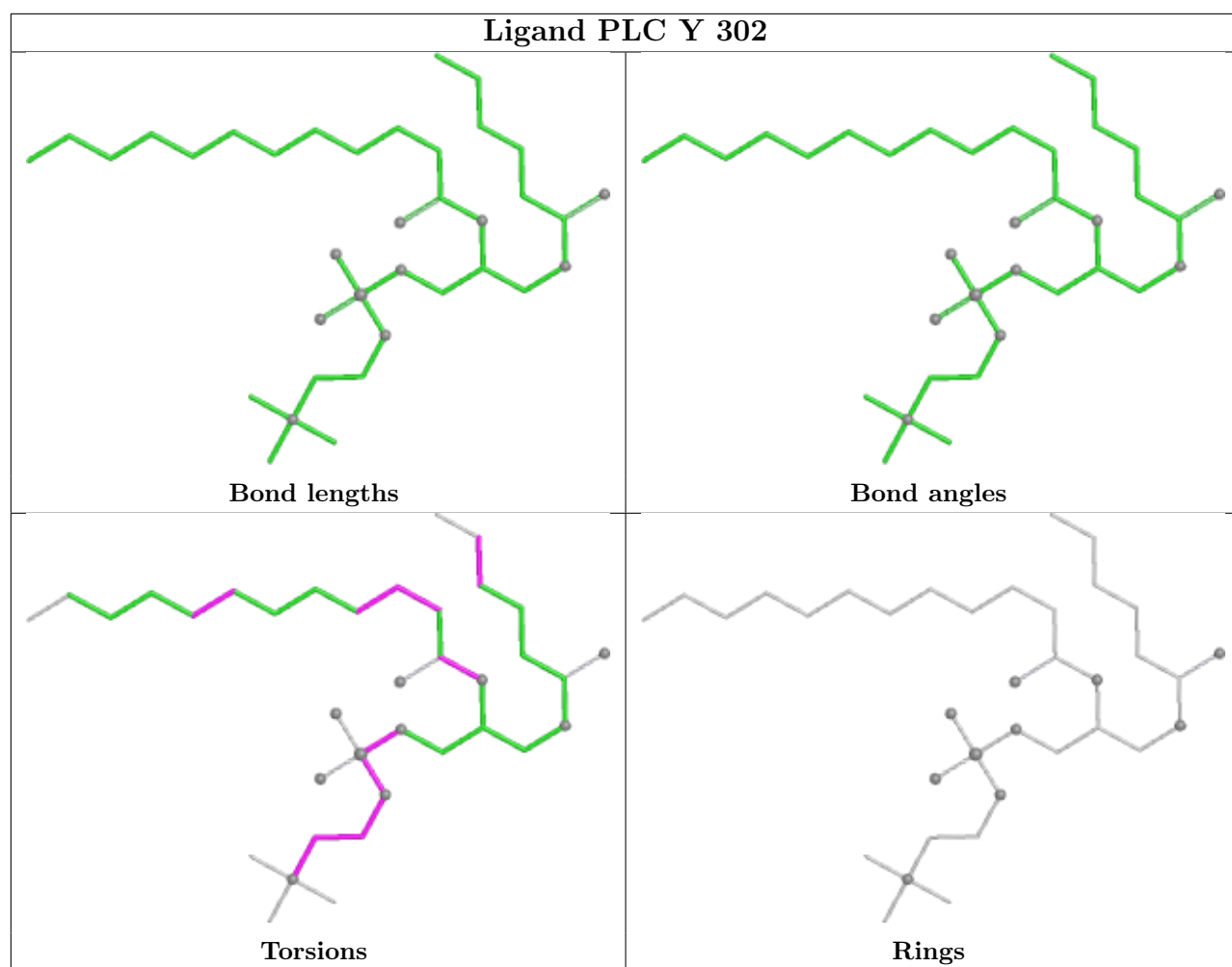


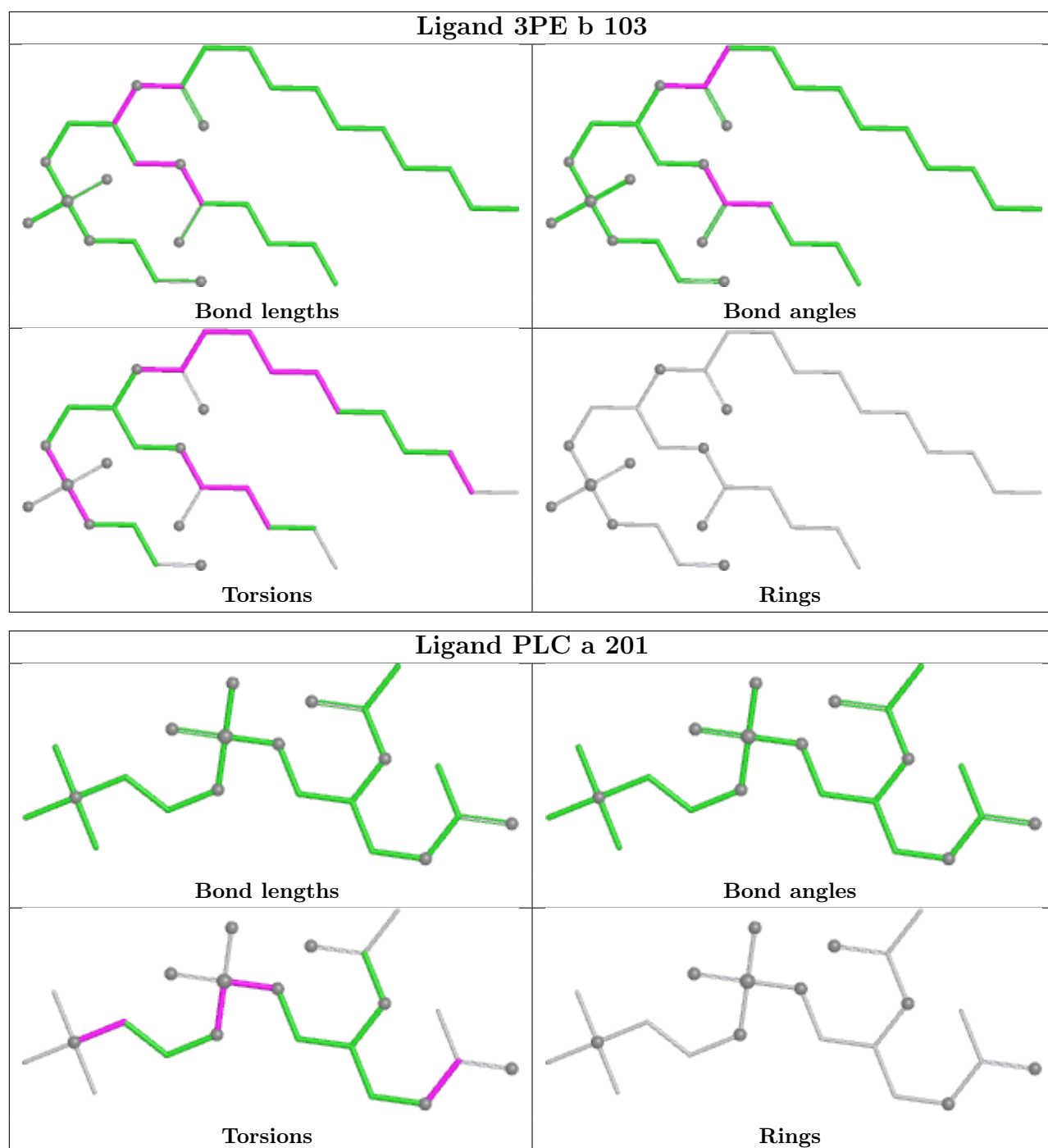


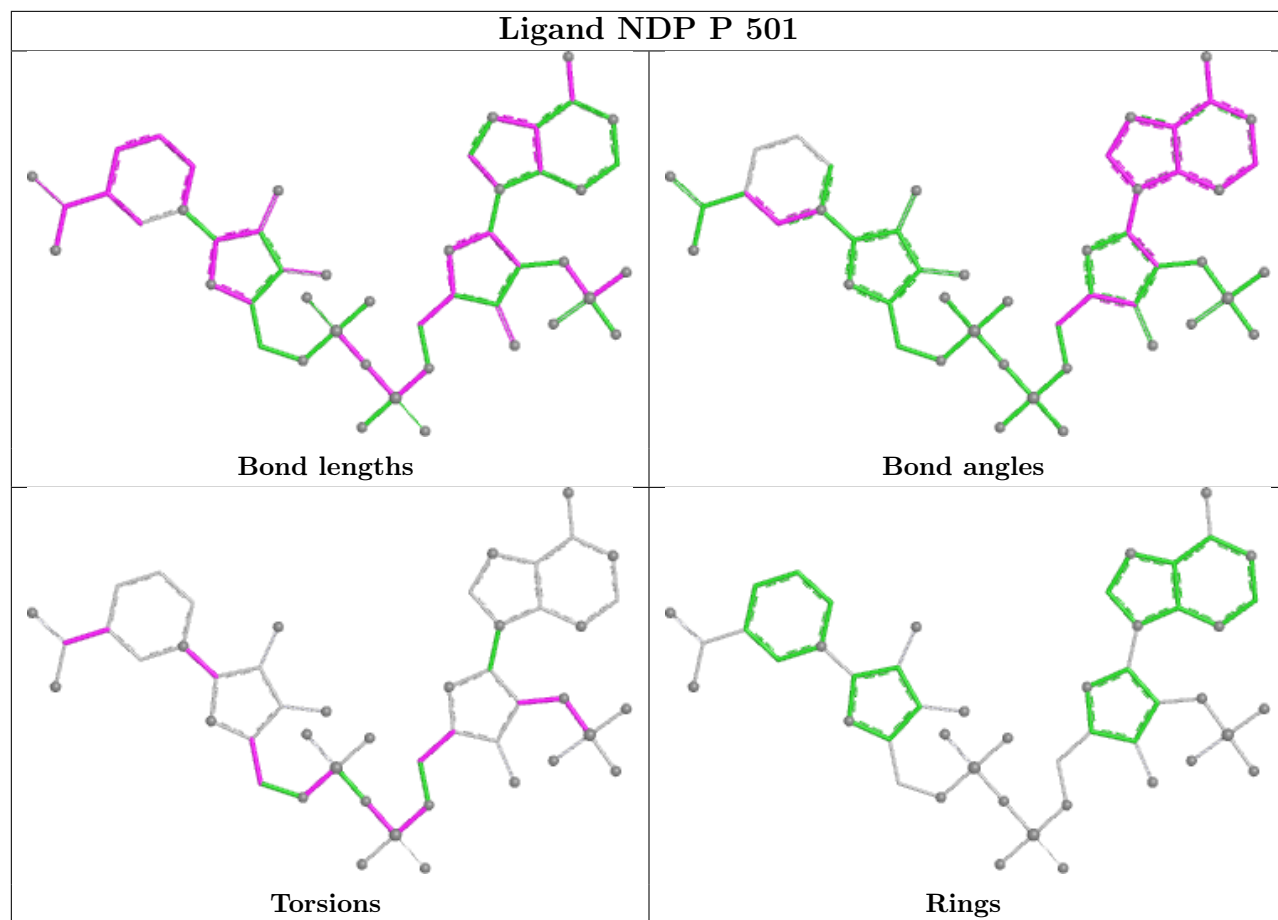


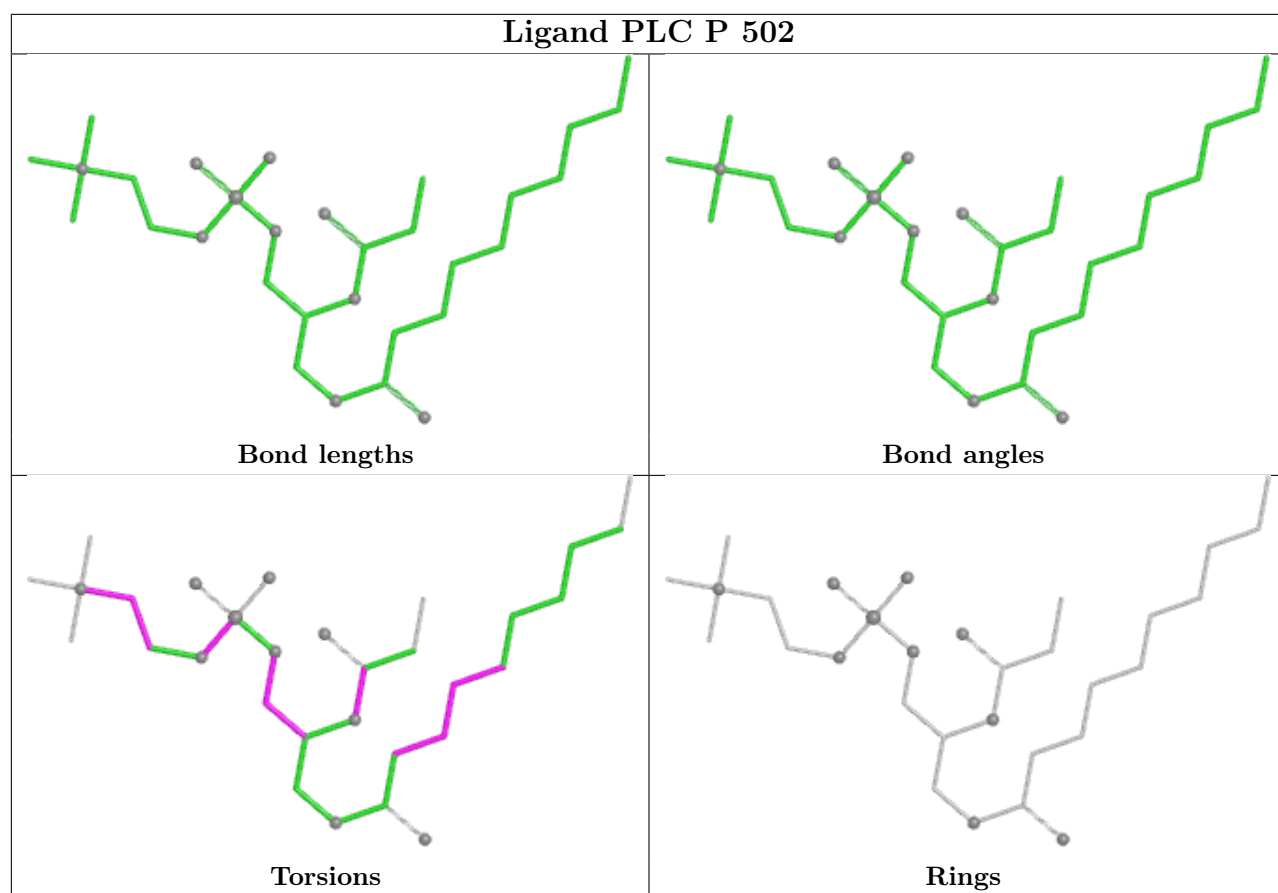


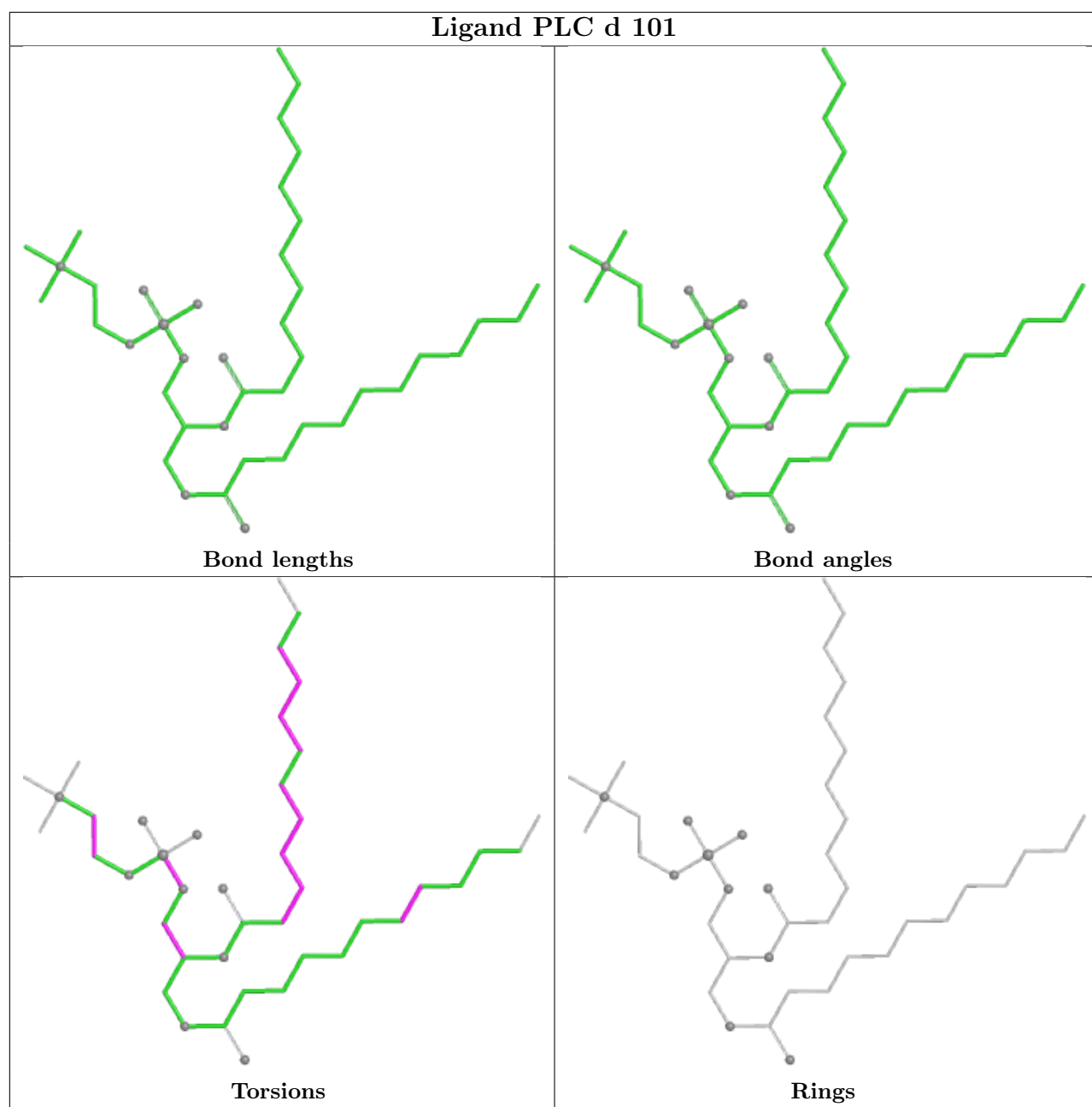




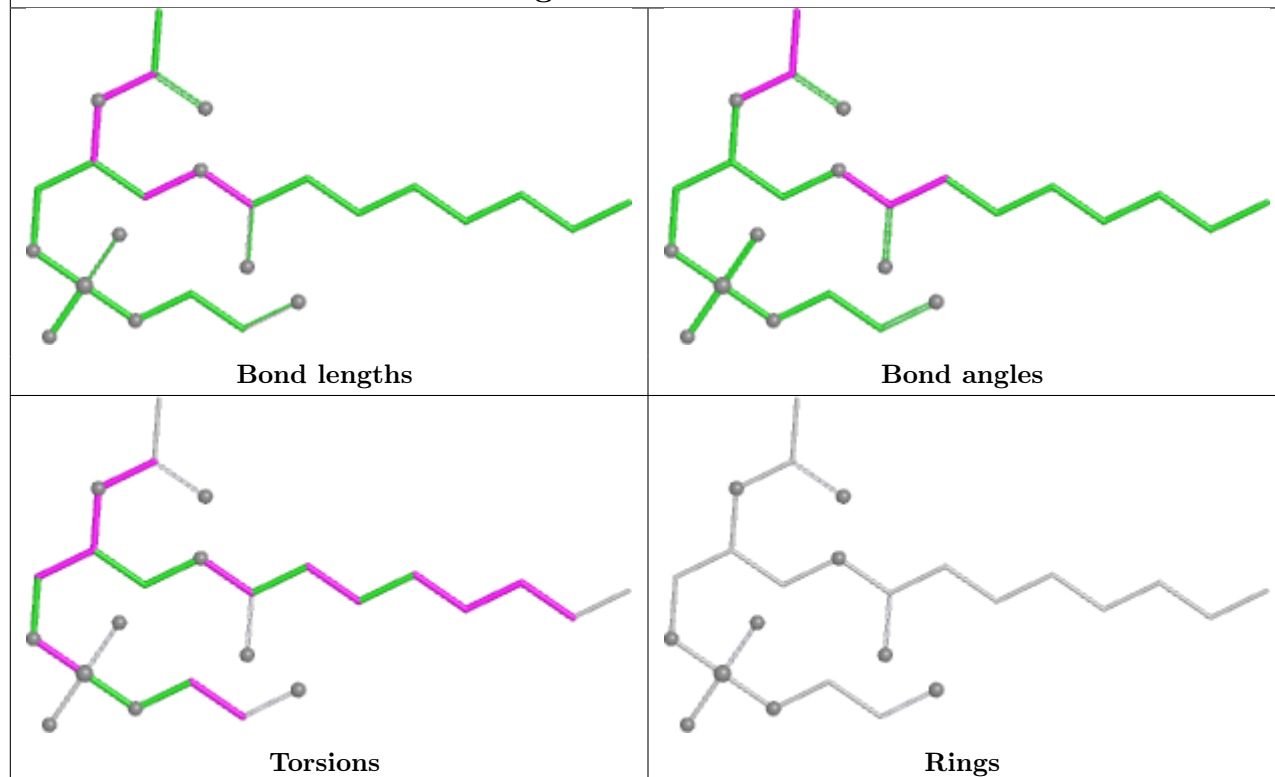




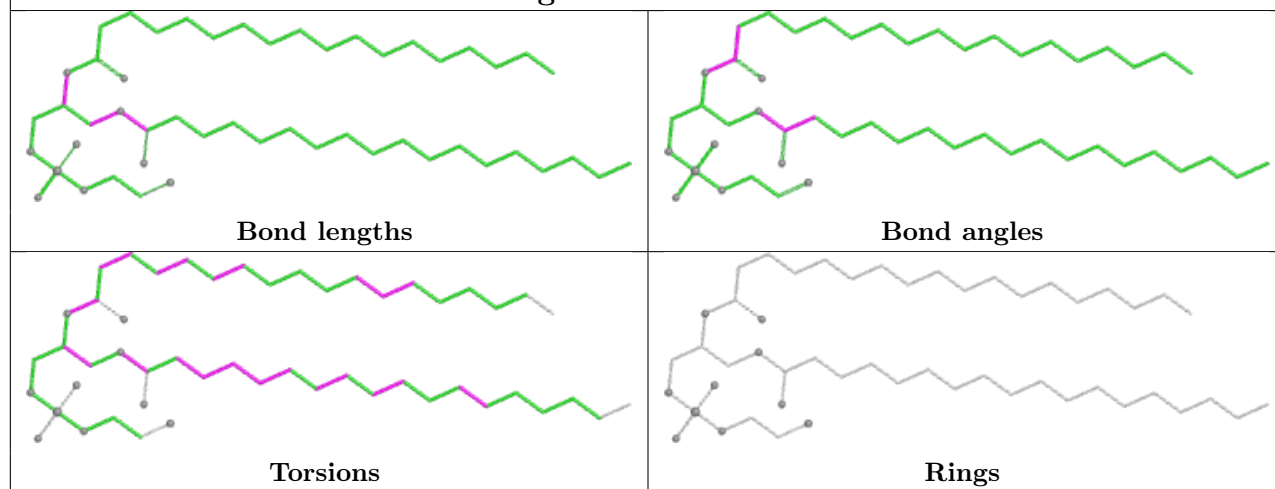


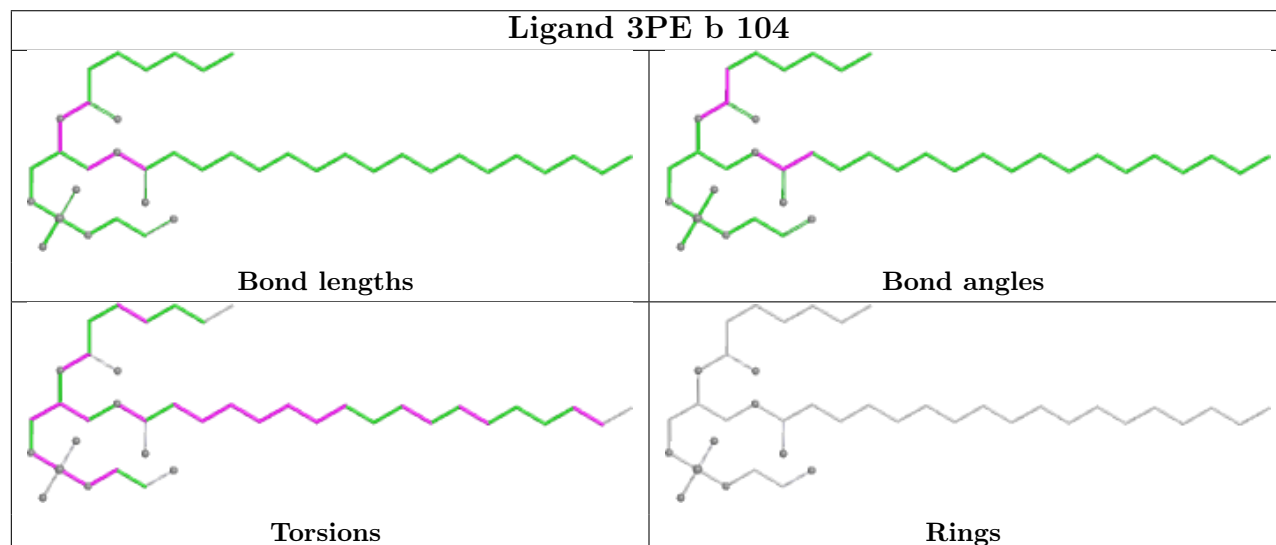
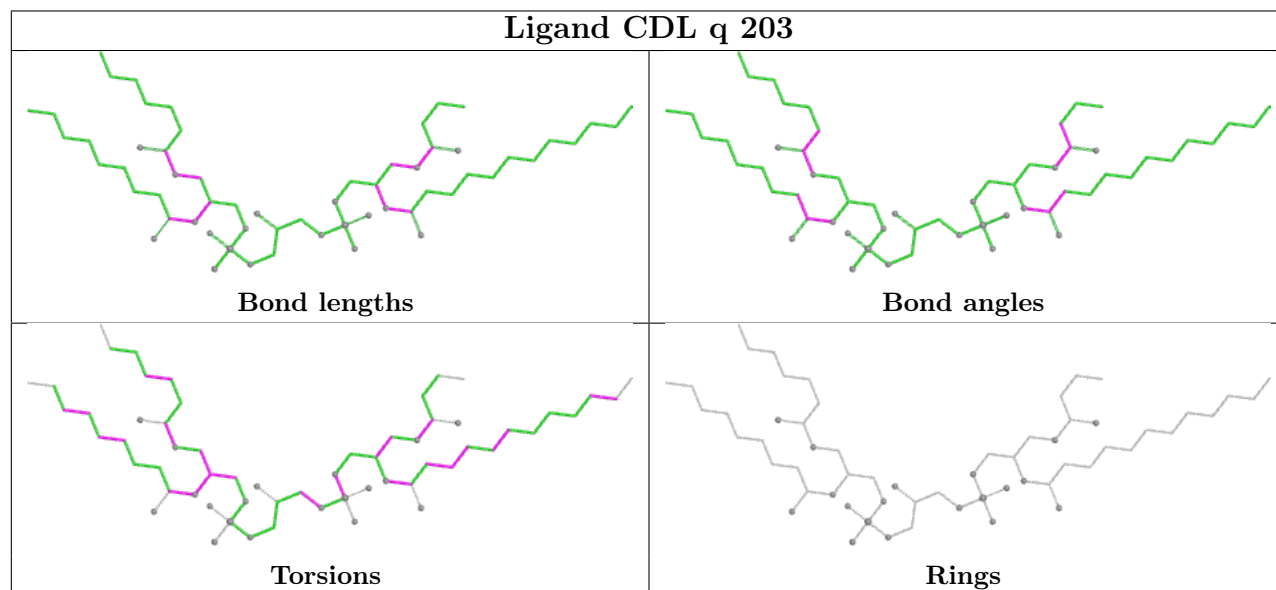
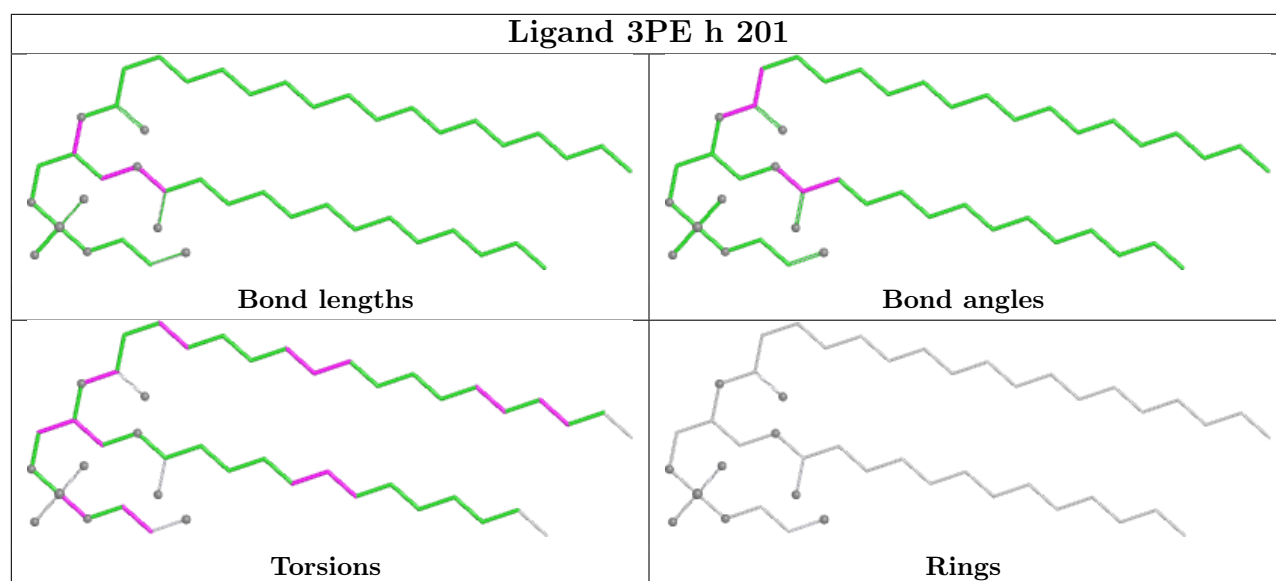


## Ligand 3PE Y 301

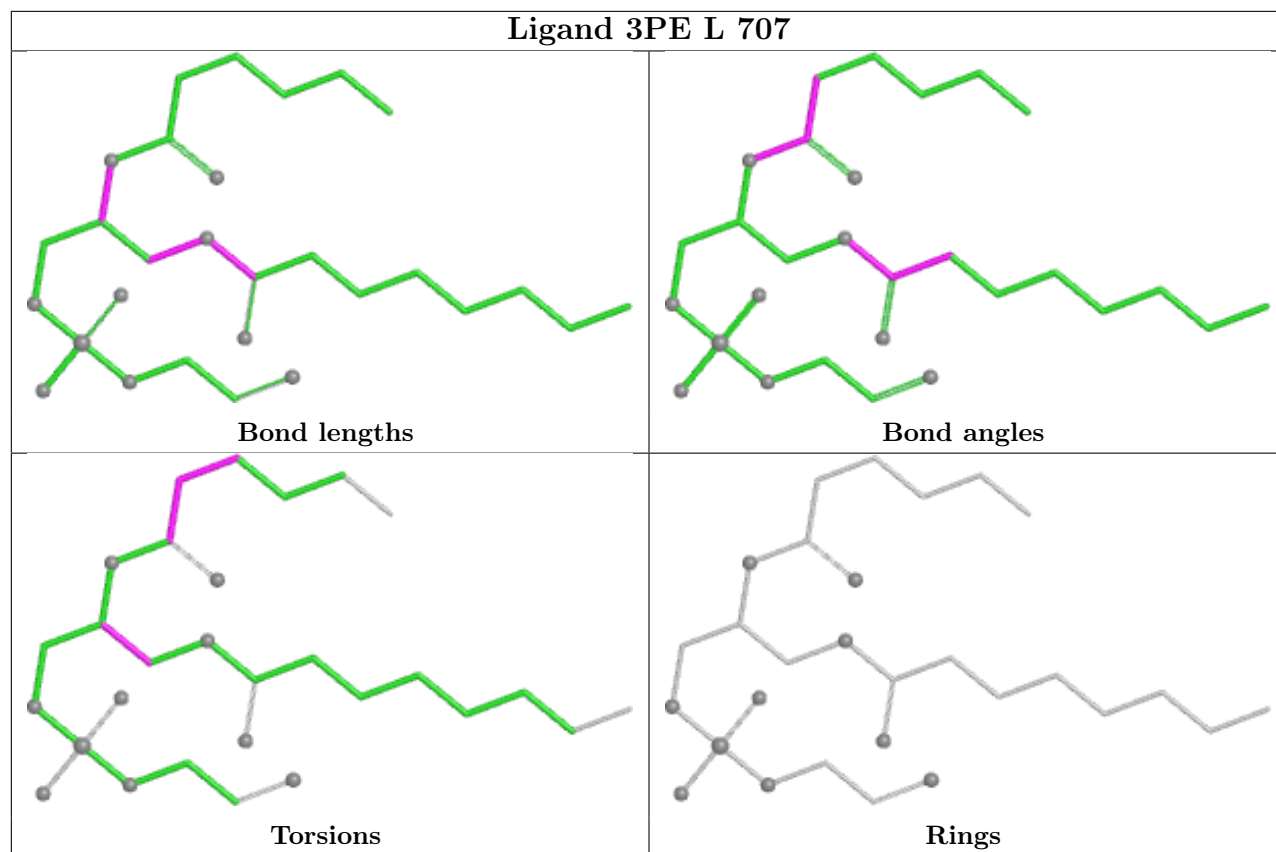


## Ligand 3PE L 702

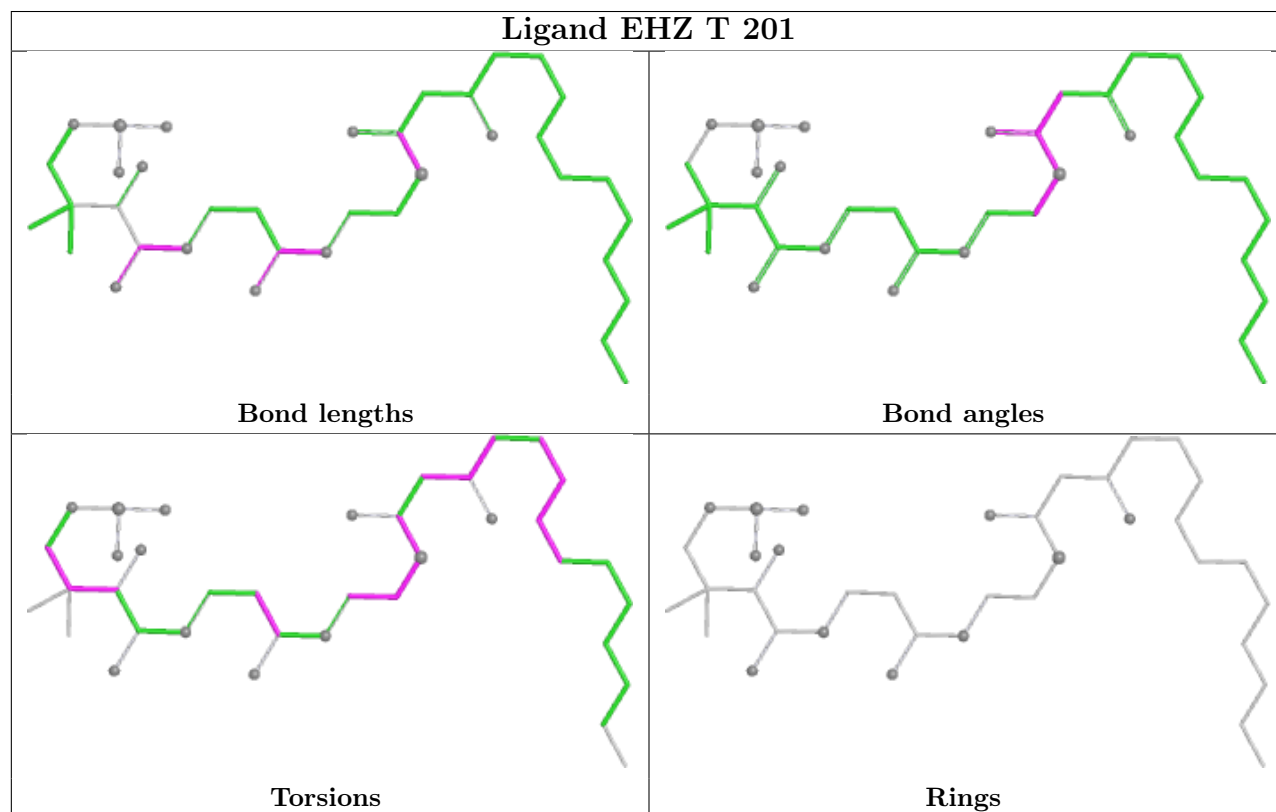


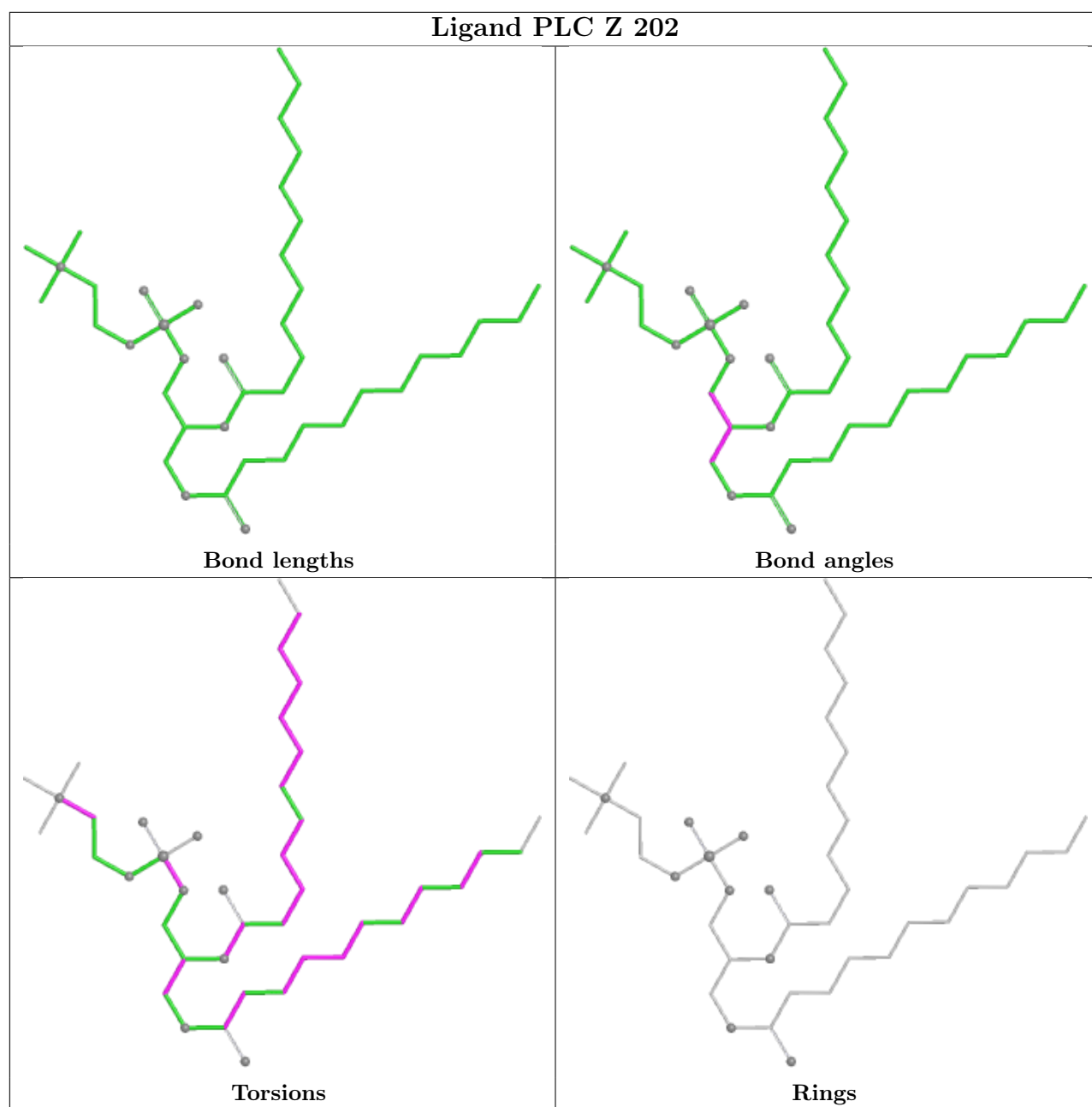


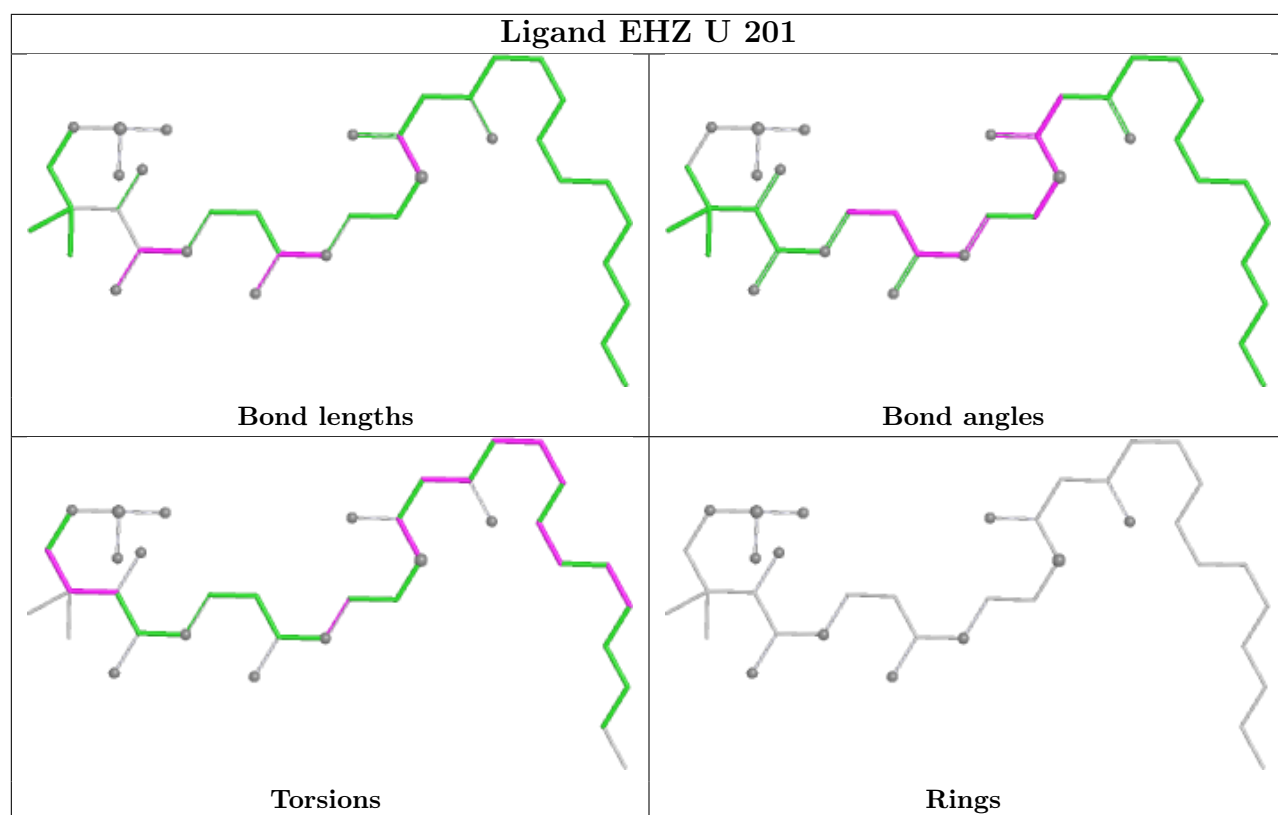
## Ligand 3PE L 707

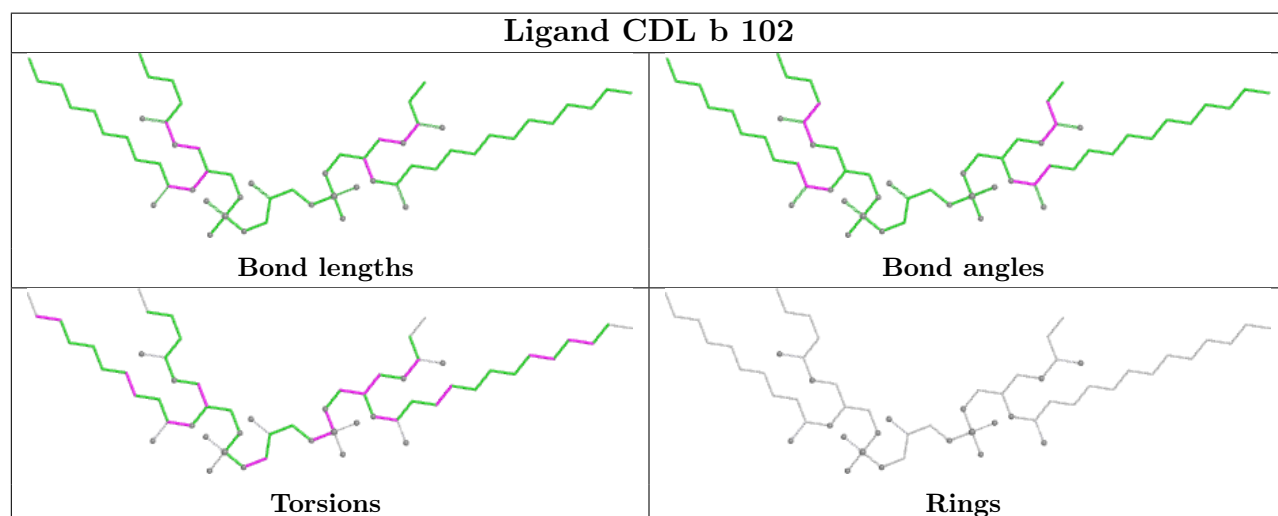
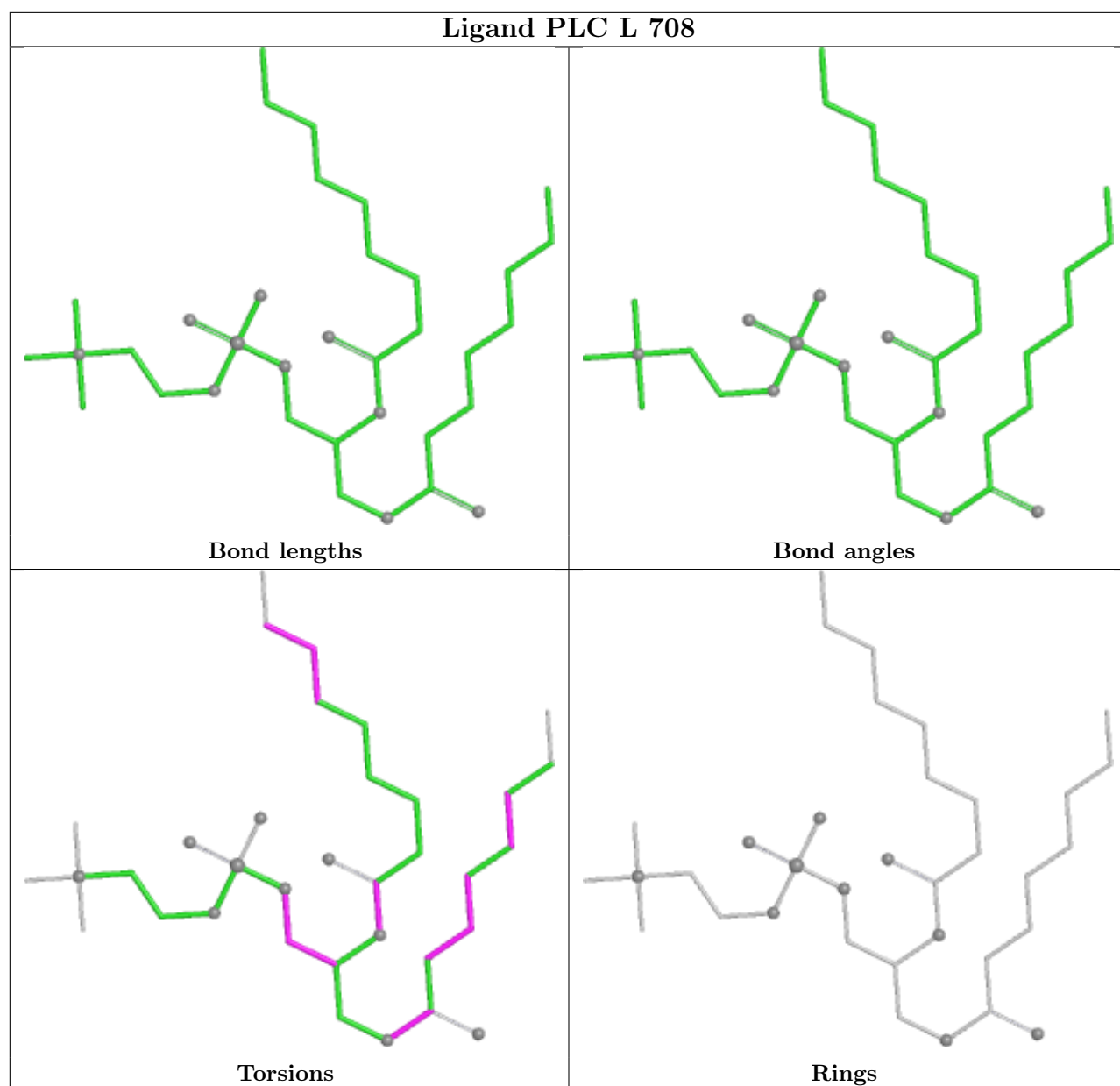


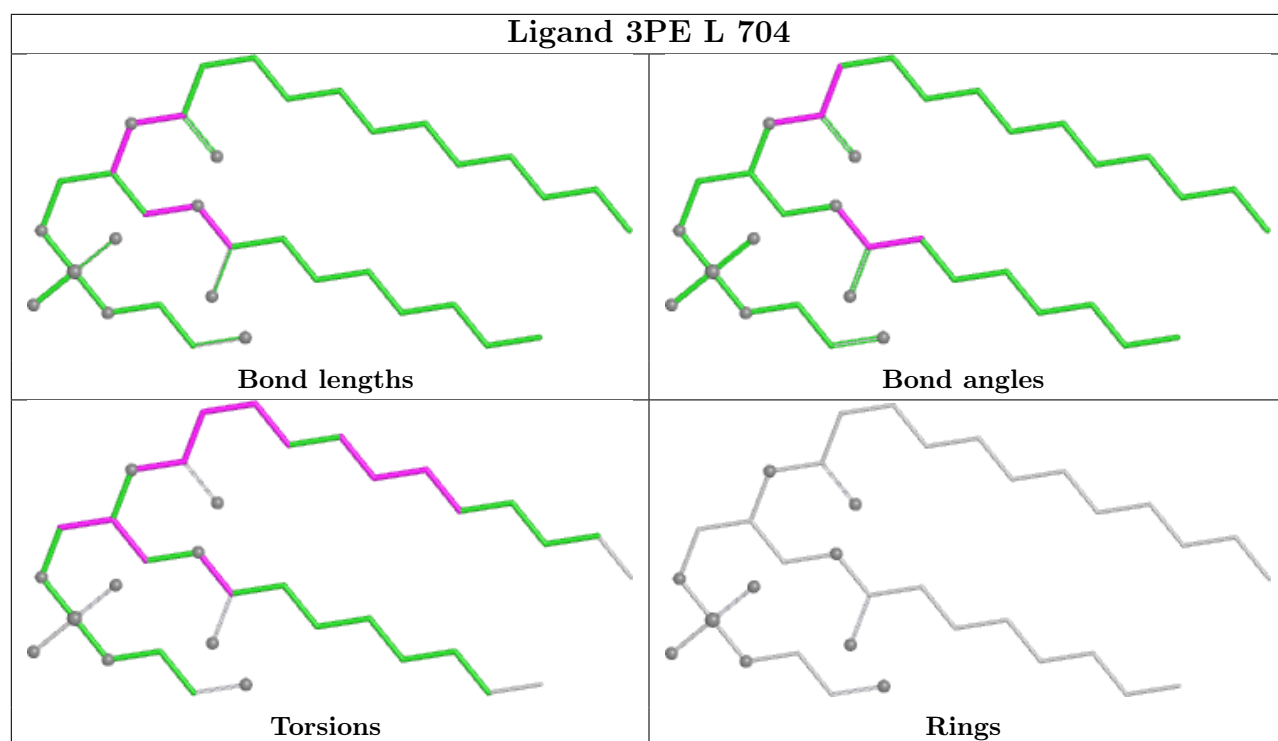
## Ligand EHZ T 201

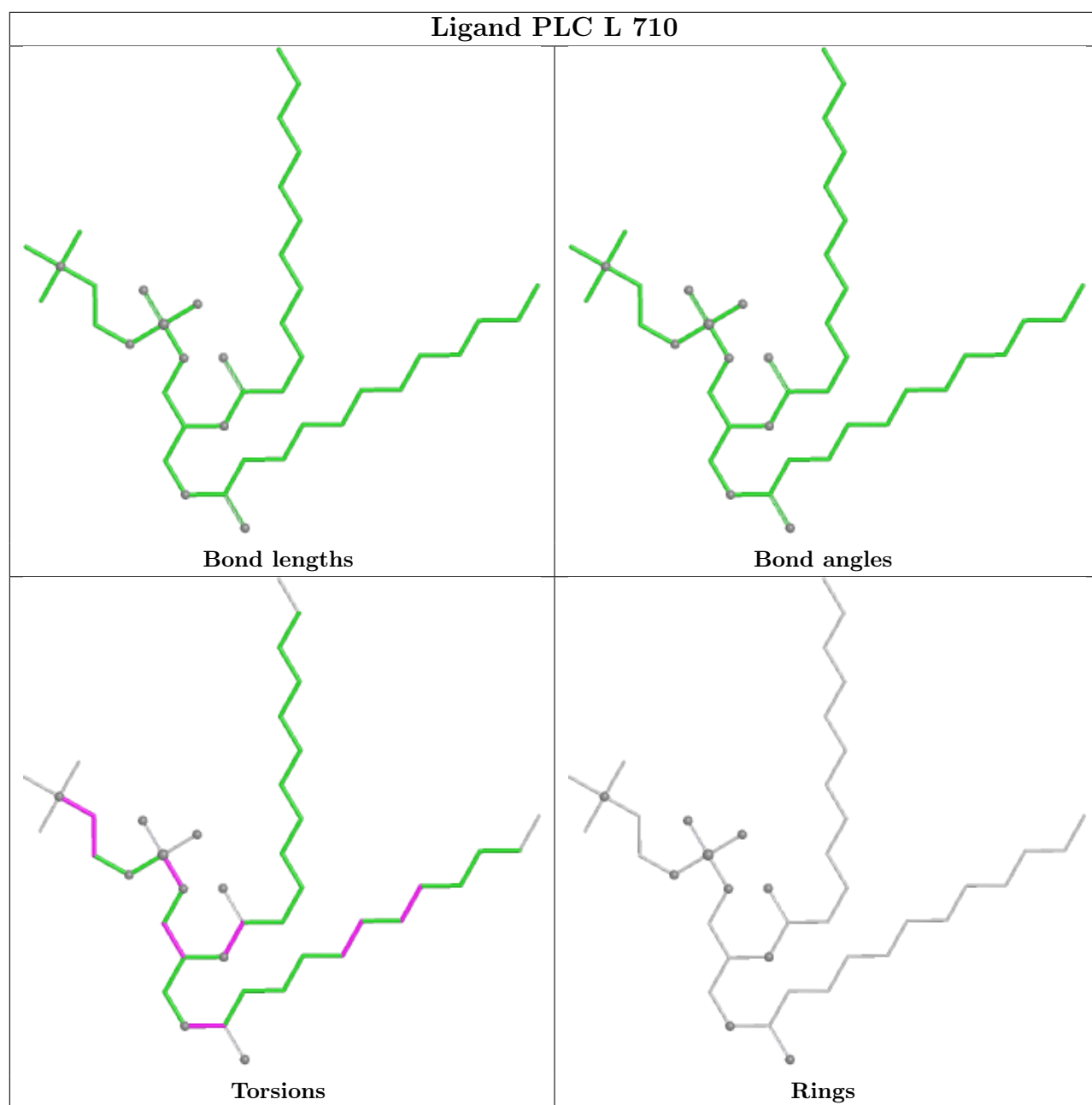


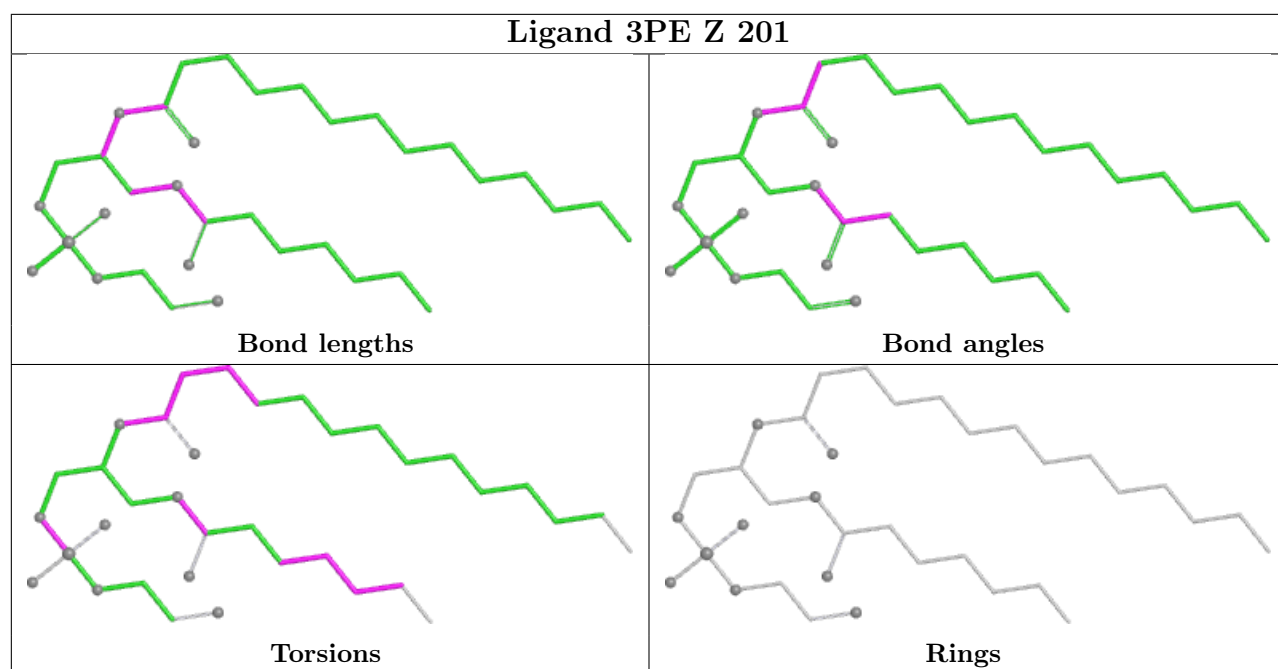


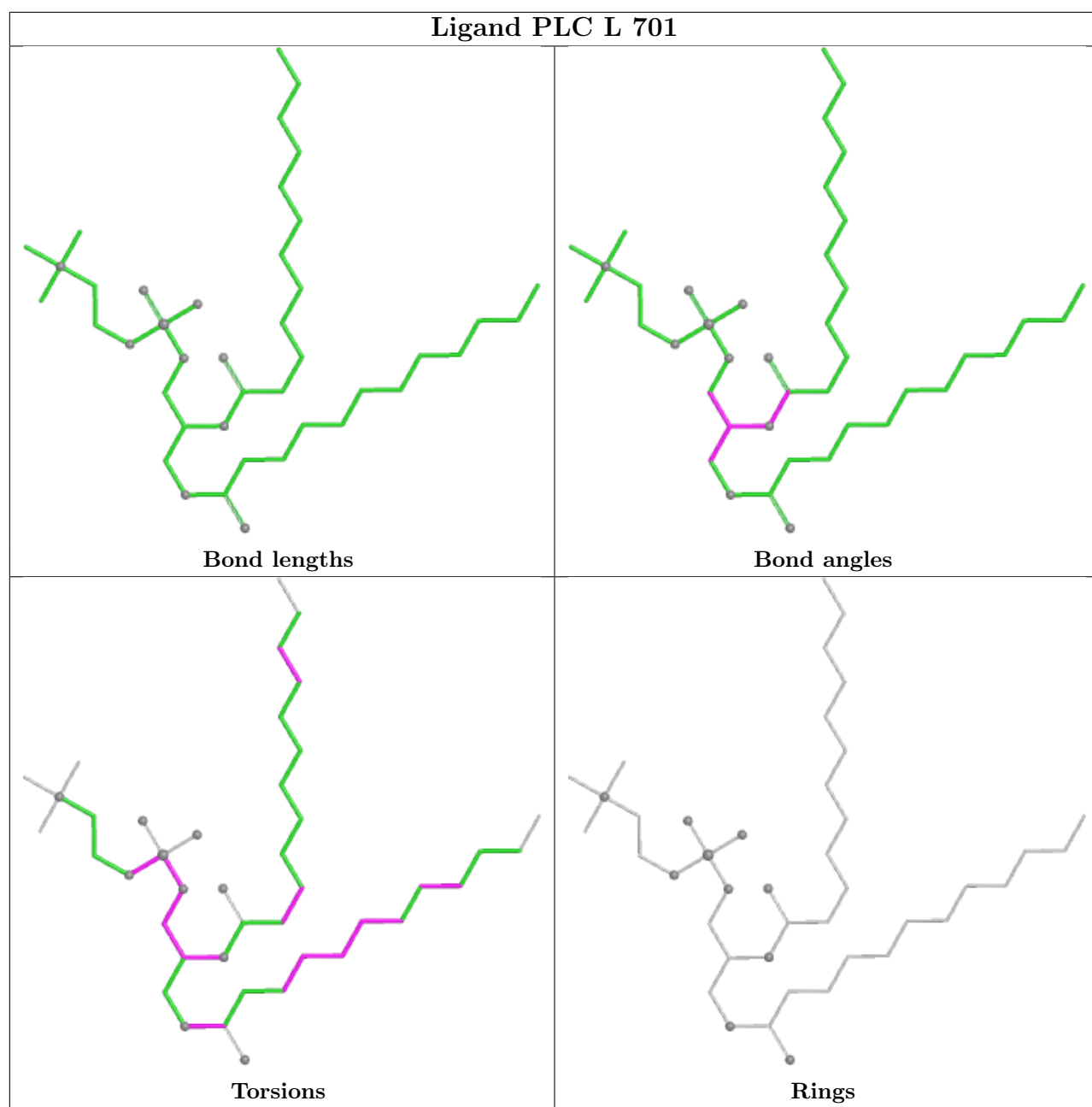


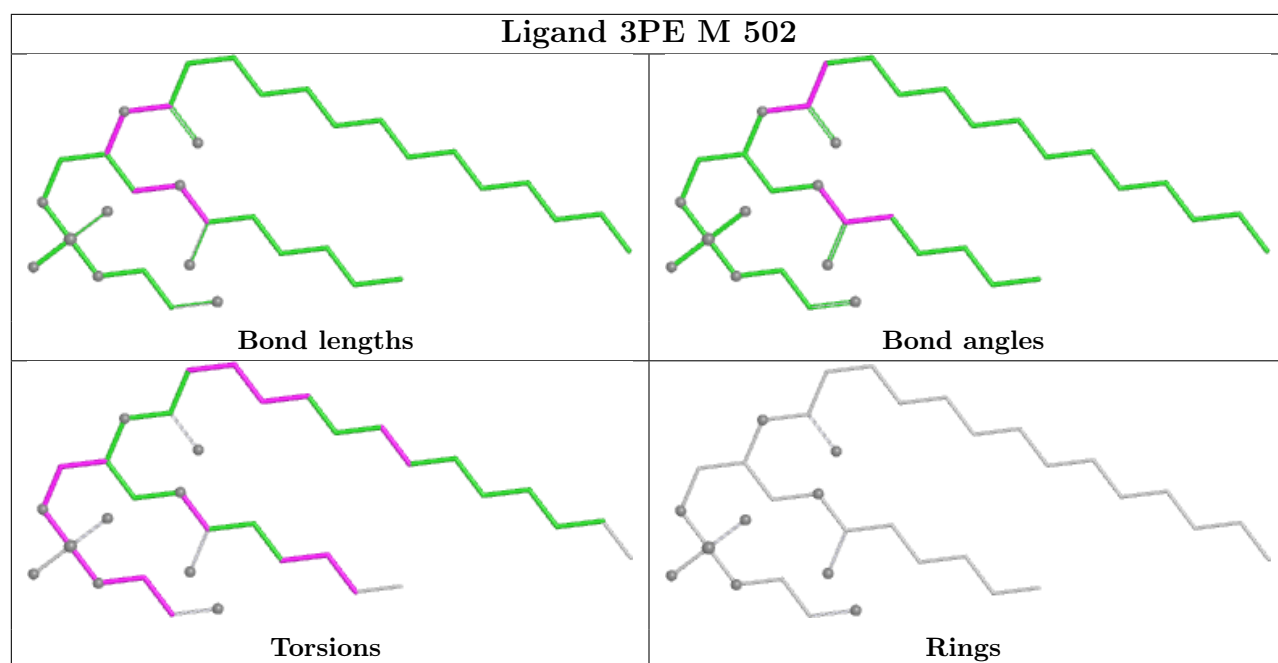


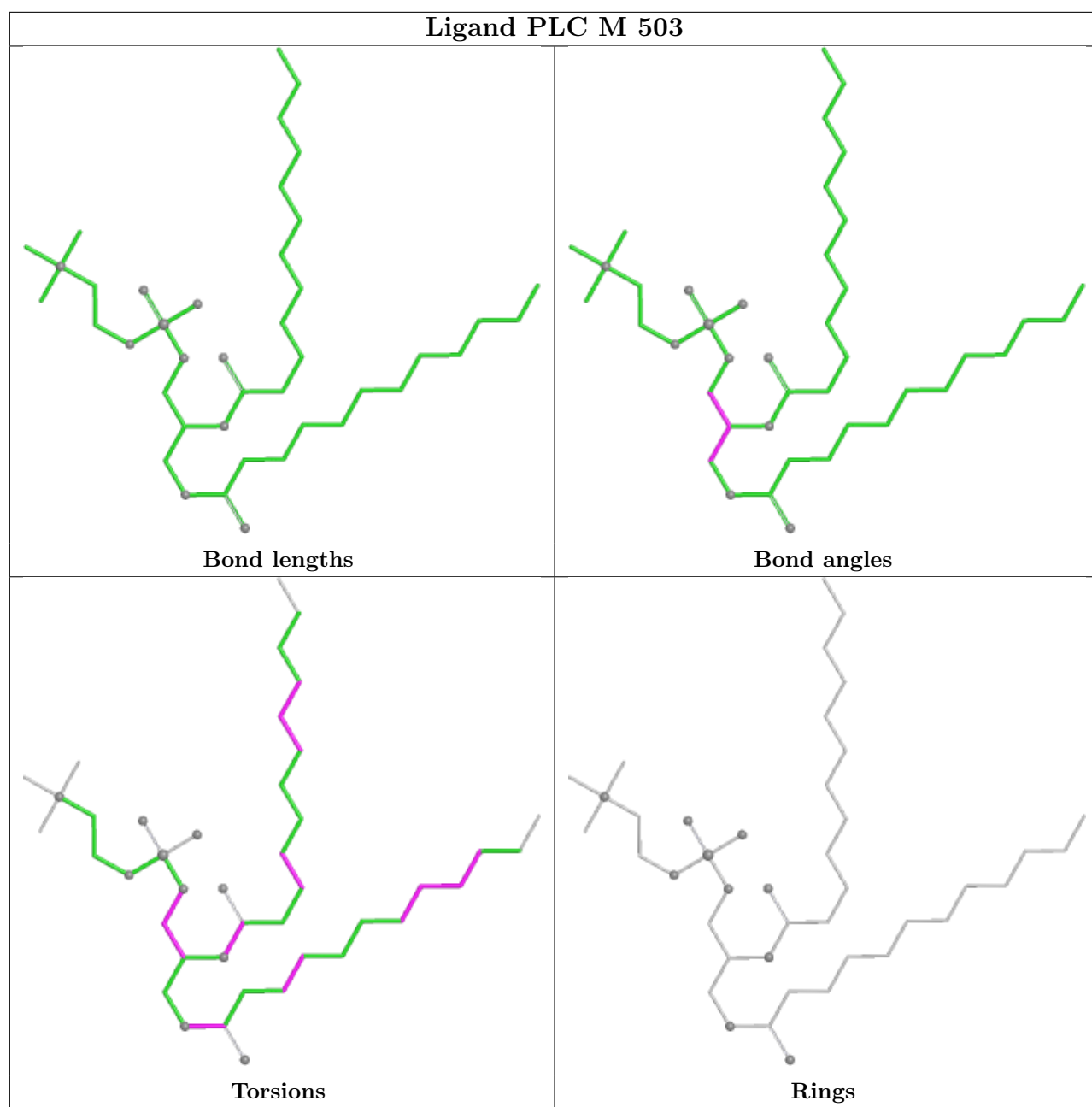


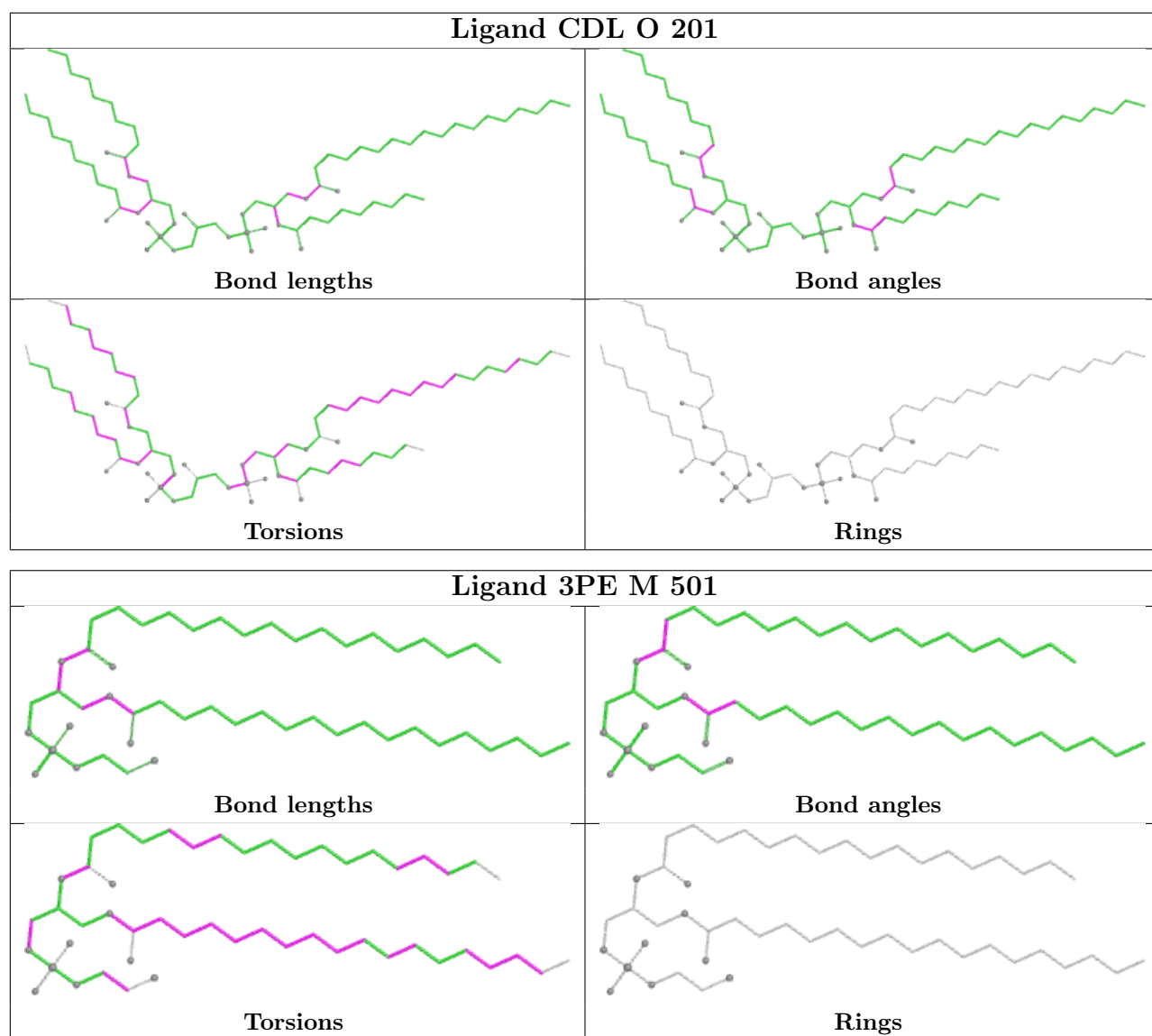


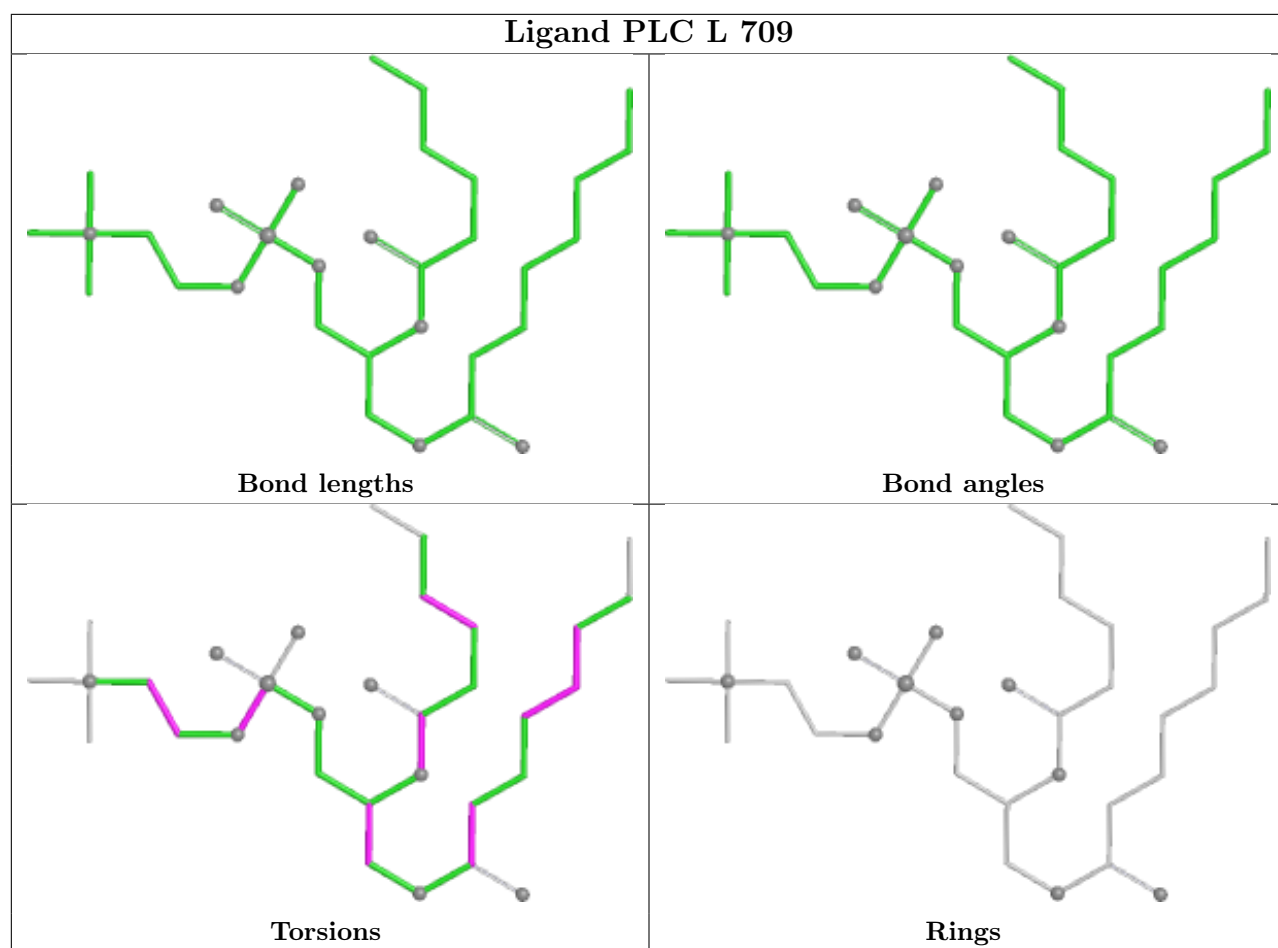


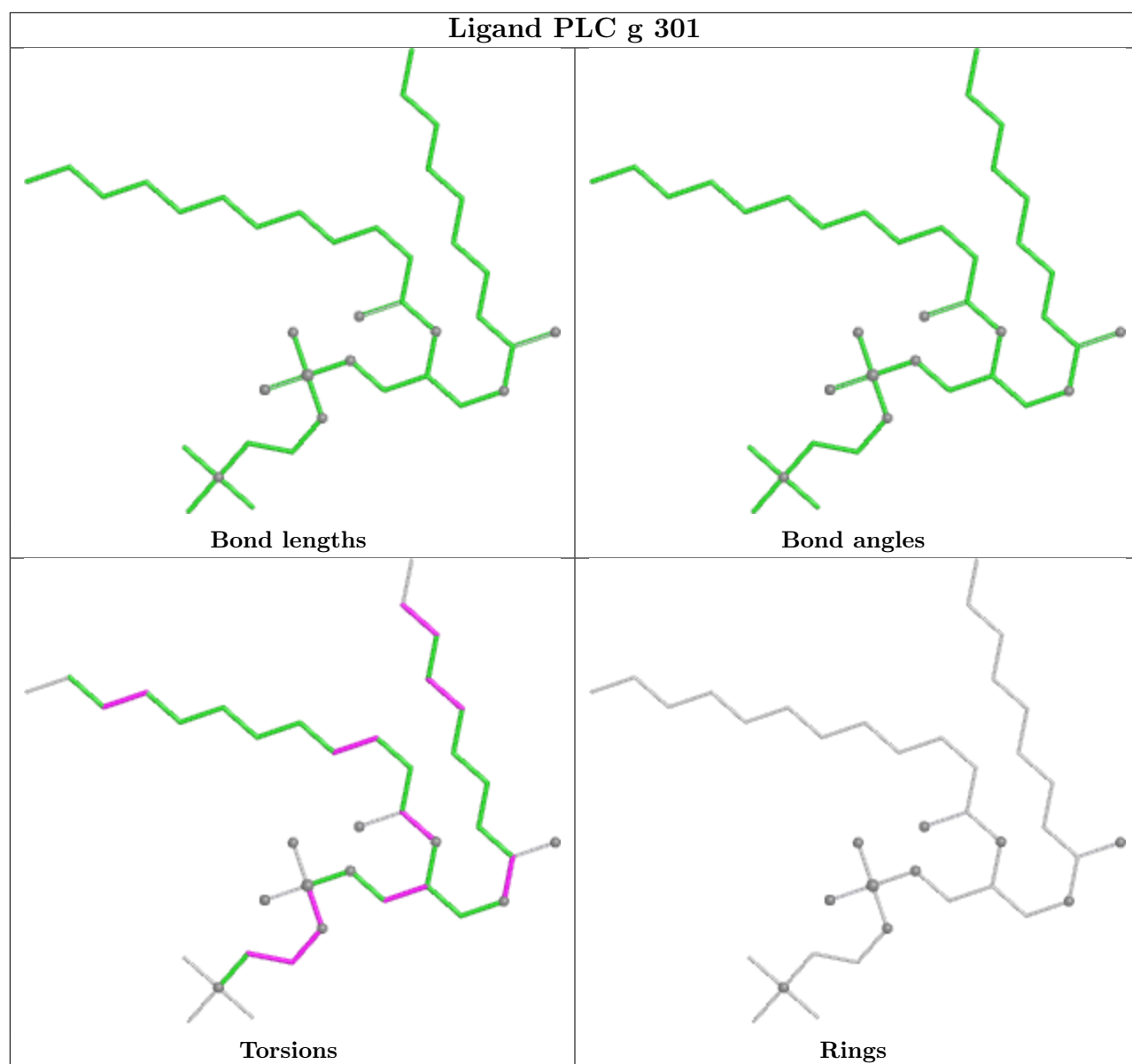


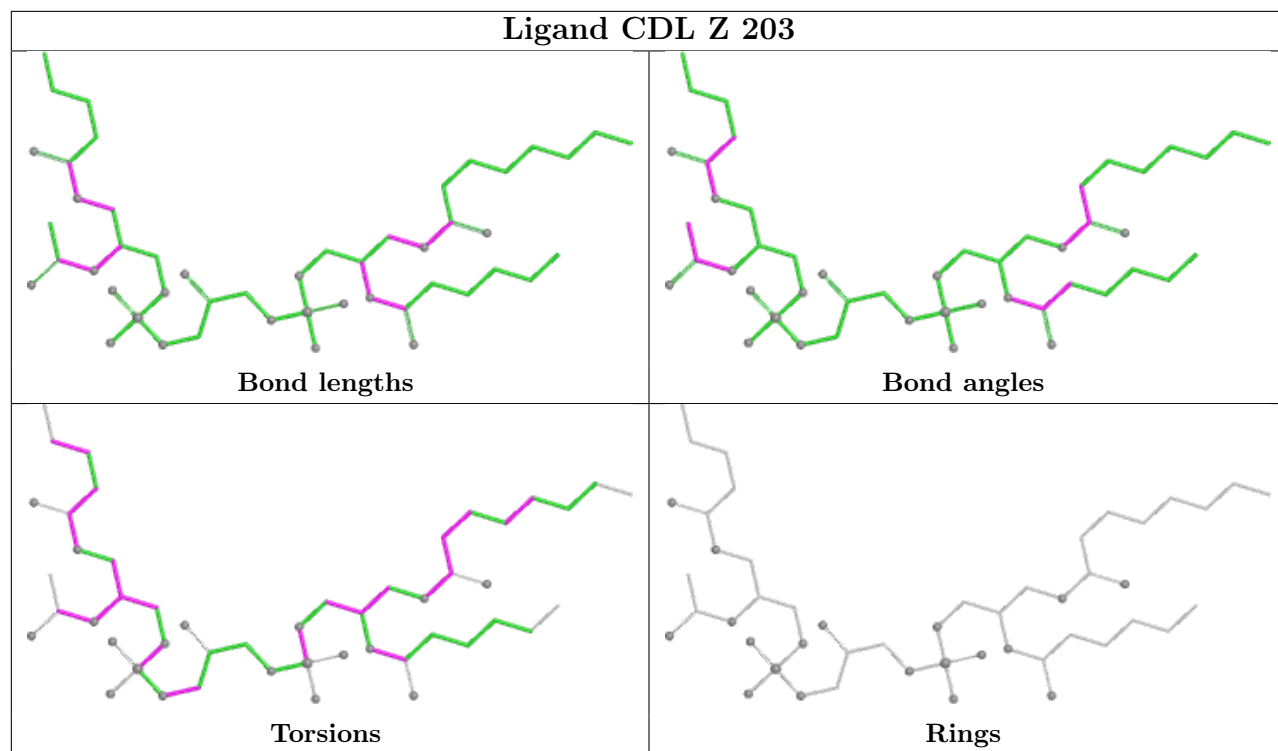


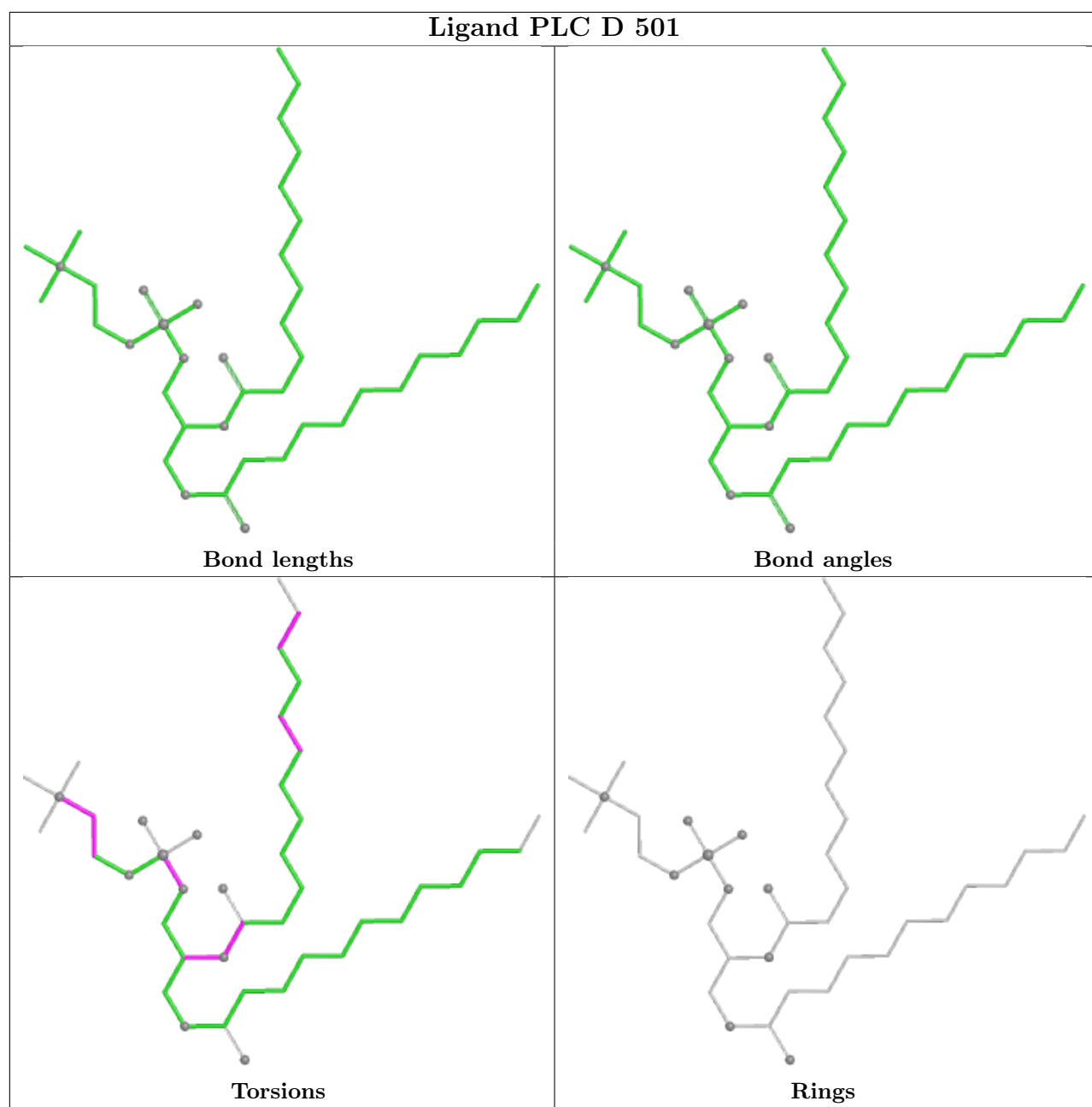


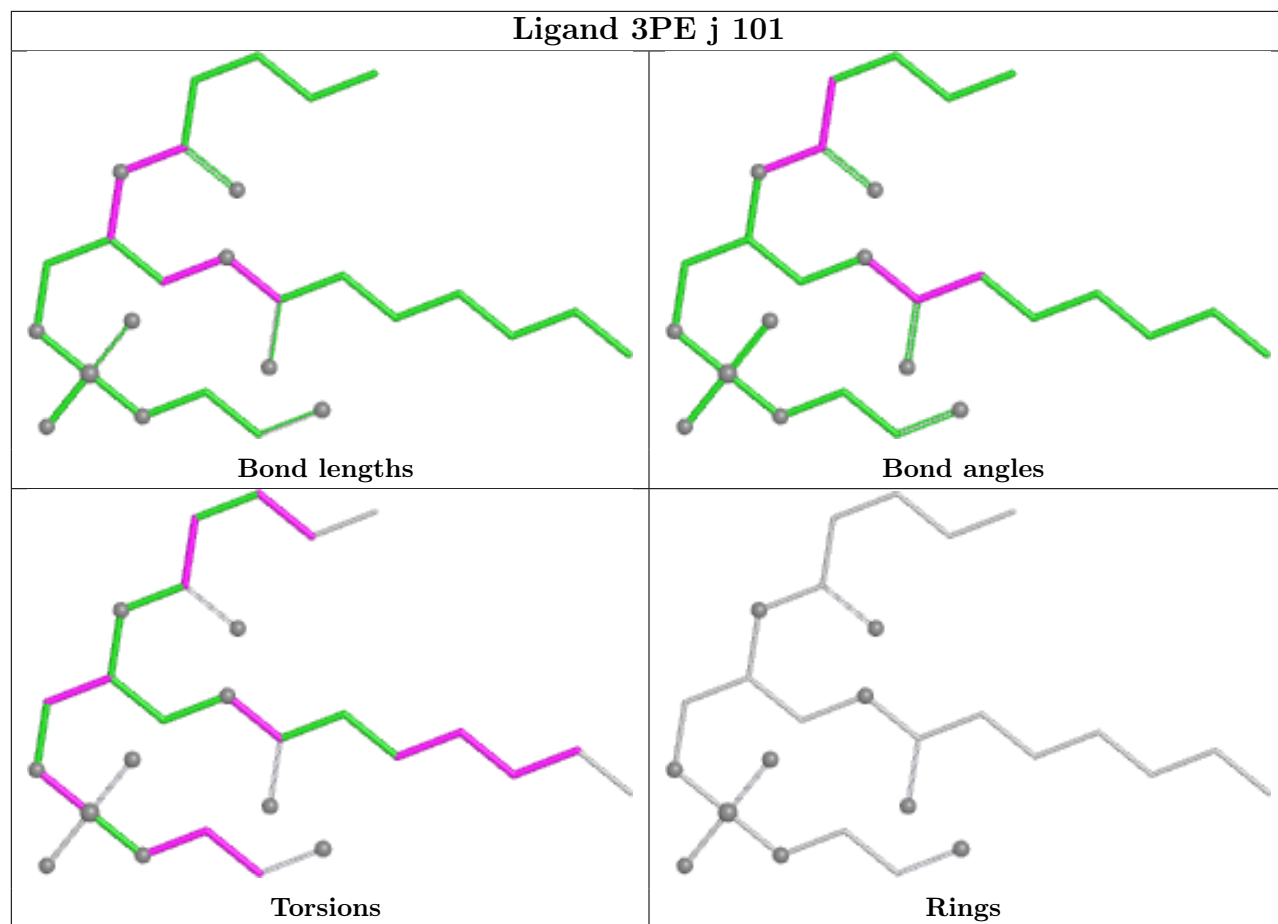


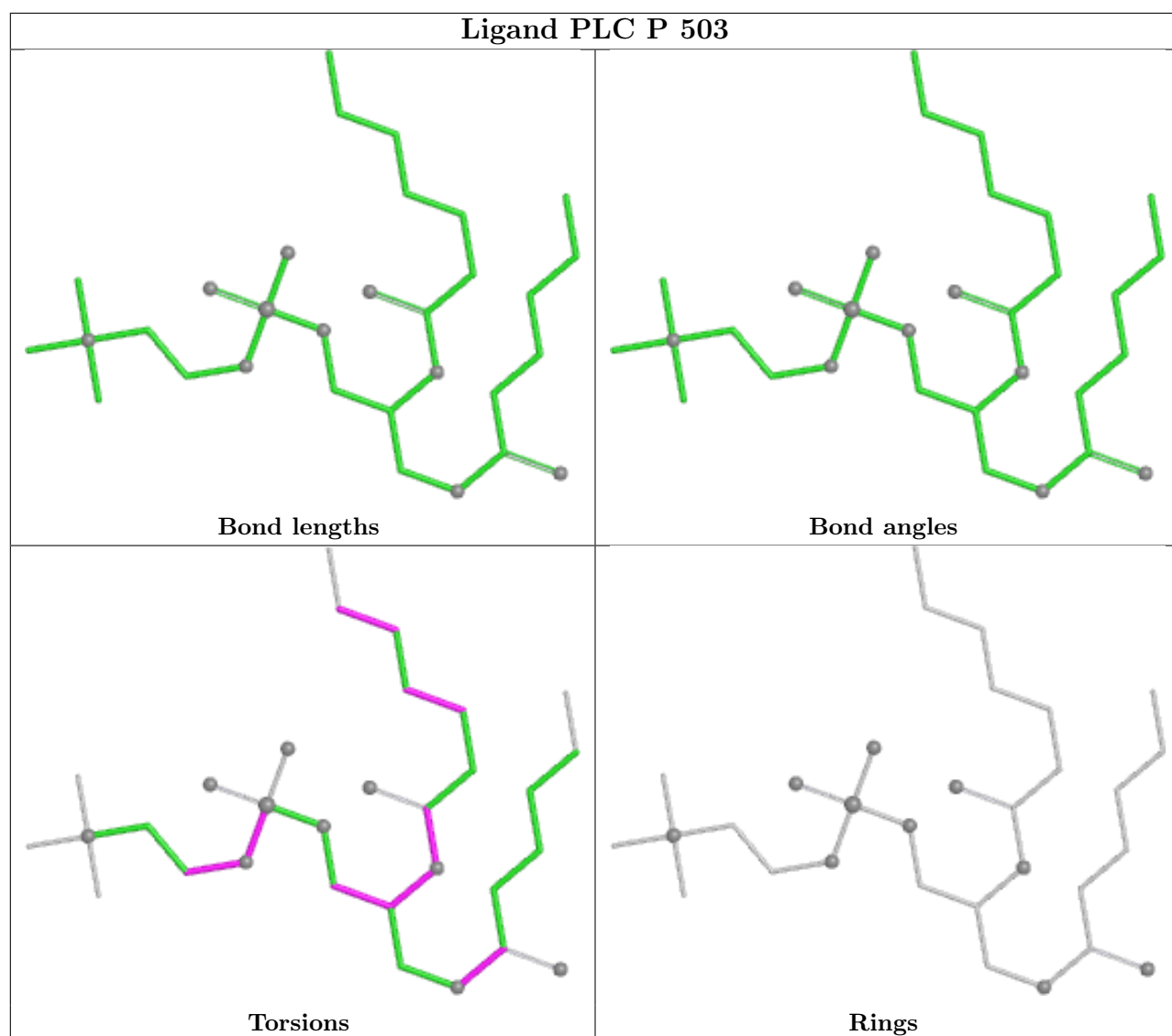


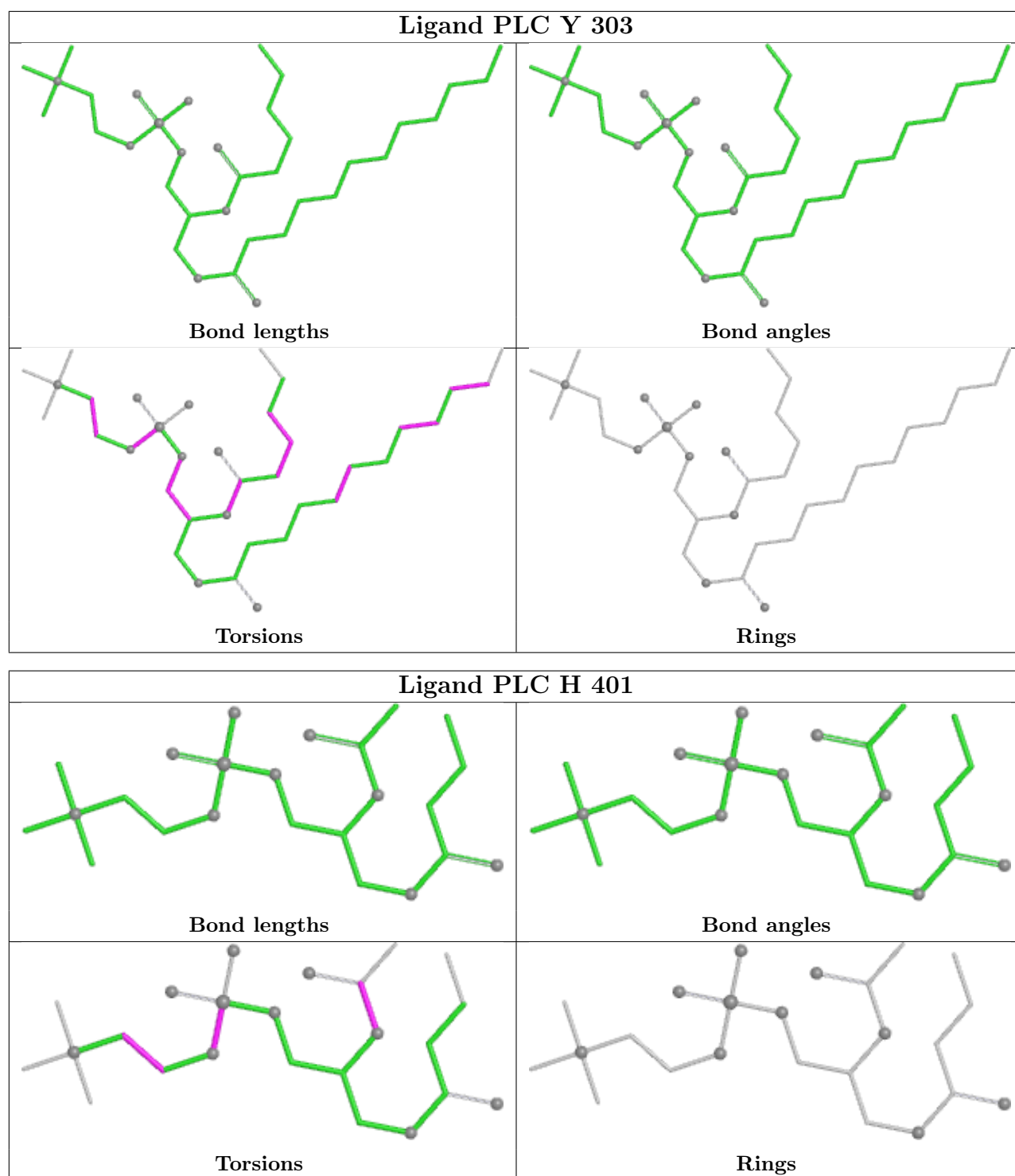












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

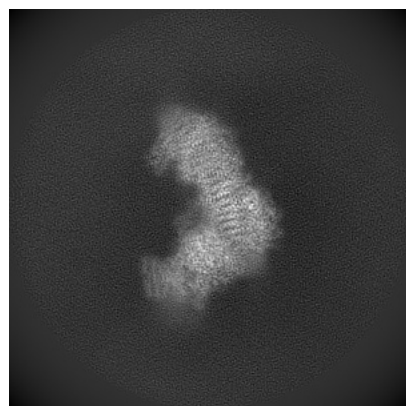
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52875. These allow visual inspection of the internal detail of the map and identification of artifacts.

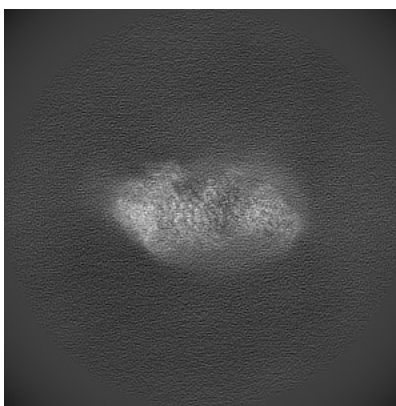
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

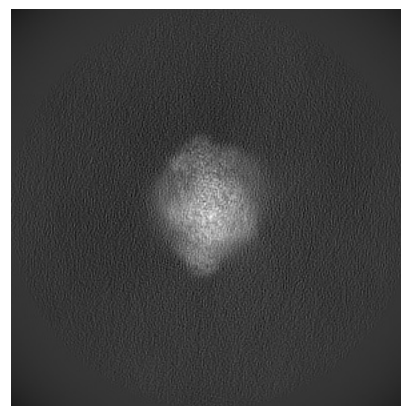
#### 6.1.1 Primary map



X

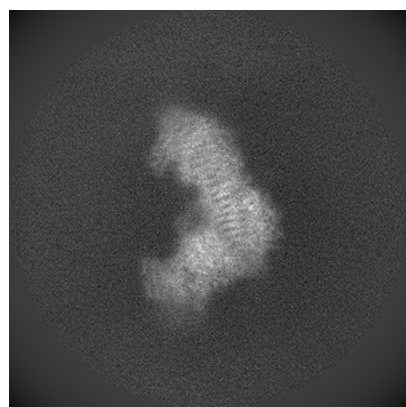


Y

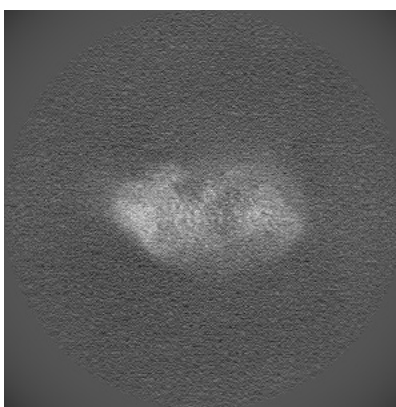


Z

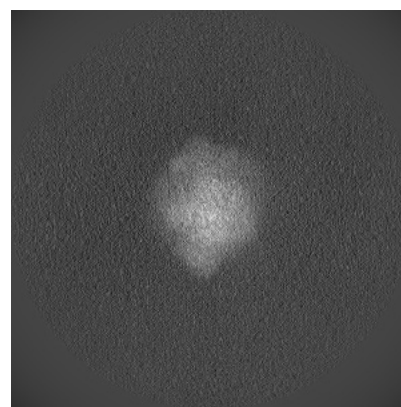
#### 6.1.2 Raw map



X



Y

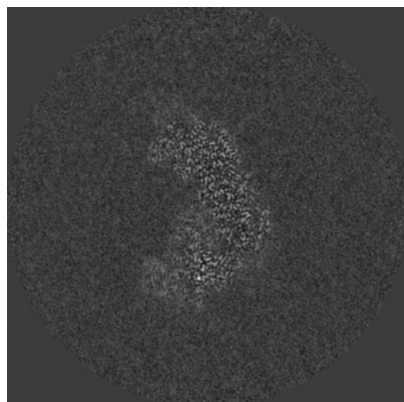


Z

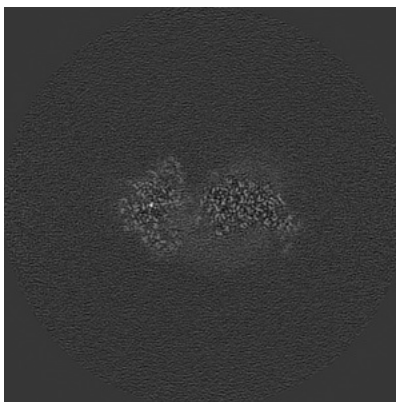
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

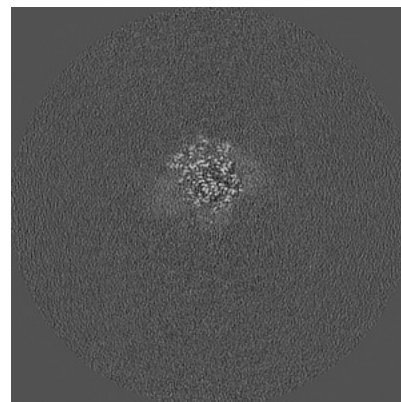
### 6.2.1 Primary map



X Index: 270

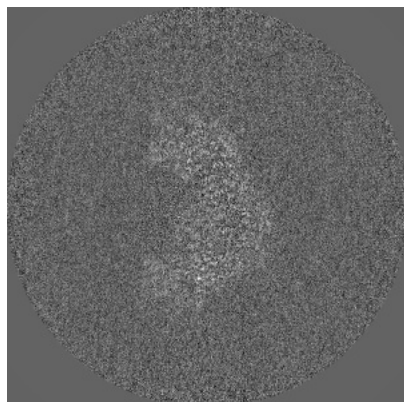


Y Index: 270

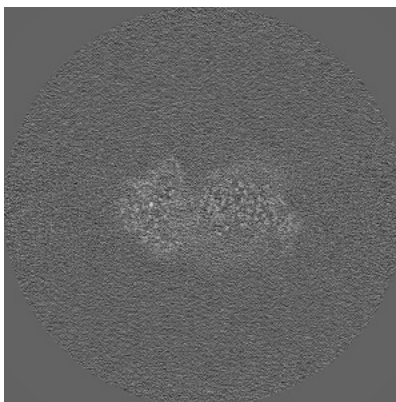


Z Index: 270

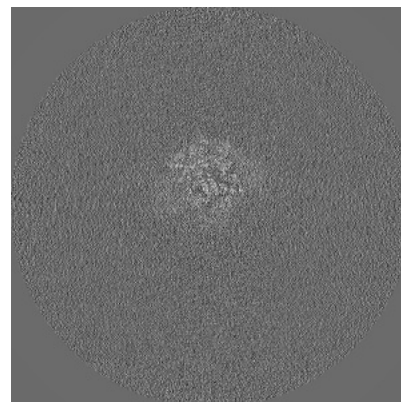
### 6.2.2 Raw map



X Index: 270



Y Index: 270

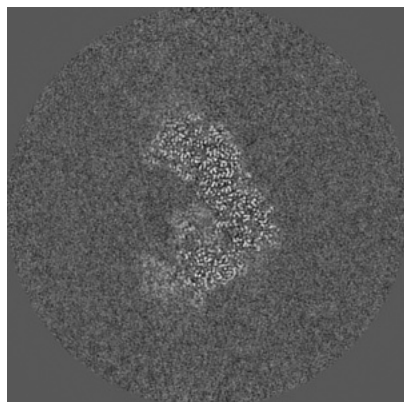


Z Index: 270

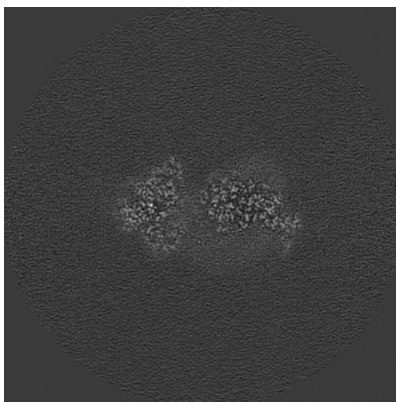
The images above show central slices of the map in three orthogonal directions.

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

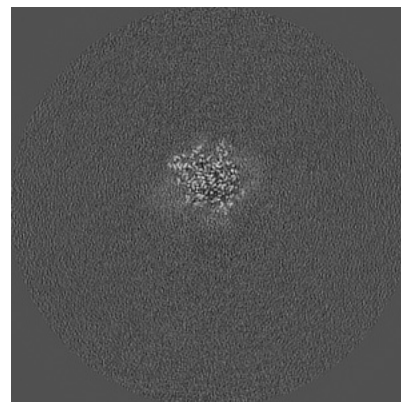
### 6.3.1 Primary map



X Index: 265

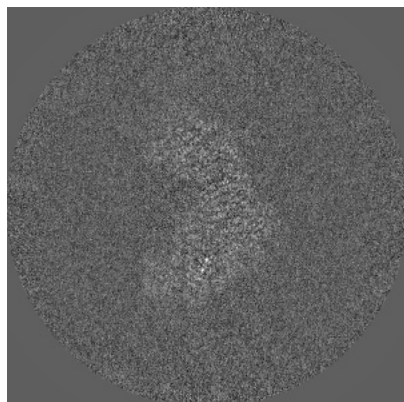


Y Index: 268

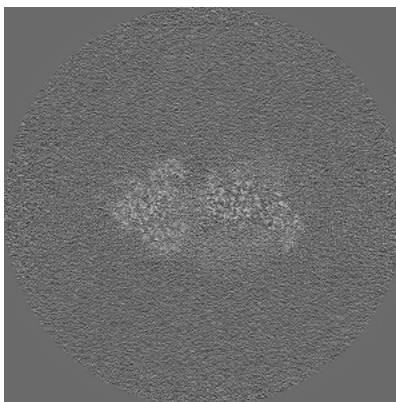


Z Index: 272

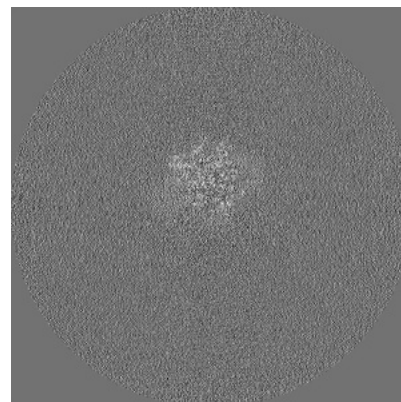
### 6.3.2 Raw map



X Index: 272



Y Index: 266

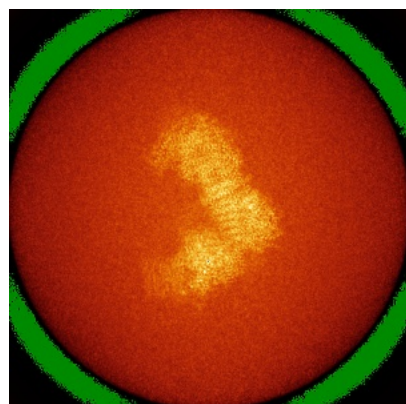


Z Index: 272

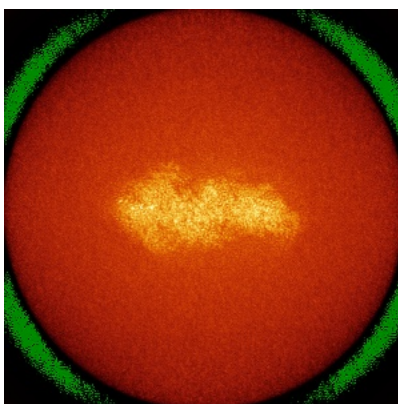
The images above show the largest variance slices of the map in three orthogonal directions.

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

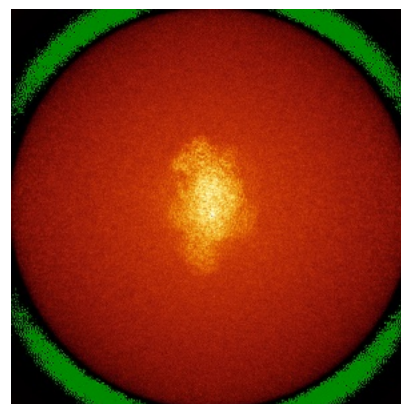
### 6.4.1 Primary map



X

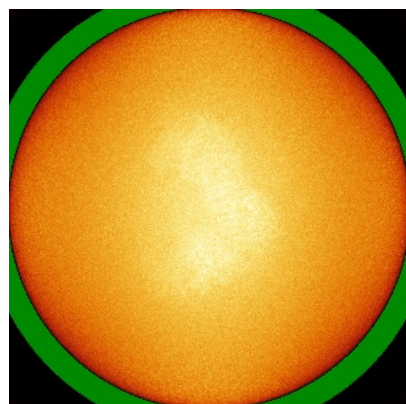


Y

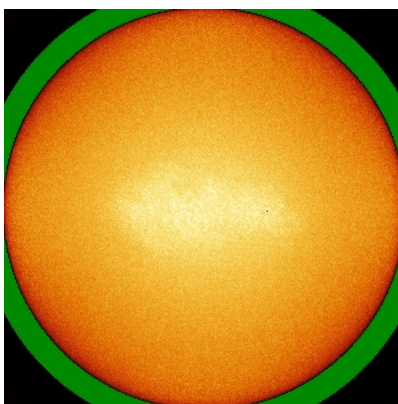


Z

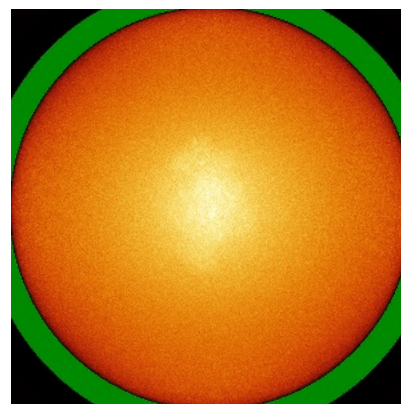
### 6.4.2 Raw map



X



Y

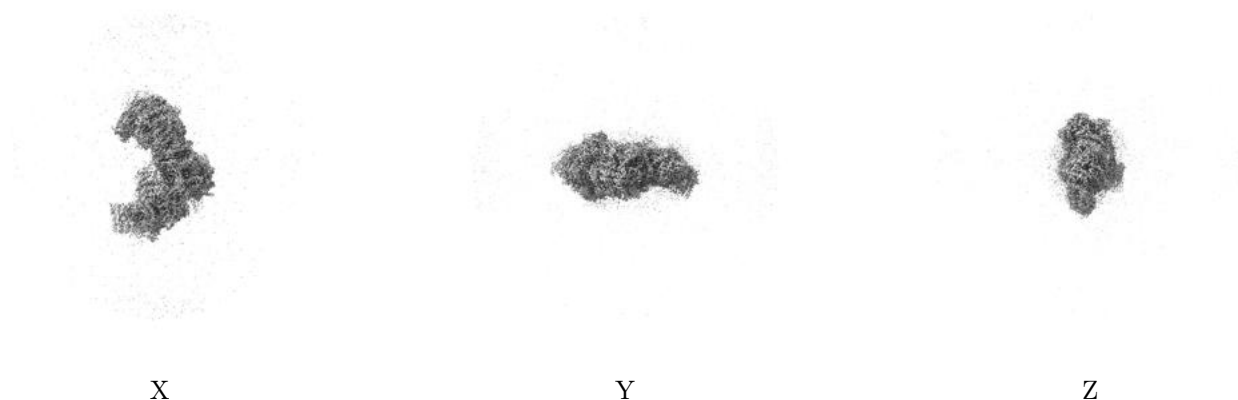


Z

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.

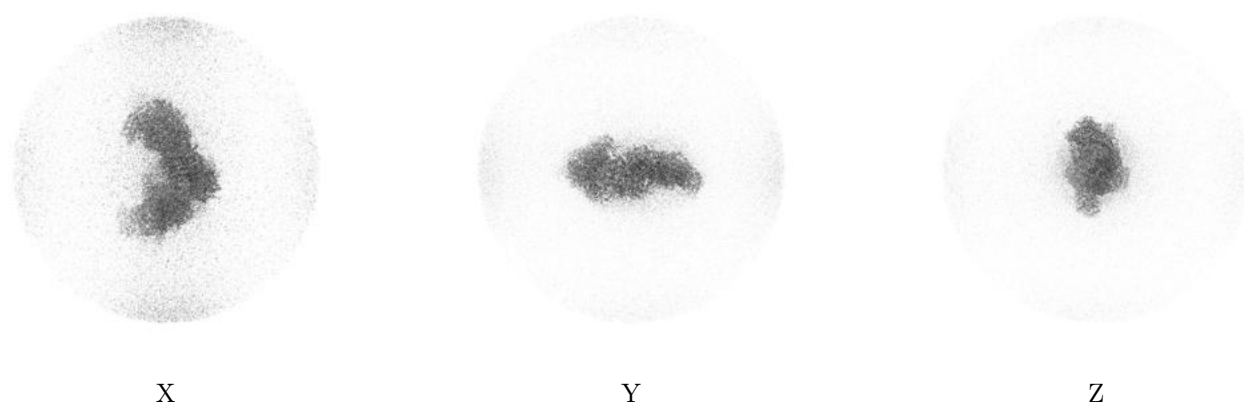
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

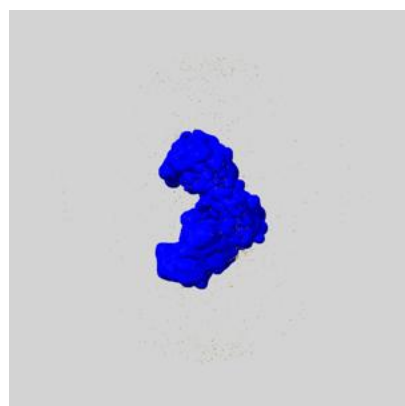
## 6.6 Mask visualisation [i](#)

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

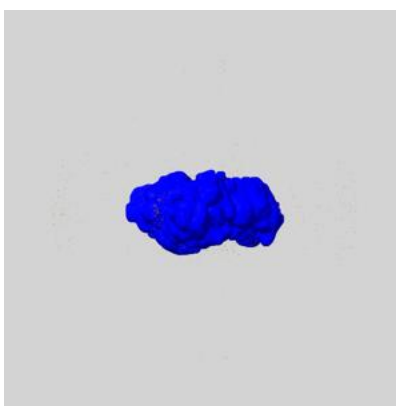
A mask typically either:

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

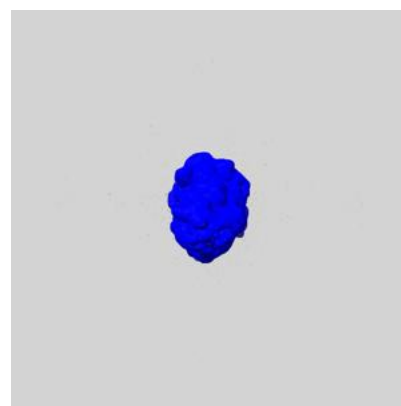
### 6.6.1 emd\_52875\_msk\_1.map [i](#)



X



Y

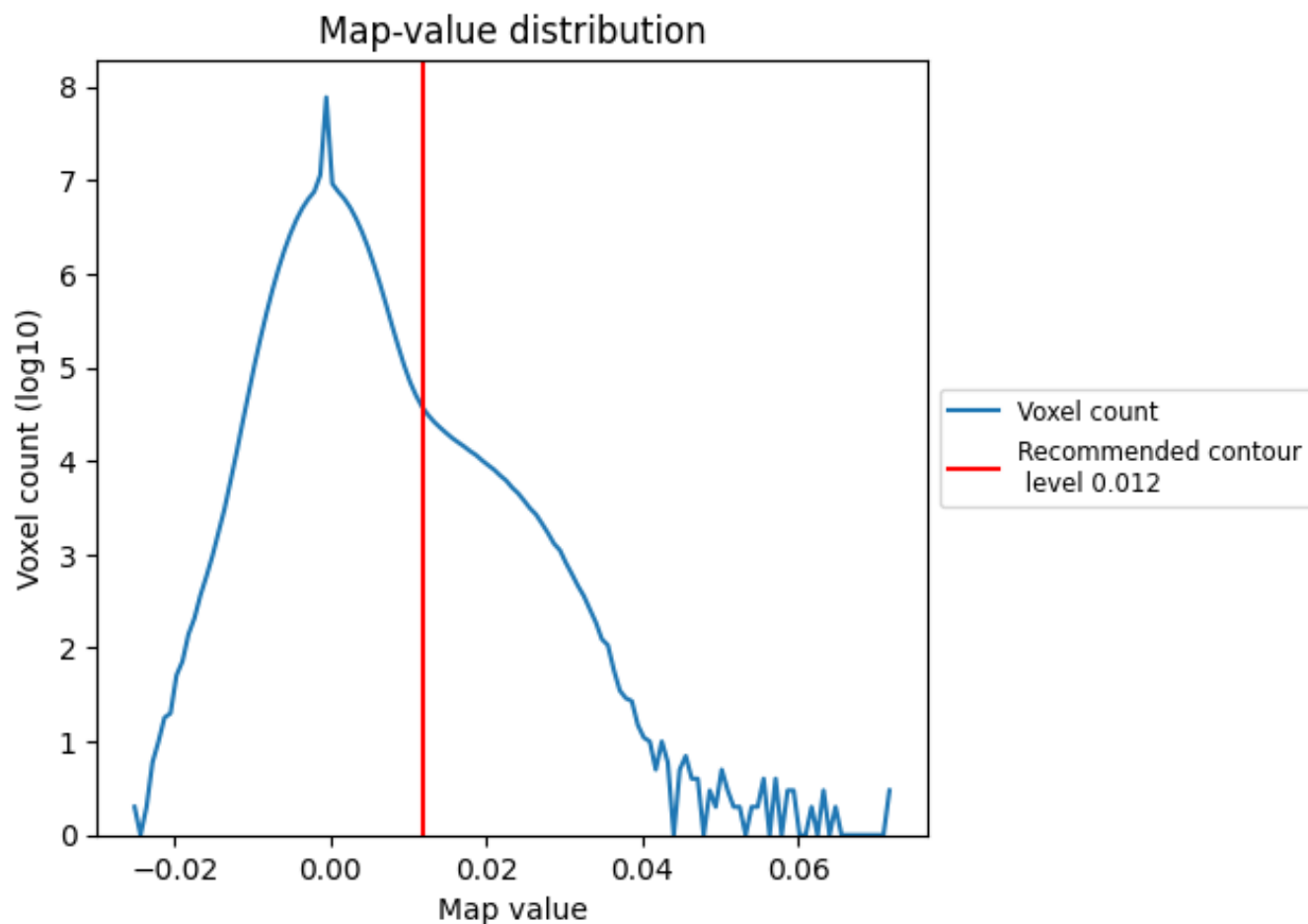


Z

## 7 Map analysis [i](#)

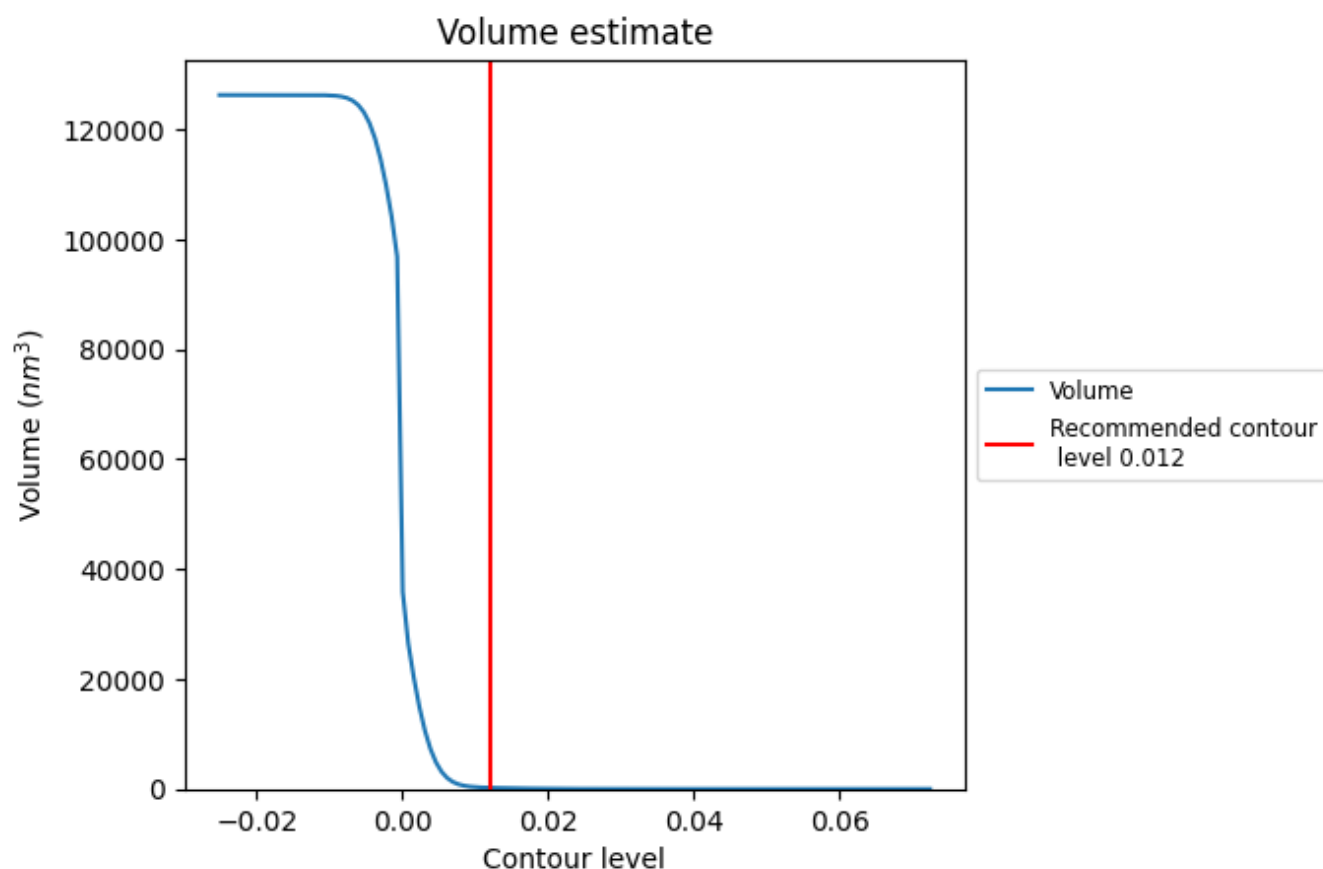
This section contains the results of statistical analysis of the map.

### 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.

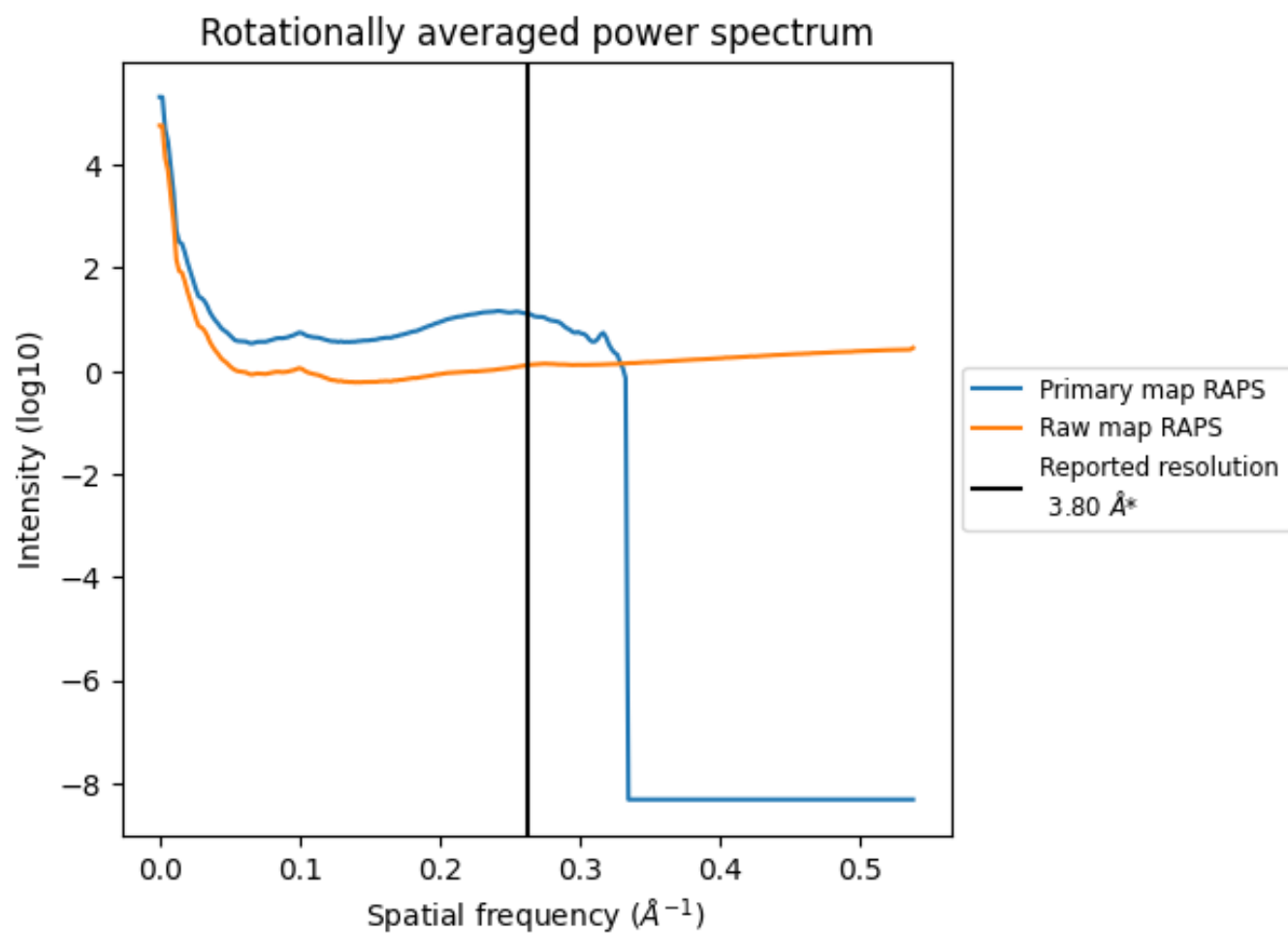
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 214  $\text{nm}^3$ ; this corresponds to an approximate mass of 193 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 ⓘ

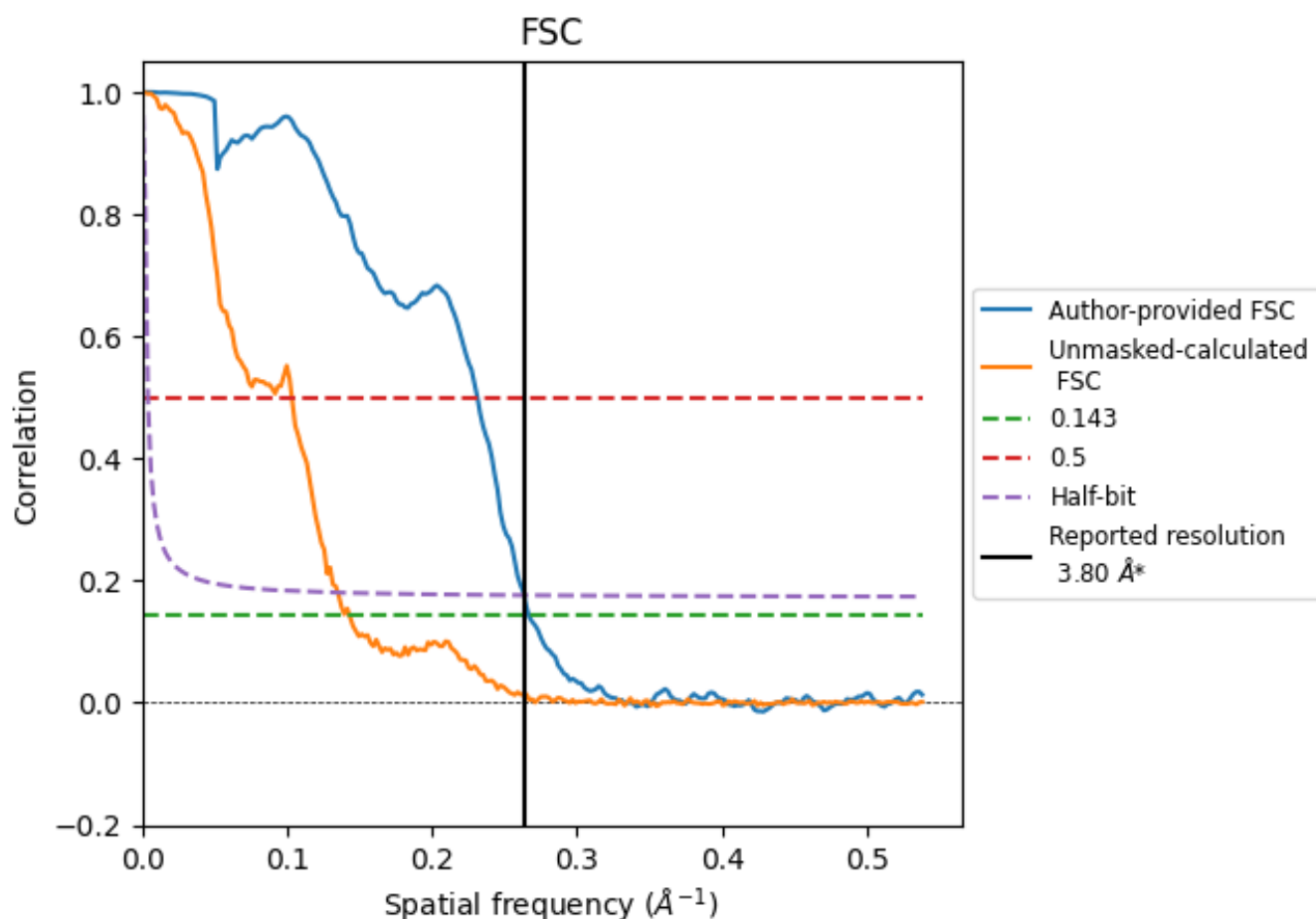


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

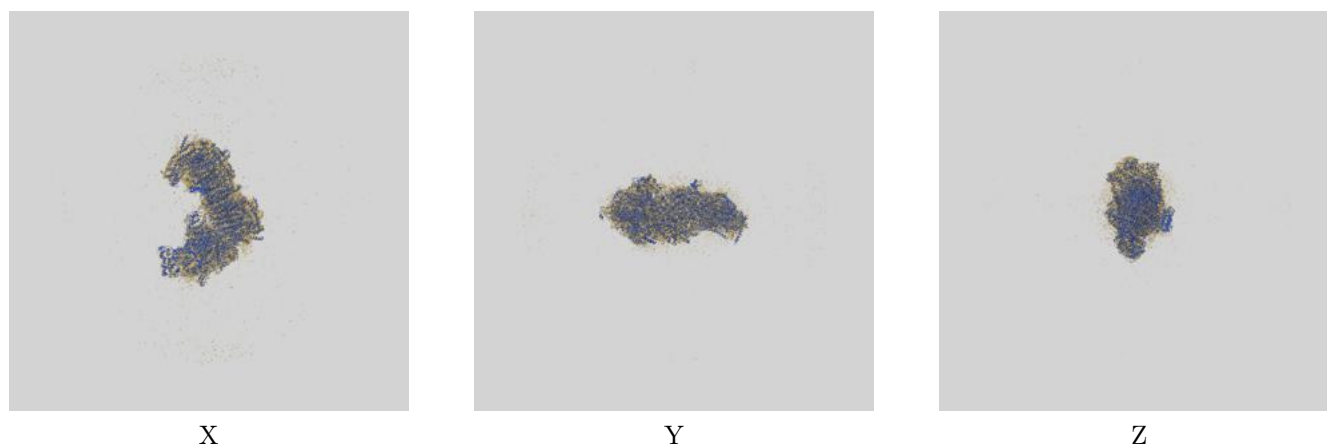
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.80                               | -    | -        |
| Author-provided FSC curve | 3.75                               | 4.32 | 3.79     |
| Unmasked-calculated*      | 6.99                               | 9.69 | 7.41     |

\*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 6.99 differs from the reported value 3.8 by more than 10 %

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

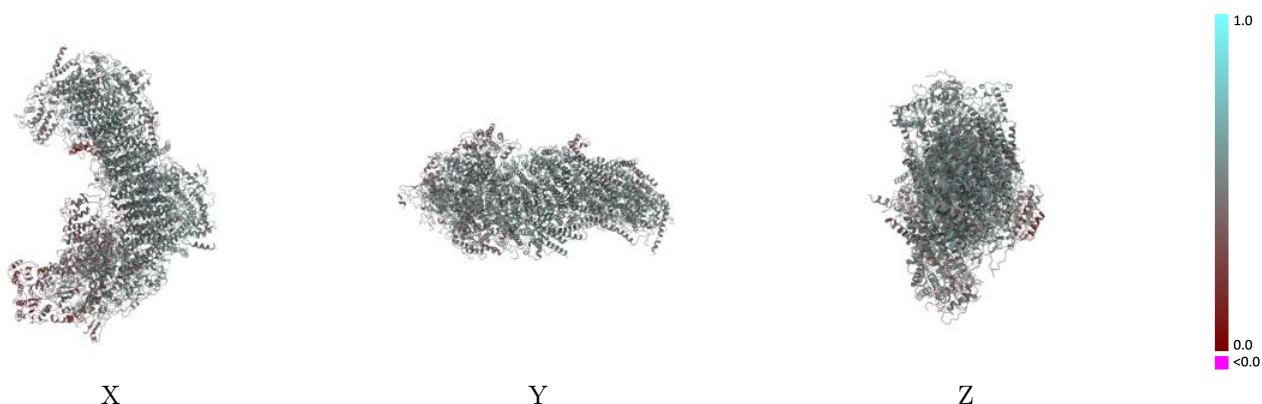
This section contains information regarding the fit between EMDB map EMD-52875 and PDB model 9IHO. Per-residue inclusion information can be found in section [3](#) on page [18](#).

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



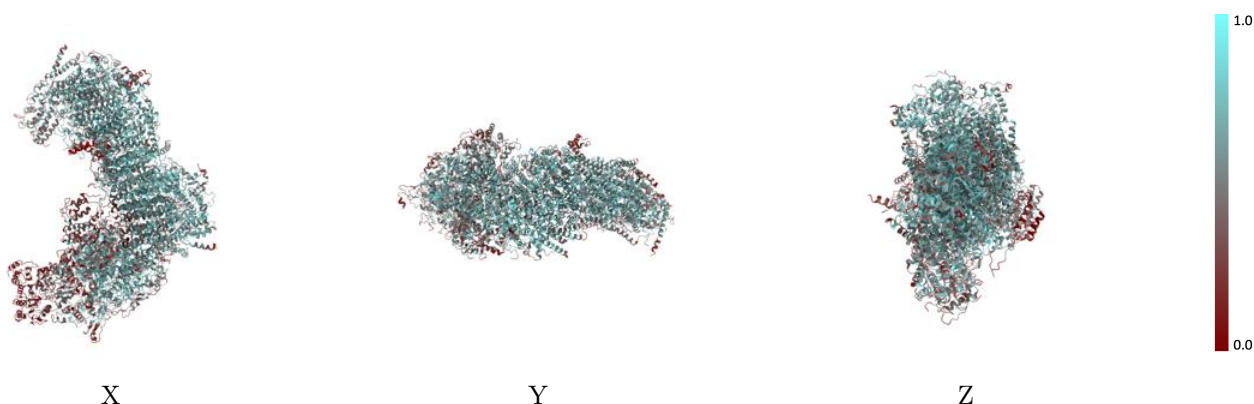
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



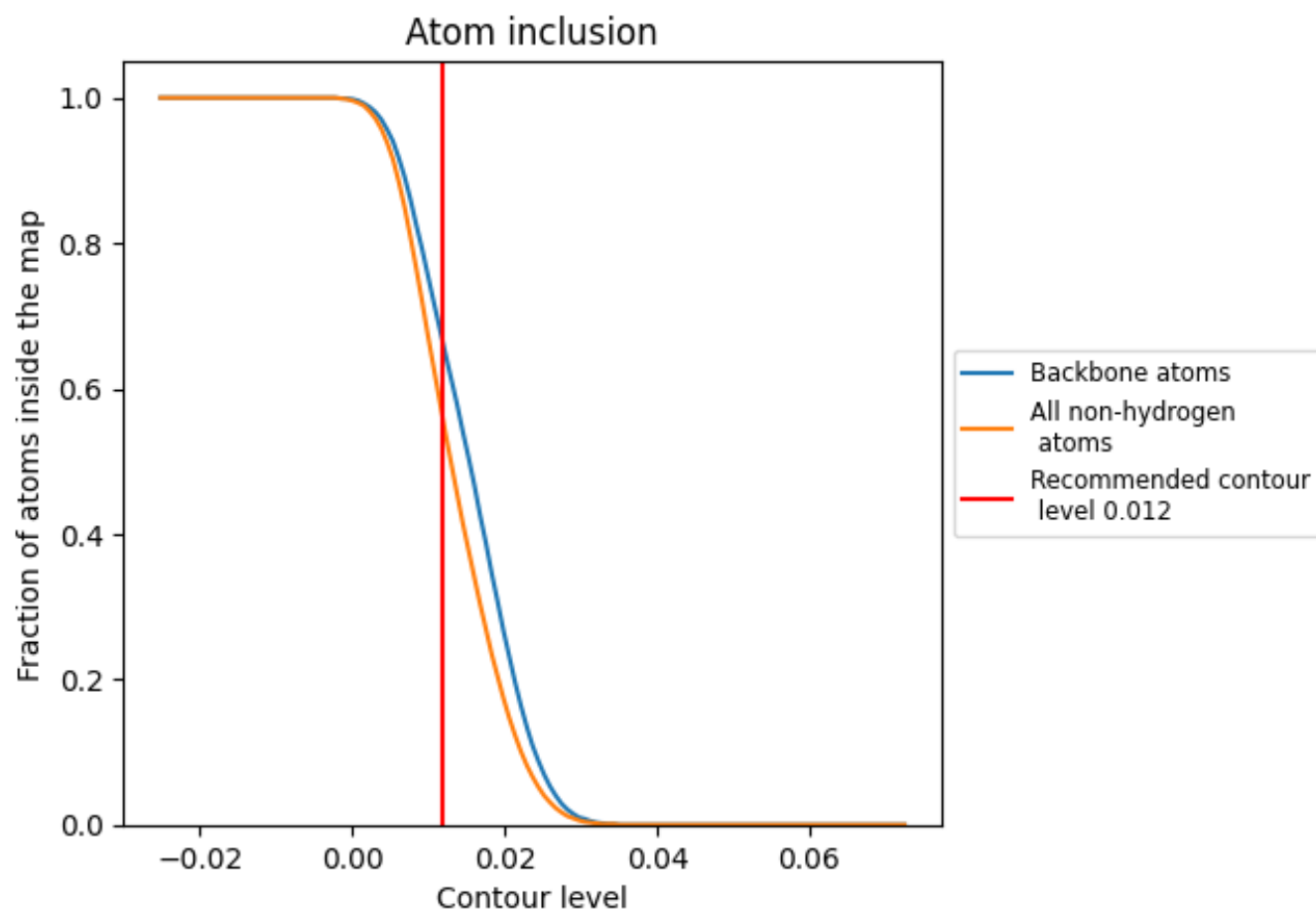
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 55% 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 (0.012) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5530   |  0.4970   |
| A     |  0.5050   |  0.4810   |
| B     |  0.6360   |  0.5220   |
| C     |  0.5140   |  0.4760   |
| D     |  0.6090   |  0.5090   |
| G     |  0.3130   |  0.3940   |
| H     |  0.6080   |  0.5200   |
| I     |  0.6780   |  0.5200   |
| J     |  0.5810   |  0.5190   |
| K     |  0.6090   |  0.5170   |
| L     |  0.6450   |  0.5340   |
| M     |  0.6850   |  0.5440   |
| N     |  0.6820   |  0.5390   |
| O     |  0.6340   |  0.5300   |
| P     |  0.4470  |  0.4570  |
| Q     |  0.4990 |  0.4730 |
| R     |  0.4520 |  0.4550 |
| S     |  0.0730 |  0.2890 |
| T     |  0.2010 |  0.4000 |
| U     |  0.4210 |  0.4660 |
| V     |  0.3970 |  0.4430 |
| W     |  0.4290 |  0.4440 |
| X     |  0.6430 |  0.5280 |
| Y     |  0.5930 |  0.5210 |
| Z     |  0.6120 |  0.5280 |
| a     |  0.6460 |  0.5350 |
| b     |  0.5810 |  0.5420 |
| c     |  0.3660 |  0.4530 |
| d     |  0.6640 |  0.5300 |
| e     |  0.6730 |  0.5310 |
| f     |  0.5800 |  0.5090 |
| g     |  0.3390 |  0.4460 |
| h     |  0.5840 |  0.5150 |
| i     |  0.5470 |  0.5010 |
| j     |  0.4880 |  0.4820 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| k     |  0.4960 |  0.4790 |
| l     |  0.5510 |  0.4960 |
| m     |  0.5690 |  0.5140 |
| n     |  0.5270 |  0.4890 |
| o     |  0.5380 |  0.4900 |
| p     |  0.6900 |  0.5330 |
| q     |  0.5500 |  0.5060 |