



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:18 AM JST

PDB ID : 7W2Y / pdb\_00007w2y  
EMDB ID : EMD-32267  
Title : Active state CI from DQ-NADH dataset, Subclass 3  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-11-24  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

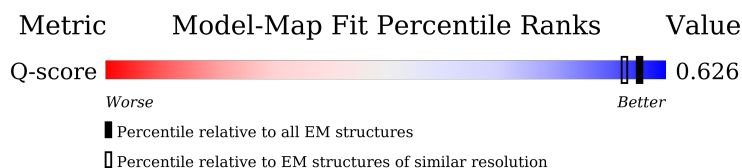
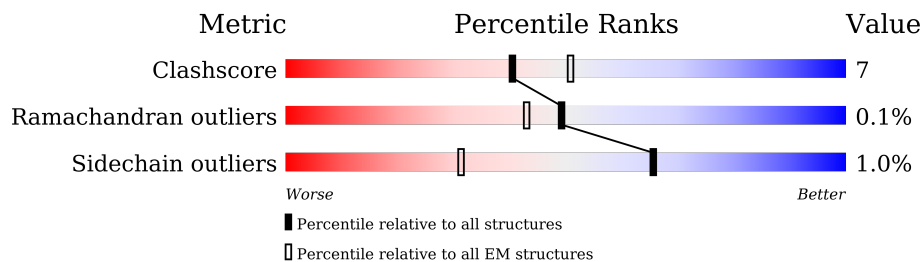
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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                       | 10327 ( 2.20 - 3.20 )                                    |

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     | 433    |                  |
| 2   | B     | 176    |                  |
| 3   | C     | 156    |                  |
| 4   | E     | 115    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | F     | 86     |                  |
| 6   | G     | 88     |                  |
| 6   | X     | 88     |                  |
| 7   | H     | 112    |                  |
| 8   | I     | 112    |                  |
| 9   | J     | 342    |                  |
| 10  | K     | 43     |                  |
| 11  | L     | 125    |                  |
| 12  | M     | 690    |                  |
| 13  | N     | 144    |                  |
| 14  | O     | 217    |                  |
| 15  | P     | 208    |                  |
| 16  | Q     | 430    |                  |
| 17  | S     | 70     |                  |
| 18  | T     | 96     |                  |
| 19  | U     | 83     |                  |
| 20  | V     | 140    |                  |
| 21  | W     | 142    |                  |
| 22  | Y     | 67     |                  |
| 23  | Z     | 80     |                  |
| 24  | a     | 138    |                  |
| 25  | b     | 126    |                  |
| 26  | c     | 156    |                  |
| 27  | d     | 175    |                  |
| 28  | e     | 104    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | f     | 49     |                  |
| 30  | g     | 122    |                  |
| 31  | h     | 105    |                  |
| 32  | i     | 347    |                  |
| 33  | j     | 115    |                  |
| 34  | k     | 98     |                  |
| 35  | l     | 606    |                  |
| 36  | m     | 175    |                  |
| 37  | n     | 56     |                  |
| 38  | o     | 128    |                  |
| 39  | p     | 178    |                  |
| 40  | r     | 459    |                  |
| 41  | s     | 318    |                  |
| 42  | u     | 171    |                  |
| 43  | v     | 125    |                  |
| 44  | w     | 320    |                  |

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 433      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3330  | 2103 | 593 | 614 | 20 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B     | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1412  | 887 | 243 | 269 | 13 |         |       |

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | C     | 156      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1248  | 794 | 227 | 213 | 14 |         |       |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | E     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 619 | 179 | 168 | 5 |         |       |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | F     | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 432 | 129 | 124 | 2 |         |       |

- Molecule 6 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | G     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 690   | 446 | 102 | 137 | 5 |         |       |
| 6   | X     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 447 | 103 | 138 | 5 |         |       |

- Molecule 7 is a protein called Complex I subunit B13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 910   | 588 | 154 | 165 | 3 |         |       |

- Molecule 8 is a protein called Complex I-B14.5a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | I     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 491 | 147 | 139 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | J     | 342      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2748  | 1782 | 481 | 476 | 9 |         |       |

- Molecule 10 is a protein called Complex I-9kD.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | K     | 43       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 366   | 228 | 68 | 69 | 1 |         |       |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | L     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 642 | 181 | 190 | 3 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 12  | M     | 690      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5296  | 3320 | 923 | 1014 | 39 |         |       |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | N     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1204  | 770 | 218 | 212 | 4 |         |       |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | O     | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1671  | 1065 | 281 | 315 | 10 |         |       |

- Molecule 15 is a protein called Complex I-30kD.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | P     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1738  | 1124 | 298 | 314 | 2 |         |       |

- Molecule 16 is a protein called Complex I-49kD.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | Q     | 430      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3459  | 2212 | 594 | 629 | 24 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 17  | S     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 566   | 364 | 103 | 94 | 5 |         |       |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 741   | 452 | 140 | 146 | 3 |         |       |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | U     | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 417 | 110 | 115 | 1 |         |       |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | V     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1021  | 651 | 174 | 190 | 6 |         |       |

- Molecule 21 is a protein called Complex I-B16.6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1161  | 749 | 197 | 206 | 9 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 22  | Y     | 67       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 584   | 385 | 95 | 103 | 1 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Z     | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 641   | 418 | 108 | 114 | 1 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | a     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1151  | 754 | 195 | 199 | 3 |         |       |

- Molecule 25 is a protein called Complex I-B17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | b     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 819   | 537 | 144 | 137 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | c     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 853 | 213 | 241 | 8 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | d     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1461  | 916 | 265 | 272 | 8 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | e     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 553 | 142 | 168 | 4 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 29  | f     | 49       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 378   | 246 | 65 | 67 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | g     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1005  | 653 | 174 | 172 | 6 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | h     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 550 | 161 | 150 | 6 |         |       |

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32  | i     | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2710  | 1782 | 420 | 462 | 46 |         |       |

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | j     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 914   | 615 | 134 | 158 | 7 |         |       |

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 34  | k     | 98       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 748   | 493 | 113 | 128 | 14 |         |       |

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 35  | l     | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4800  | 3182 | 744 | 823 | 51 |         |       |

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 36  | m     | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1277  | 852 | 187 | 225 | 13 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37  | n     | 56       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 479   | 311 | 88 | 79 | 1 |         |       |

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 38  | o     | 128      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1062  | 691 | 182 | 189 |  |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | p     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1534  | 982 | 279 | 265 | 8 |         |       |

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 40  | r     | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3631  | 2412 | 572 | 609 | 38 |         |       |

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41  | s     | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2508  | 1678 | 385 | 424 | 21 |         |       |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 42  | u     | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1398  | 887 | 250 | 251 | 10 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | v     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1028  | 642 | 195 | 182 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| v     | 1       | MYR      | -      | acetylation | UNP F1SCH1 |

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

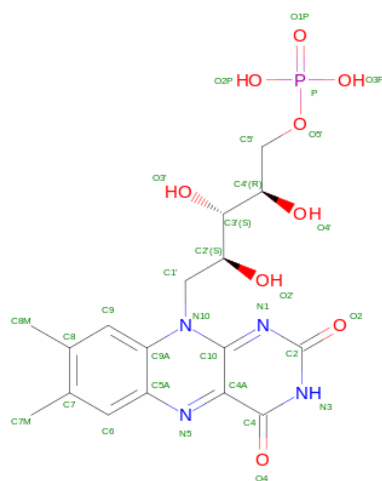
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | w     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2582  | 1643 | 438 | 491 | 10 |         |       |

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



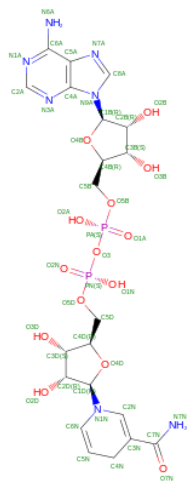
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $C_{17}H_{21}N_4O_9P$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula:  $C_{21}H_{29}N_7O_{14}P_2$ ) (labeled as "Ligand of Interest" by depositor).



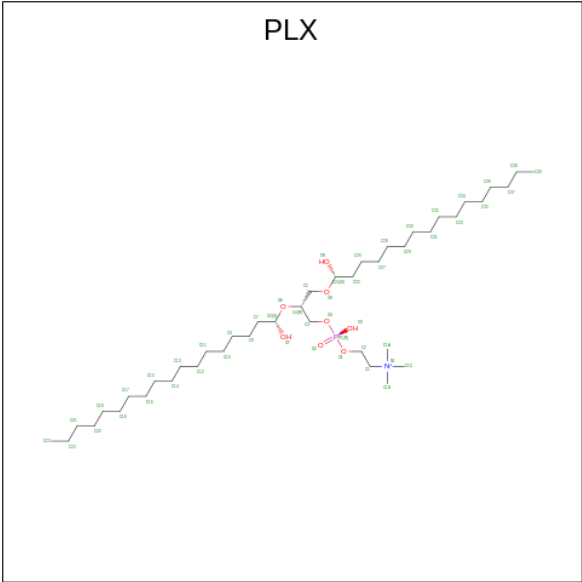
| Mol | Chain | Residues | Atoms       |         |        |         |        | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 47  | A     | 1        | Total<br>44 | C<br>21 | N<br>7 | O<br>14 | P<br>2 | 0       |

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



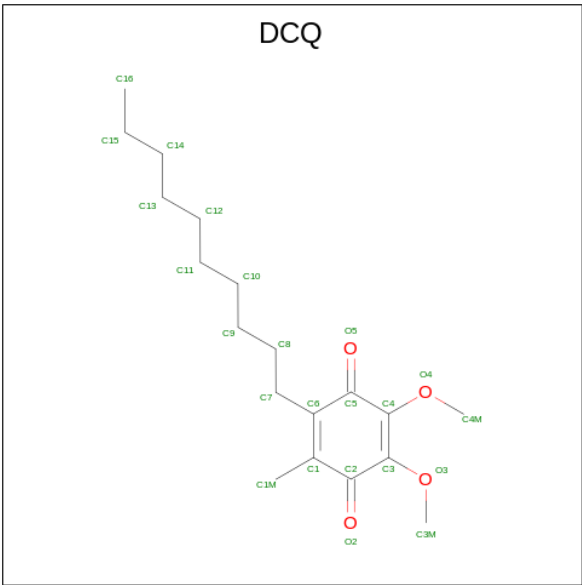
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | B     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 48  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | V     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 40    | 30 | 1 | 8 | 1 |         |
| 48  | W     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 48  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 48  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 1 | 8 | 1 |         |
| 48  | l     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 48  | l     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 48  | r     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |

- Molecule 49 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY]METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



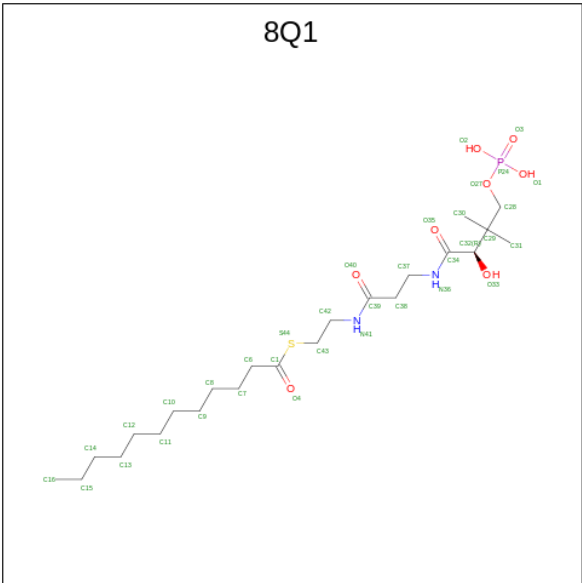
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 49  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | a     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | e     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | g     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | j     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | r     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

- Molecule 50 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C<sub>19</sub>H<sub>30</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



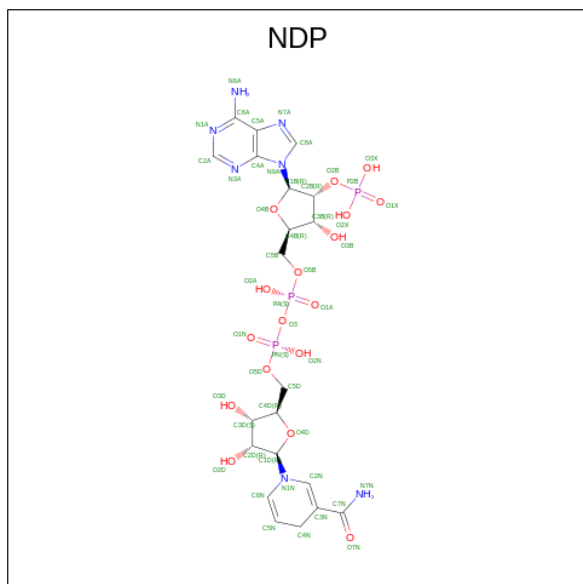
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 50  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 23    | 19 | 4 |         |

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-a  
lanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>2</sub>O<sub>8</sub>PS) (labeled as  
"Ligand of Interest" by depositor).



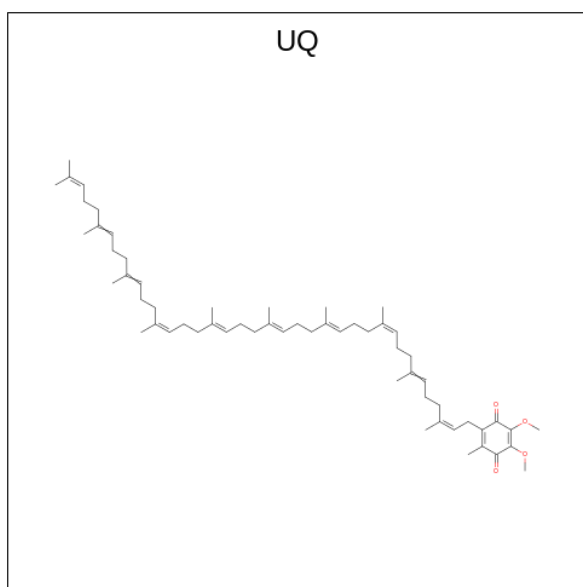
| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 51  | G     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 35    | 23 | 2 | 8 | 1 | 1 |         |
| 51  | X     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 35    | 23 | 2 | 8 | 1 | 1 |         |

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



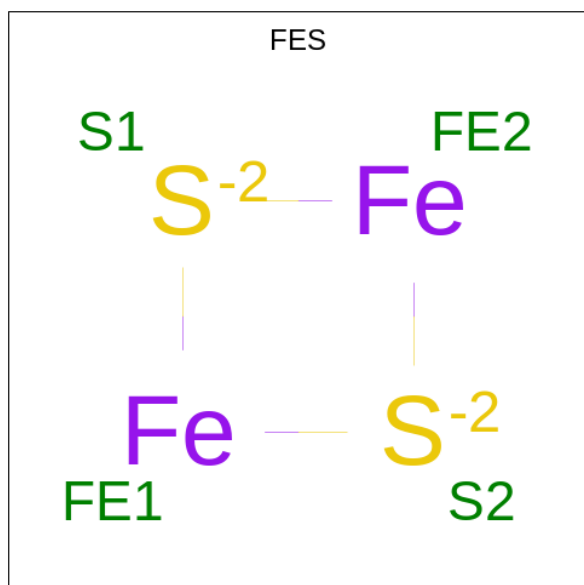
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 52  | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 53 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula:  $C_{59}H_{90}O_4$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 53  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 29 | 4 |         |
| 53  | s     | 1        | Total | C  | O | 0       |
|     |       |          | 38    | 34 | 4 |         |

- Molecule 54 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

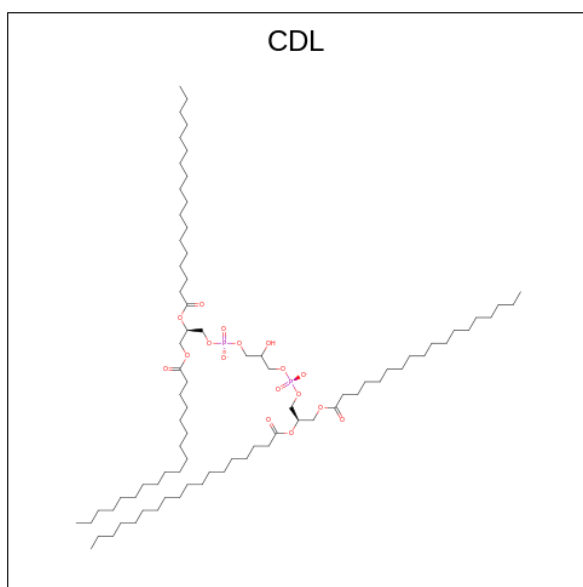


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 54  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 54  | O     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 56 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

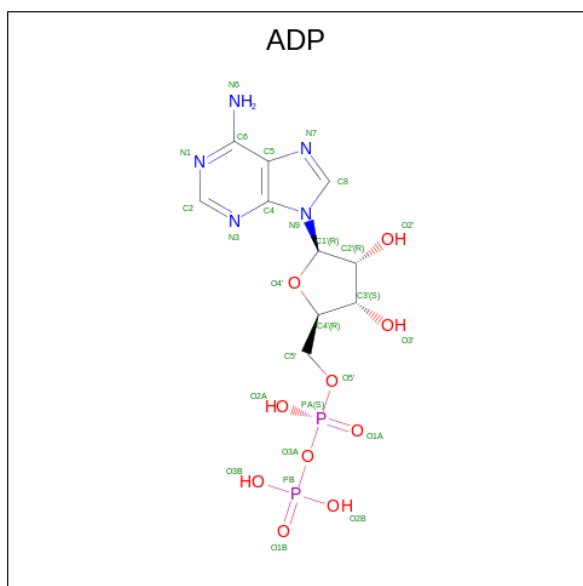


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 56  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 32 | 17 | 2 |         |
| 56  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 94    | 75 | 17 | 2 |         |
| 56  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 56  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 56  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 56  | i     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 87    | 68 | 17 | 2 |         |
| 56  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 99    | 80 | 17 | 2 |         |
| 56  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 92    | 73 | 17 | 2 |         |
| 56  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 55    | 36 | 17 | 2 |         |
| 56  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 56  | s     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 89    | 70 | 17 | 2 |         |

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 57  | T     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

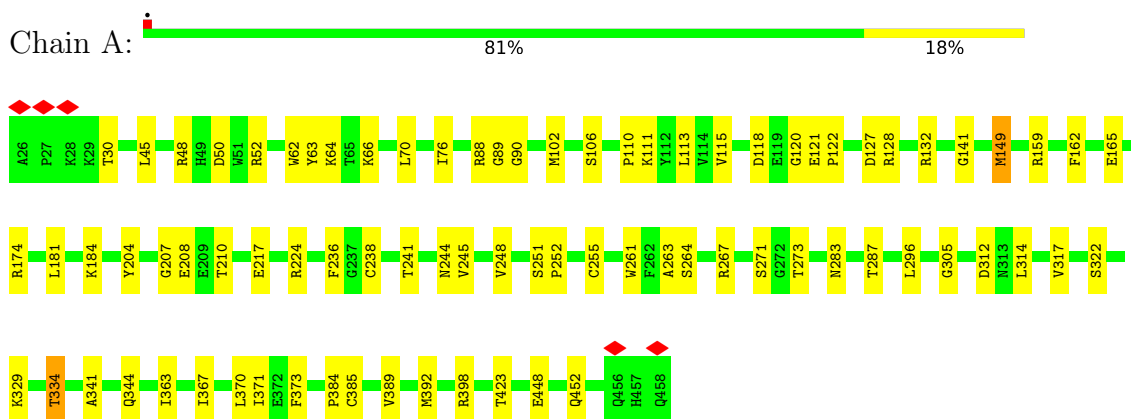


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 58  | w     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

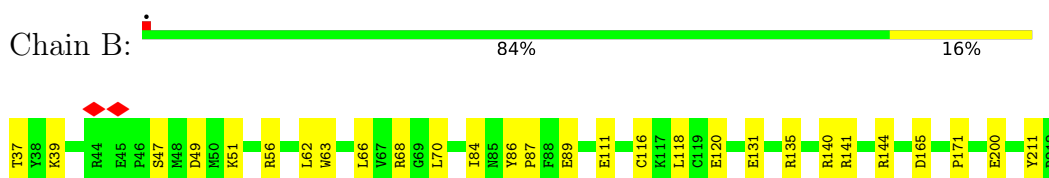
### 3 Residue-property plots

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

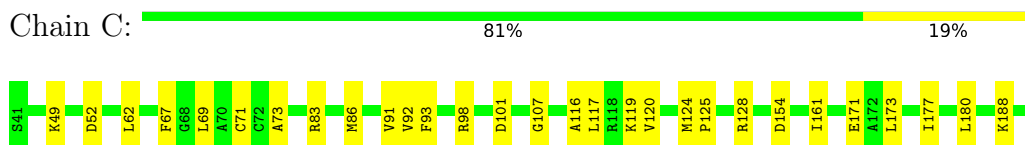
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



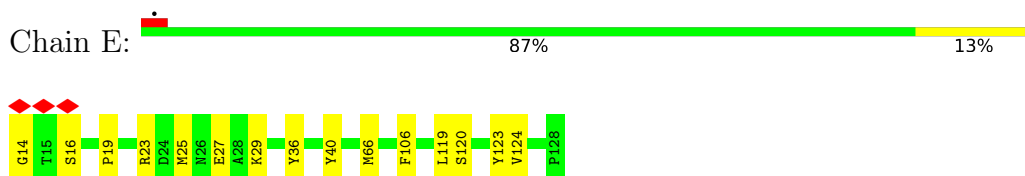
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



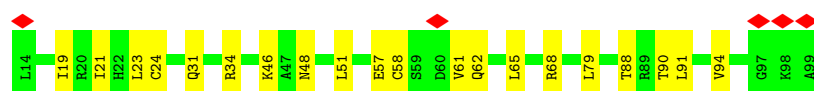
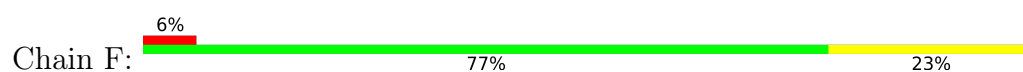
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



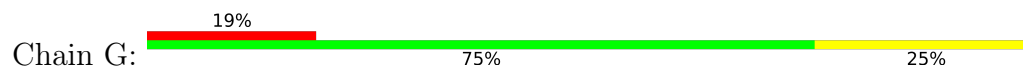
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



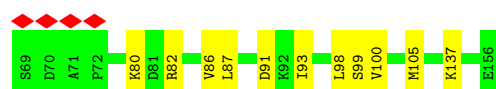
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



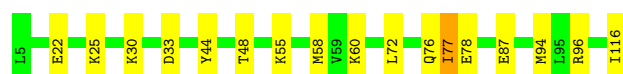
- Molecule 6: Acyl carrier protein



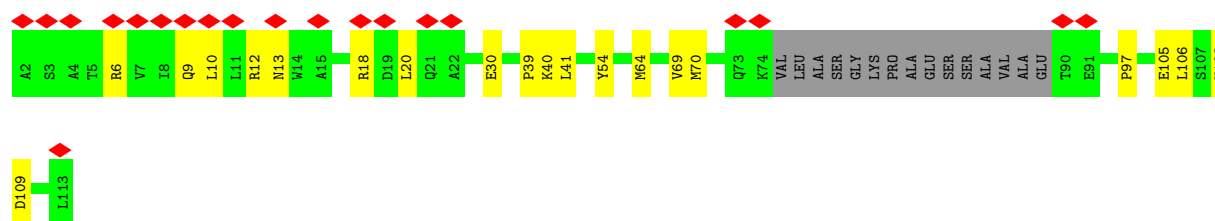
- Molecule 6: Acyl carrier protein



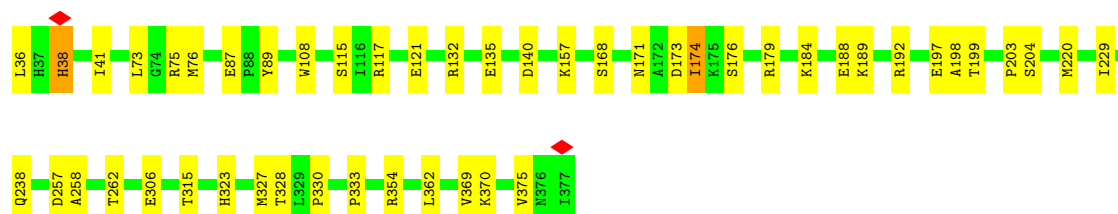
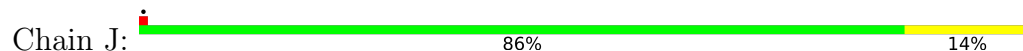
- Molecule 7: Complex I subunit B13



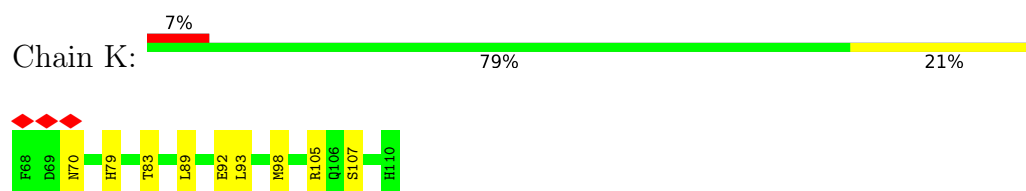
- Molecule 8: Complex I-B14.5a



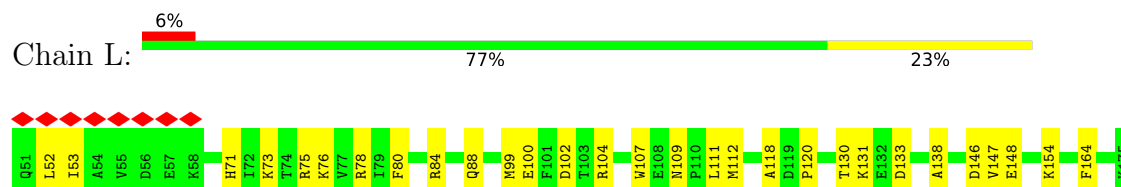
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



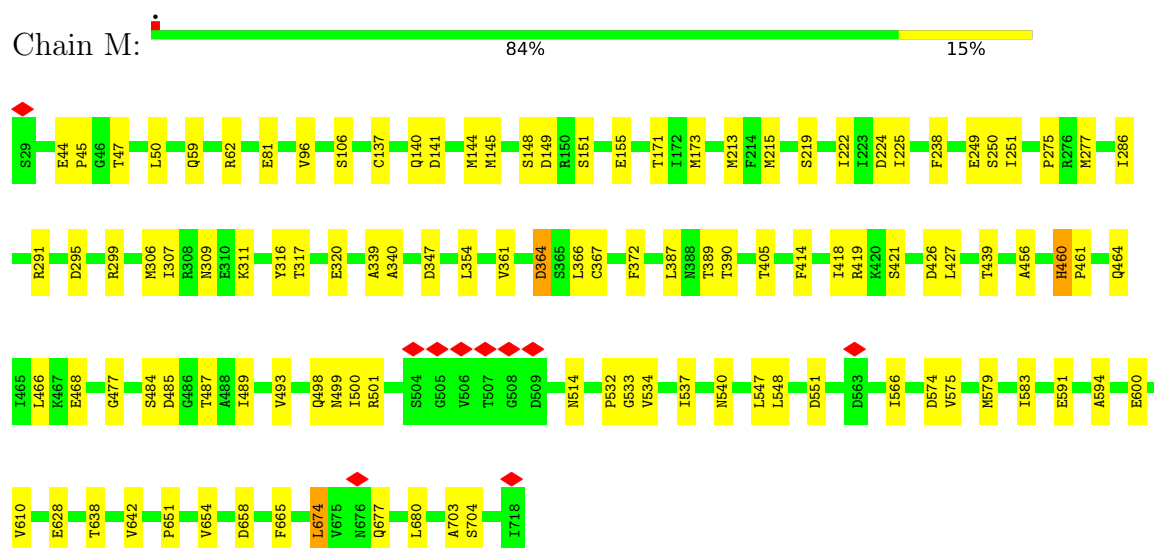
- Molecule 10: Complex I-9kD



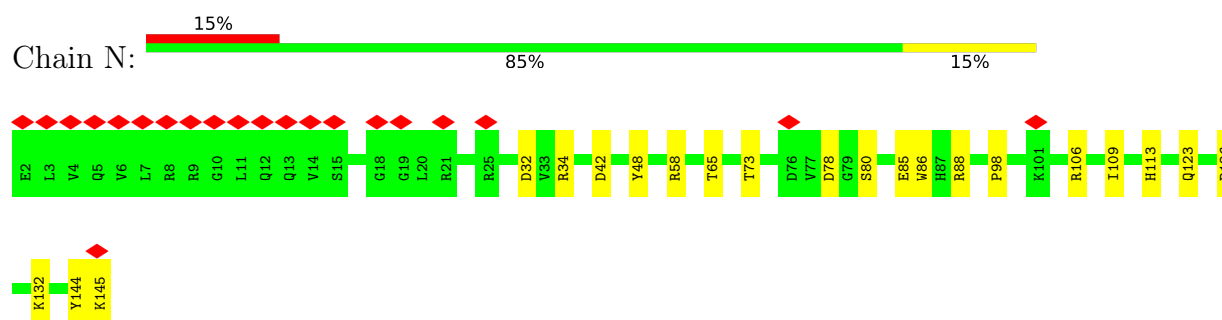
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



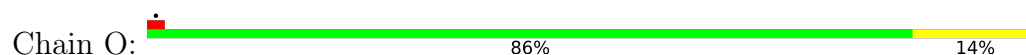
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





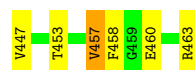
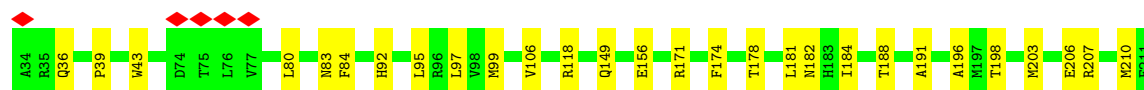
• Molecule 15: Complex I-30kD

Chain P: 84% 16%



• Molecule 16: Complex I-49kD

Chain Q: 84% 15%



• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 84% 16%



• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 8% 89% 10%



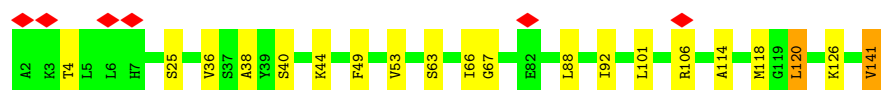
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 5% 90% 10%



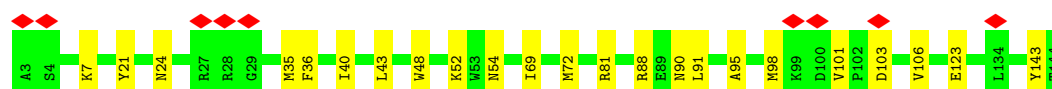
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  86% 13%



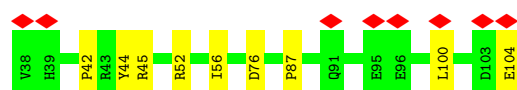
- Molecule 21: Complex I-B16.6

Chain W:  84% 16% 6%



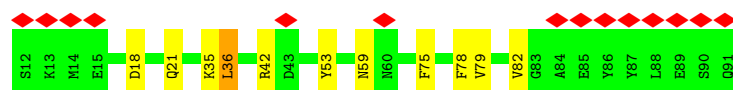
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  87% 13% 12%



- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:  86% 12% 18%



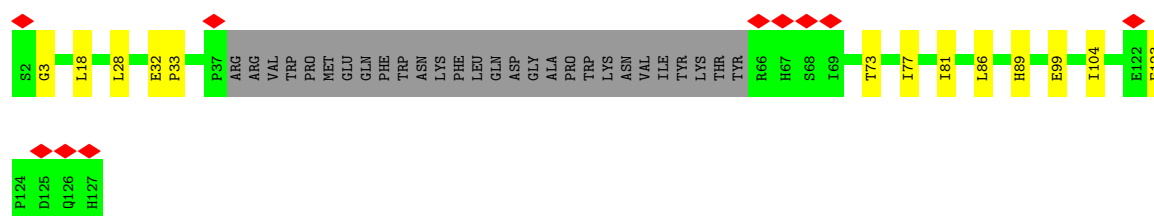
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  89% 11%

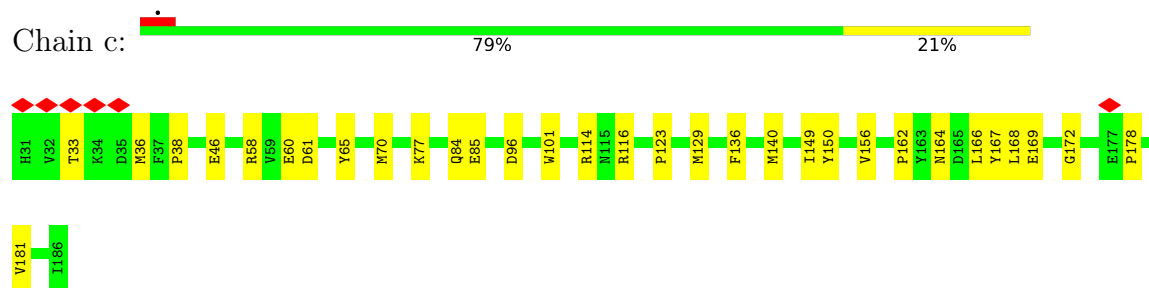


- Molecule 25: Complex I-B17

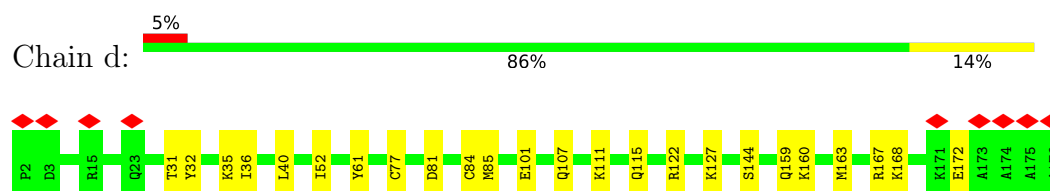
Chain b:  67% 10% 22% 8%



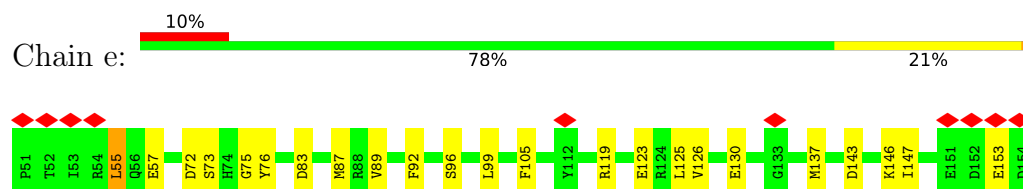
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



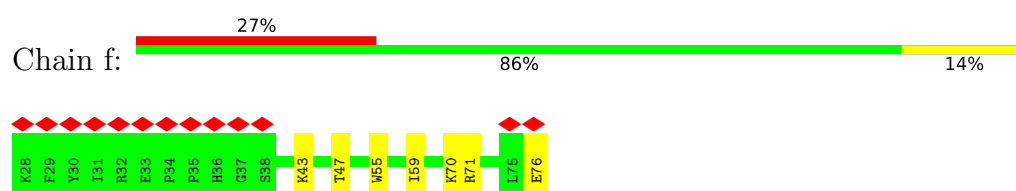
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



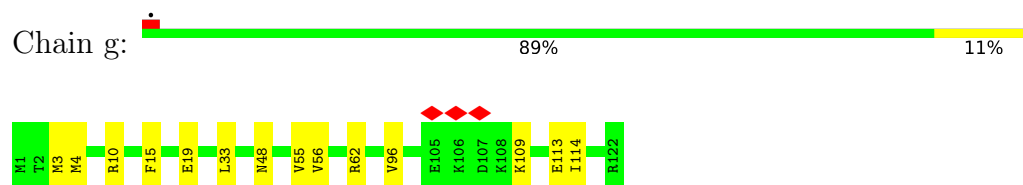
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



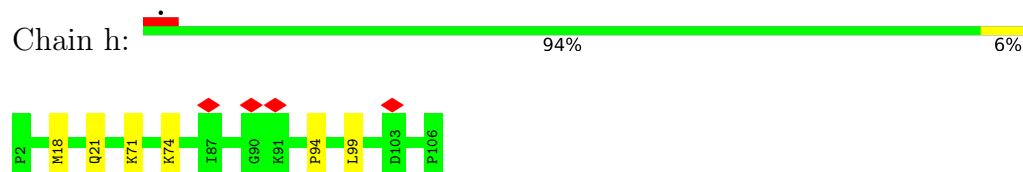
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



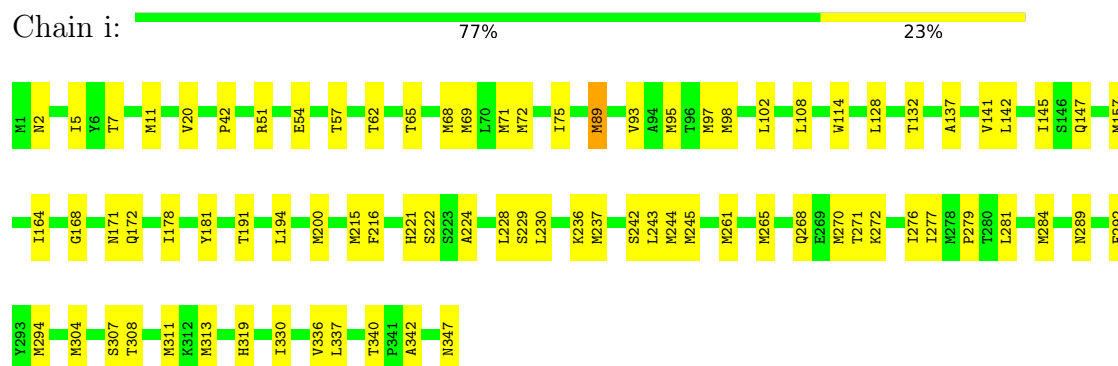
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



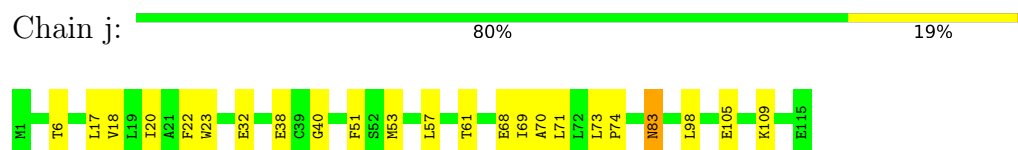
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



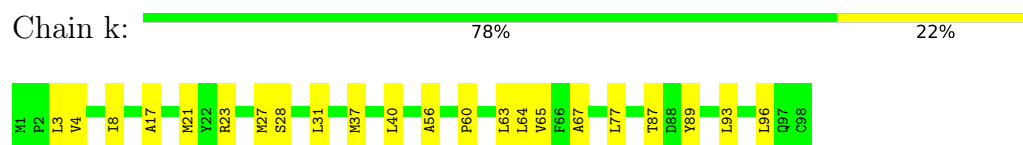
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



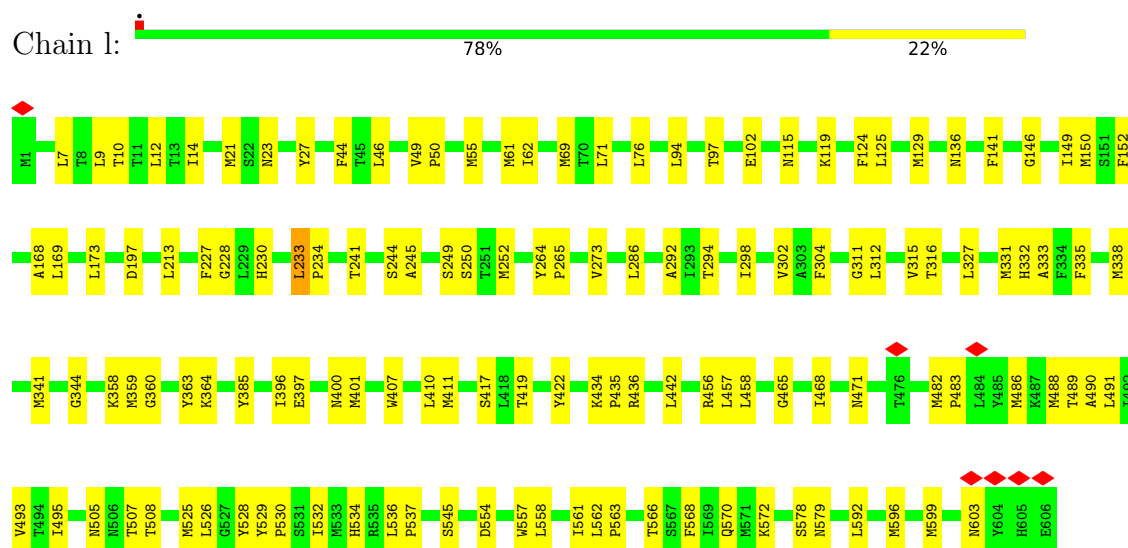
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



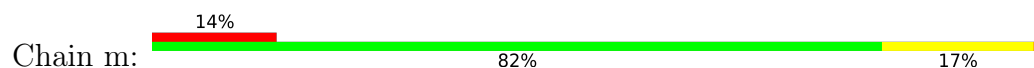
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

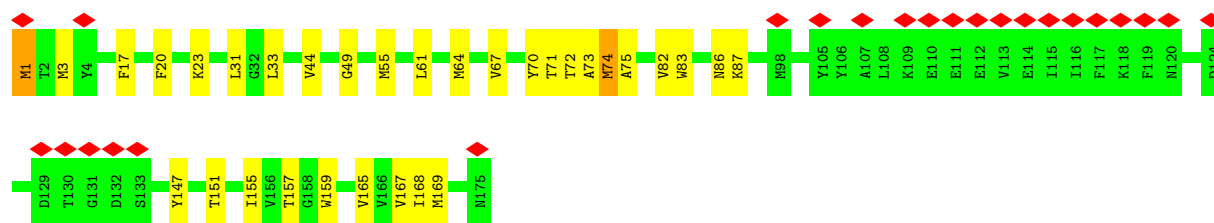


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

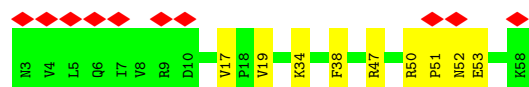
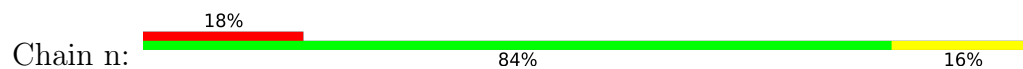


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

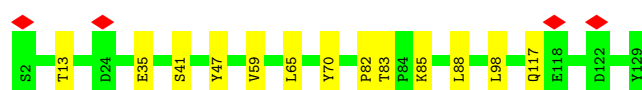




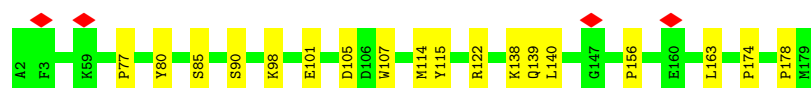
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



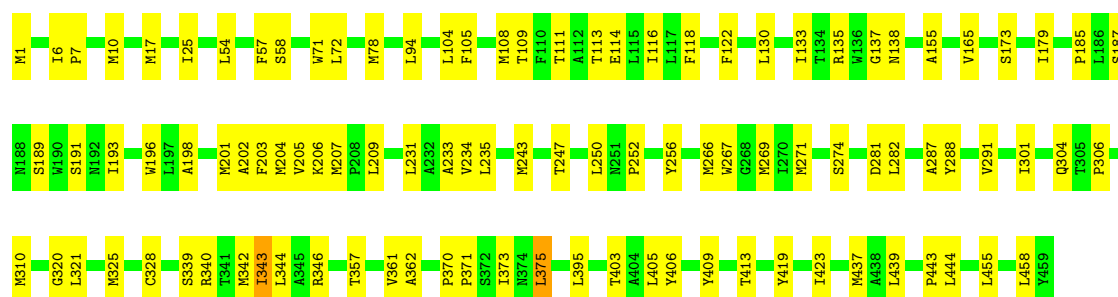
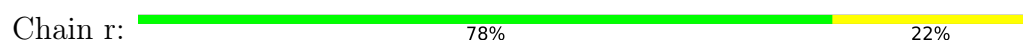
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



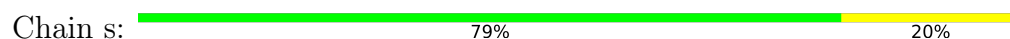
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

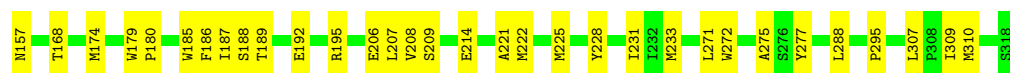


- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

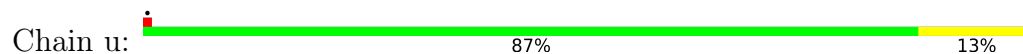


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

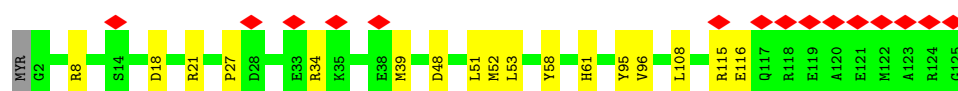
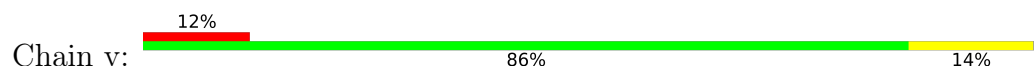




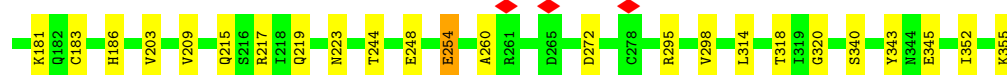
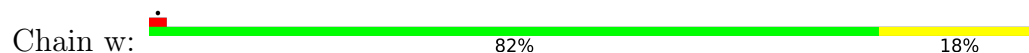
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 184754                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1300                                    | Depositor |
| Maximum defocus (nm)                 | 1800                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.191                                   | Depositor |
| Minimum map value                    | -0.109                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.0254                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 333.002, 333.002, 333.002               | wwPDB     |
| Map dimensions                       | 310, 310, 310                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0742, 1.0742, 1.0742                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, NAI, NDP, FMN, DCQ, MG, 8Q1, ADP, 2MR, PLX, ZN, SF4, UQ, PEE

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     | 0.12         | 0/3406  | 0.31        | 0/4603        |
| 2   | B     | 0.13         | 0/1443  | 0.31        | 0/1952        |
| 3   | C     | 0.17         | 0/1279  | 0.37        | 0/1730        |
| 4   | E     | 0.12         | 0/995   | 0.30        | 0/1340        |
| 5   | F     | 0.14         | 0/698   | 0.37        | 0/940         |
| 6   | G     | 0.13         | 0/702   | 0.34        | 0/952         |
| 6   | X     | 0.11         | 0/704   | 0.29        | 0/953         |
| 7   | H     | 0.13         | 0/929   | 0.36        | 0/1258        |
| 8   | I     | 0.14         | 0/798   | 0.36        | 0/1079        |
| 9   | J     | 0.13         | 0/2825  | 0.32        | 0/3830        |
| 10  | K     | 0.09         | 0/377   | 0.25        | 0/509         |
| 11  | L     | 0.16         | 0/1039  | 0.42        | 1/1403 (0.1%) |
| 12  | M     | 0.14         | 0/5384  | 0.35        | 2/7295 (0.0%) |
| 13  | N     | 0.13         | 0/1245  | 0.31        | 0/1694        |
| 14  | O     | 0.13         | 0/1711  | 0.35        | 0/2328        |
| 15  | P     | 0.14         | 0/1789  | 0.40        | 2/2436 (0.1%) |
| 16  | Q     | 0.14         | 0/3538  | 0.32        | 0/4796        |
| 17  | S     | 0.15         | 0/581   | 0.40        | 0/781         |
| 18  | T     | 0.10         | 0/755   | 0.28        | 0/1018        |
| 19  | U     | 0.11         | 0/664   | 0.26        | 0/912         |
| 20  | V     | 0.11         | 0/1042  | 0.25        | 0/1411        |
| 21  | W     | 0.13         | 0/1192  | 0.29        | 0/1610        |
| 22  | Y     | 0.12         | 0/610   | 0.31        | 0/836         |
| 23  | Z     | 0.10         | 0/660   | 0.29        | 0/892         |
| 24  | a     | 0.13         | 0/1184  | 0.31        | 0/1603        |
| 25  | b     | 0.15         | 0/844   | 0.37        | 0/1149        |
| 26  | c     | 0.12         | 0/1371  | 0.34        | 0/1875        |
| 27  | d     | 0.12         | 0/1494  | 0.30        | 0/2015        |
| 28  | e     | 0.13         | 0/891   | 0.33        | 0/1210        |
| 29  | f     | 0.11         | 0/386   | 0.28        | 0/523         |
| 30  | g     | 0.12         | 0/1036  | 0.29        | 0/1401        |
| 31  | h     | 0.13         | 0/889   | 0.32        | 0/1190        |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 32  | i     | 0.16         | 0/2773  | 0.35        | 0/3768         |
| 33  | j     | 0.14         | 0/938   | 0.34        | 0/1281         |
| 34  | k     | 0.16         | 0/759   | 0.32        | 0/1029         |
| 35  | l     | 0.14         | 0/4929  | 0.34        | 0/6704         |
| 36  | m     | 0.15         | 0/1309  | 0.35        | 0/1780         |
| 37  | n     | 0.12         | 0/491   | 0.30        | 0/663          |
| 38  | o     | 0.13         | 0/1092  | 0.32        | 0/1481         |
| 39  | p     | 0.12         | 0/1590  | 0.28        | 0/2155         |
| 40  | r     | 0.16         | 0/3723  | 0.35        | 0/5078         |
| 41  | s     | 0.17         | 0/2581  | 0.38        | 0/3529         |
| 42  | u     | 0.11         | 0/1436  | 0.31        | 0/1938         |
| 43  | v     | 0.13         | 0/1052  | 0.32        | 0/1411         |
| 44  | w     | 0.12         | 0/2642  | 0.31        | 0/3580         |
| All | All   | 0.14         | 0/67776 | 0.33        | 5/91921 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 11  | L     | 73  | LYS  | N-CA-C | 6.55 | 118.21      | 111.14   |
| 15  | P     | 44  | ARG  | CA-C-N | 5.85 | 125.55      | 119.05   |
| 15  | P     | 44  | ARG  | C-N-CA | 5.85 | 125.55      | 119.05   |
| 12  | M     | 460 | HIS  | CA-C-N | 5.59 | 125.25      | 119.05   |
| 12  | M     | 460 | HIS  | C-N-CA | 5.59 | 125.25      | 119.05   |

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     | 3330  | 0        | 3292     | 56      | 0            |
| 2   | B     | 1412  | 0        | 1363     | 23      | 0            |
| 3   | C     | 1248  | 0        | 1254     | 24      | 0            |
| 4   | E     | 971   | 0        | 975      | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | F     | 687   | 0        | 700      | 12      | 0            |
| 6   | G     | 690   | 0        | 669      | 13      | 0            |
| 6   | X     | 693   | 0        | 671      | 9       | 0            |
| 7   | H     | 910   | 0        | 950      | 13      | 0            |
| 8   | I     | 780   | 0        | 808      | 17      | 0            |
| 9   | J     | 2748  | 0        | 2771     | 30      | 0            |
| 10  | K     | 366   | 0        | 338      | 7       | 0            |
| 11  | L     | 1016  | 0        | 1016     | 25      | 0            |
| 12  | M     | 5296  | 0        | 5326     | 64      | 0            |
| 13  | N     | 1204  | 0        | 1162     | 18      | 0            |
| 14  | O     | 1671  | 0        | 1673     | 20      | 0            |
| 15  | P     | 1738  | 0        | 1693     | 31      | 0            |
| 16  | Q     | 3459  | 0        | 3396     | 43      | 0            |
| 17  | S     | 566   | 0        | 561      | 8       | 0            |
| 18  | T     | 741   | 0        | 701      | 7       | 0            |
| 19  | U     | 643   | 0        | 642      | 6       | 0            |
| 20  | V     | 1021  | 0        | 1025     | 16      | 0            |
| 21  | W     | 1161  | 0        | 1144     | 20      | 0            |
| 22  | Y     | 584   | 0        | 529      | 6       | 0            |
| 23  | Z     | 641   | 0        | 620      | 8       | 0            |
| 24  | a     | 1151  | 0        | 1164     | 14      | 0            |
| 25  | b     | 819   | 0        | 835      | 12      | 0            |
| 26  | c     | 1315  | 0        | 1208     | 25      | 0            |
| 27  | d     | 1461  | 0        | 1429     | 16      | 0            |
| 28  | e     | 867   | 0        | 817      | 24      | 0            |
| 29  | f     | 378   | 0        | 356      | 5       | 0            |
| 30  | g     | 1005  | 0        | 999      | 12      | 0            |
| 31  | h     | 867   | 0        | 871      | 3       | 0            |
| 32  | i     | 2710  | 0        | 2874     | 62      | 0            |
| 33  | j     | 914   | 0        | 951      | 22      | 0            |
| 34  | k     | 748   | 0        | 799      | 21      | 0            |
| 35  | l     | 4800  | 0        | 4939     | 101     | 0            |
| 36  | m     | 1277  | 0        | 1239     | 31      | 0            |
| 37  | n     | 479   | 0        | 486      | 5       | 0            |
| 38  | o     | 1062  | 0        | 1072     | 12      | 0            |
| 39  | p     | 1534  | 0        | 1470     | 12      | 0            |
| 40  | r     | 3631  | 0        | 3839     | 73      | 0            |
| 41  | s     | 2508  | 0        | 2607     | 52      | 0            |
| 42  | u     | 1398  | 0        | 1374     | 18      | 0            |
| 43  | v     | 1028  | 0        | 982      | 15      | 0            |
| 44  | w     | 2582  | 0        | 2531     | 34      | 0            |
| 45  | A     | 8     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45  | B     | 16    | 0        | 0        | 0       | 0            |
| 45  | C     | 8     | 0        | 0        | 1       | 0            |
| 45  | M     | 16    | 0        | 0        | 0       | 0            |
| 46  | A     | 31    | 0        | 19       | 5       | 0            |
| 47  | A     | 44    | 0        | 27       | 7       | 0            |
| 48  | B     | 51    | 0        | 82       | 5       | 0            |
| 48  | C     | 47    | 0        | 71       | 3       | 0            |
| 48  | V     | 40    | 0        | 54       | 2       | 0            |
| 48  | W     | 41    | 0        | 59       | 0       | 0            |
| 48  | j     | 92    | 0        | 141      | 8       | 0            |
| 48  | l     | 97    | 0        | 151      | 6       | 0            |
| 48  | r     | 51    | 0        | 82       | 8       | 0            |
| 49  | C     | 52    | 0        | 88       | 4       | 0            |
| 49  | J     | 52    | 0        | 88       | 8       | 0            |
| 49  | a     | 52    | 0        | 88       | 2       | 0            |
| 49  | e     | 52    | 0        | 88       | 5       | 0            |
| 49  | g     | 52    | 0        | 88       | 3       | 0            |
| 49  | j     | 52    | 0        | 88       | 5       | 0            |
| 49  | r     | 52    | 0        | 88       | 6       | 0            |
| 50  | C     | 23    | 0        | 30       | 2       | 0            |
| 51  | G     | 35    | 0        | 0        | 0       | 0            |
| 51  | X     | 35    | 0        | 0        | 0       | 0            |
| 52  | J     | 48    | 0        | 25       | 2       | 0            |
| 53  | J     | 33    | 0        | 39       | 1       | 0            |
| 53  | s     | 38    | 0        | 47       | 2       | 0            |
| 54  | M     | 4     | 0        | 0        | 0       | 0            |
| 54  | O     | 4     | 0        | 0        | 0       | 0            |
| 55  | M     | 1     | 0        | 0        | 0       | 0            |
| 56  | N     | 51    | 0        | 46       | 0       | 0            |
| 56  | V     | 294   | 0        | 450      | 25      | 0            |
| 56  | a     | 100   | 0        | 156      | 7       | 0            |
| 56  | i     | 87    | 0        | 124      | 4       | 0            |
| 56  | l     | 191   | 0        | 288      | 19      | 0            |
| 56  | n     | 55    | 0        | 54       | 1       | 0            |
| 56  | r     | 100   | 0        | 156      | 10      | 0            |
| 56  | s     | 89    | 0        | 125      | 5       | 0            |
| 57  | T     | 1     | 0        | 0        | 0       | 0            |
| 58  | w     | 27    | 0        | 11       | 2       | 0            |
| All | All   | 68232 | 0        | 68974    | 955     | 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 7.

All (955) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 15:P:44:ARG:CB   | 15:P:45:PRO:HD3   | 1.58                     | 1.33              |
| 15:P:44:ARG:HB3  | 15:P:45:PRO:CD    | 1.57                     | 1.31              |
| 47:A:503:NAI:C1B | 47:A:503:NAI:O4B  | 1.63                     | 1.23              |
| 52:J:401:NDP:O4D | 52:J:401:NDP:C4D  | 1.68                     | 1.11              |
| 41:s:24:GLU:OE1  | 41:s:271:LEU:HD22 | 1.77                     | 0.85              |
| 35:l:360:GLY:HA3 | 35:l:435:PRO:HA   | 1.60                     | 0.83              |
| 1:A:121:GLU:HG2  | 47:A:503:NAI:H42N | 1.61                     | 0.82              |
| 36:m:72:THR:HG21 | 41:s:133:LEU:HD21 | 1.62                     | 0.81              |
| 41:s:222:MET:HA  | 41:s:225:MET:HE2  | 1.63                     | 0.80              |
| 32:i:236:LYS:HG3 | 32:i:237:MET:HG3  | 1.63                     | 0.79              |
| 16:Q:83:ASN:HB2  | 33:j:38:GLU:HG2   | 1.64                     | 0.78              |
| 36:m:82:VAL:HG21 | 56:s:401:CDL:HB31 | 1.65                     | 0.77              |
| 15:P:44:ARG:HB3  | 15:P:45:PRO:HD3   | 0.79                     | 0.76              |
| 44:w:113:SER:HB3 | 44:w:116:LYS:HG2  | 1.68                     | 0.76              |
| 8:I:40:LYS:HB3   | 21:W:7:LYS:H      | 1.51                     | 0.76              |
| 12:M:149:ASP:HB2 | 16:Q:361:ALA:HB3  | 1.68                     | 0.75              |
| 41:s:195:ARG:HD3 | 41:s:231:ILE:HD11 | 1.67                     | 0.75              |
| 3:C:98:ARG:HD2   | 41:s:61:LEU:HD21  | 1.71                     | 0.73              |
| 33:j:70:ALA:HA   | 36:m:55:MET:HE2   | 1.69                     | 0.73              |
| 15:P:44:ARG:CG   | 15:P:45:PRO:HD3   | 2.19                     | 0.73              |
| 40:r:17:MET:HE3  | 56:r:503:CDL:H581 | 1.71                     | 0.73              |
| 37:n:47:ARG:NH1  | 37:n:53:GLU:OE2   | 2.21                     | 0.73              |
| 15:P:83:GLU:OE1  | 15:P:142:ARG:NH2  | 2.22                     | 0.72              |
| 44:w:125:ASP:O   | 44:w:130:ARG:NH2  | 2.22                     | 0.72              |
| 1:A:149:MET:HE3  | 1:A:241:THR:HB    | 1.71                     | 0.72              |
| 21:W:81:ARG:NH2  | 42:u:64:ASN:OD1   | 2.23                     | 0.71              |
| 35:l:483:PRO:HD2 | 35:l:486:MET:HE3  | 1.72                     | 0.71              |
| 35:l:69:MET:HE3  | 35:l:71:LEU:HD21  | 1.73                     | 0.70              |
| 11:L:109:ASN:ND2 | 11:L:111:LEU:O    | 2.25                     | 0.70              |
| 1:A:398:ARG:NH1  | 12:M:155:GLU:OE2  | 2.25                     | 0.70              |
| 27:d:31:THR:HG22 | 27:d:35:LYS:HE2   | 1.74                     | 0.70              |
| 32:i:268:GLN:HA  | 40:r:165:VAL:HG11 | 1.73                     | 0.69              |
| 12:M:213:MET:HB3 | 12:M:215:MET:HG2  | 1.74                     | 0.69              |
| 25:b:86:LEU:HD11 | 35:l:9:LEU:HD12   | 1.73                     | 0.69              |
| 40:r:191:SER:HB3 | 48:r:501:PEE:H2   | 1.76                     | 0.68              |
| 9:J:132:ARG:HH21 | 52:J:401:NDP:H51A | 1.59                     | 0.68              |
| 16:Q:302:LEU:HB2 | 16:Q:401:GLU:HB2  | 1.76                     | 0.68              |
| 35:l:102:GLU:OE2 | 35:l:456:ARG:NH2  | 2.27                     | 0.67              |
| 32:i:270:MET:HE3 | 32:i:279:PRO:HG3  | 1.77                     | 0.67              |
| 12:M:456:ALA:O   | 12:M:499:ASN:ND2  | 2.27                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 56:r:503:CDL:H401 | 56:r:503:CDL:H221 | 1.74                     | 0.67              |
| 2:B:47:SER:O      | 2:B:56:ARG:NH2    | 2.27                     | 0.67              |
| 33:j:57:LEU:HD21  | 36:m:169:MET:HE3  | 1.77                     | 0.67              |
| 44:w:47:GLU:OE2   | 44:w:52:LYS:NZ    | 2.27                     | 0.67              |
| 12:M:501:ARG:HH21 | 12:M:665:PHE:HD2  | 1.42                     | 0.66              |
| 14:O:38:LEU:O     | 14:O:124:ARG:NH2  | 2.28                     | 0.66              |
| 30:g:56:VAL:HG21  | 40:r:17:MET:HE1   | 1.77                     | 0.66              |
| 9:J:328:THR:HG22  | 9:J:330:PRO:HD3   | 1.78                     | 0.66              |
| 14:O:182:ASN:HB3  | 14:O:194:GLU:HB2  | 1.77                     | 0.66              |
| 28:e:119:ARG:O    | 28:e:123:GLU:HG3  | 1.96                     | 0.65              |
| 9:J:192:ARG:NH1   | 9:J:198:ALA:O     | 2.30                     | 0.65              |
| 16:Q:149:GLN:NE2  | 16:Q:309:ASP:OD2  | 2.28                     | 0.64              |
| 3:C:119:LYS:NZ    | 33:j:32:GLU:OE1   | 2.28                     | 0.64              |
| 2:B:63:TRP:HB3    | 2:B:66:LEU:HD12   | 1.80                     | 0.64              |
| 11:L:75:ARG:HD2   | 11:L:104:ARG:NH2  | 2.13                     | 0.64              |
| 34:k:65:VAL:HG11  | 36:m:157:THR:HG23 | 1.78                     | 0.64              |
| 1:A:102:MET:O     | 1:A:111:LYS:NZ    | 2.31                     | 0.64              |
| 10:K:105:ARG:NH2  | 12:M:426:ASP:OD2  | 2.28                     | 0.64              |
| 24:a:78:THR:HG21  | 28:e:96:SER:HA    | 1.78                     | 0.64              |
| 26:c:36:MET:HA    | 26:c:36:MET:HE2   | 1.80                     | 0.64              |
| 40:r:72:LEU:HD11  | 40:r:233:ALA:HB3  | 1.80                     | 0.64              |
| 26:c:168:LEU:HA   | 26:c:172:GLY:HA2  | 1.80                     | 0.64              |
| 41:s:221:ALA:O    | 41:s:225:MET:HG3  | 1.98                     | 0.63              |
| 1:A:385:CYS:HB2   | 45:A:501:SF4:S4   | 2.39                     | 0.63              |
| 29:f:55:TRP:O     | 29:f:59:ILE:HG12  | 1.98                     | 0.63              |
| 26:c:116:ARG:HG2  | 48:l:703:PEE:H49  | 1.79                     | 0.63              |
| 12:M:224:ASP:OD1  | 12:M:291:ARG:NH1  | 2.32                     | 0.63              |
| 30:g:10:ARG:NH2   | 32:i:347:ASN:O    | 2.32                     | 0.63              |
| 56:l:701:CDL:H432 | 56:l:701:CDL:H621 | 1.80                     | 0.63              |
| 56:l:702:CDL:H322 | 56:l:702:CDL:H121 | 1.80                     | 0.63              |
| 35:l:525:MET:HE2  | 39:p:77:PRO:HB3   | 1.81                     | 0.63              |
| 44:w:139:ARG:NH1  | 44:w:166:ASP:OD1  | 2.33                     | 0.62              |
| 32:i:171:ASN:ND2  | 35:l:578:SER:OG   | 2.25                     | 0.62              |
| 23:Z:75:PHE:O     | 23:Z:79:VAL:HG23  | 1.99                     | 0.62              |
| 34:k:23:ARG:HG3   | 36:m:23:LYS:HE2   | 1.80                     | 0.62              |
| 35:l:227:PHE:O    | 35:l:230:HIS:ND1  | 2.33                     | 0.62              |
| 5:F:65:LEU:HB2    | 5:F:79:LEU:HD11   | 1.82                     | 0.62              |
| 16:Q:424:ILE:HB   | 16:Q:463:ARG:HD2  | 1.82                     | 0.62              |
| 30:g:15:PHE:HB2   | 49:g:201:PLX:H6   | 1.82                     | 0.62              |
| 1:A:448:GLU:O     | 1:A:452:GLN:HG2   | 2.00                     | 0.62              |
| 3:C:125:PRO:HG2   | 41:s:58:LYS:HE3   | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:P:113:ASP:OD1  | 16:Q:423:LYS:NZ   | 2.33                     | 0.61              |
| 35:l:173:LEU:HD12 | 40:r:405:LEU:HD21 | 1.80                     | 0.61              |
| 12:M:460:HIS:ND1  | 12:M:461:PRO:HD2  | 2.15                     | 0.61              |
| 8:I:6:ARG:HH21    | 8:I:10:LEU:HD11   | 1.65                     | 0.61              |
| 32:i:265:MET:O    | 32:i:268:GLN:HG3  | 1.99                     | 0.61              |
| 39:p:105:ASP:OD1  | 39:p:122:ARG:NH1  | 2.22                     | 0.61              |
| 3:C:73:ALA:HB3    | 50:C:304:DCQ:H4MB | 1.83                     | 0.61              |
| 30:g:62:ARG:NH2   | 44:w:355:LYS:O    | 2.34                     | 0.61              |
| 34:k:28:SER:HB3   | 36:m:23:LYS:HG2   | 1.81                     | 0.61              |
| 9:J:117:ARG:O     | 9:J:121:GLU:HG3   | 2.00                     | 0.61              |
| 38:o:59:VAL:HG22  | 40:r:423:ILE:HG12 | 1.83                     | 0.60              |
| 3:C:69:LEU:HB2    | 3:C:107:GLY:HA3   | 1.83                     | 0.60              |
| 12:M:387:LEU:HD12 | 12:M:514:ASN:HB3  | 1.83                     | 0.60              |
| 3:C:52:ASP:HB3    | 49:C:303:PLX:H251 | 1.83                     | 0.60              |
| 44:w:139:ARG:HH12 | 58:w:401:ADP:HN61 | 1.49                     | 0.60              |
| 3:C:92:VAL:HG11   | 53:s:402:UQ:H103  | 1.83                     | 0.60              |
| 8:I:12:ARG:HB3    | 8:I:20:LEU:HD12   | 1.83                     | 0.60              |
| 1:A:48:ARG:NH1    | 10:K:70:ASN:O     | 2.32                     | 0.60              |
| 6:G:79:ILE:HG22   | 6:G:145:VAL:HG12  | 1.83                     | 0.60              |
| 40:r:78:MET:HE1   | 40:r:439:LEU:HD12 | 1.84                     | 0.60              |
| 41:s:63:PRO:HB2   | 41:s:66:SER:HB3   | 1.83                     | 0.60              |
| 1:A:121:GLU:HG2   | 47:A:503:NAI:C4N  | 2.31                     | 0.59              |
| 13:N:106:ARG:HB2  | 13:N:109:ILE:HG13 | 1.84                     | 0.59              |
| 56:s:401:CDL:HA61 | 56:s:401:CDL:H132 | 1.84                     | 0.59              |
| 42:u:137:LEU:HD12 | 42:u:138:PRO:HD2  | 1.83                     | 0.59              |
| 9:J:174:ILE:HD11  | 9:J:189:LYS:HE2   | 1.84                     | 0.59              |
| 11:L:84:ARG:NH1   | 11:L:88:GLN:O     | 2.35                     | 0.59              |
| 12:M:59:GLN:HE21  | 12:M:62:ARG:HH12  | 1.50                     | 0.59              |
| 12:M:306:MET:HB2  | 12:M:583:ILE:HB   | 1.84                     | 0.59              |
| 16:Q:387:GLU:OE2  | 16:Q:390:GLN:NE2  | 2.35                     | 0.59              |
| 40:r:306:PRO:HB3  | 40:r:458:LEU:HD12 | 1.84                     | 0.59              |
| 42:u:49:GLU:OE1   | 42:u:135:ARG:NH2  | 2.34                     | 0.59              |
| 1:A:244:ASN:ND2   | 46:A:502:FMN:O2   | 2.32                     | 0.59              |
| 32:i:71:MET:HE3   | 34:k:63:LEU:HD21  | 1.83                     | 0.59              |
| 32:i:93:VAL:HG22  | 35:l:603:ASN:HD21 | 1.66                     | 0.59              |
| 35:l:491:LEU:O    | 35:l:495:ILE:HD12 | 2.02                     | 0.59              |
| 48:r:501:PEE:H79  | 48:r:501:PEE:H37  | 1.85                     | 0.59              |
| 14:O:207:GLU:HG2  | 14:O:212:LYS:HB2  | 1.83                     | 0.59              |
| 32:i:42:PRO:HG2   | 36:m:167:VAL:HG22 | 1.85                     | 0.59              |
| 35:l:410:LEU:HD23 | 35:l:411:MET:HE2  | 1.85                     | 0.59              |
| 39:p:98:LYS:HG2   | 39:p:178:PRO:HG3  | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:r:201:MET:HG3  | 48:r:501:PEE:H34  | 1.84                     | 0.59              |
| 41:s:109:SER:OG   | 41:s:192:GLU:OE2  | 2.20                     | 0.59              |
| 1:A:113:LEU:HD13  | 1:A:149:MET:HE1   | 1.83                     | 0.59              |
| 16:Q:181:LEU:HD23 | 16:Q:207:ARG:HG2  | 1.84                     | 0.59              |
| 56:V:204:CDL:H812 | 34:k:17:ALA:HB2   | 1.85                     | 0.59              |
| 49:e:201:PLX:H202 | 56:l:701:CDL:H801 | 1.84                     | 0.59              |
| 8:I:9:GLN:O       | 8:I:13:ASN:ND2    | 2.36                     | 0.59              |
| 40:r:1:MET:HE3    | 40:r:111:THR:HG21 | 1.84                     | 0.59              |
| 44:w:118:TYR:OH   | 58:w:401:ADP:O2'  | 2.21                     | 0.59              |
| 56:V:204:CDL:H332 | 56:V:204:CDL:H222 | 1.84                     | 0.58              |
| 40:r:310:MET:HB3  | 40:r:455:LEU:HD22 | 1.86                     | 0.58              |
| 16:Q:184:ILE:O    | 16:Q:188:THR:OG1  | 2.20                     | 0.58              |
| 6:G:94:ASP:OD1    | 6:G:97:LYS:N      | 2.36                     | 0.58              |
| 20:V:88:LEU:O     | 20:V:92:ILE:HG13  | 2.03                     | 0.58              |
| 32:i:7:THR:HG23   | 56:i:401:CDL:H522 | 1.85                     | 0.58              |
| 2:B:62:LEU:HD12   | 21:W:35:MET:HE3   | 1.86                     | 0.58              |
| 41:s:307:LEU:HA   | 41:s:310:MET:HE2  | 1.85                     | 0.58              |
| 12:M:275:PRO:HG3  | 12:M:286:ILE:HG12 | 1.86                     | 0.58              |
| 35:l:545:SER:OG   | 40:r:274:SER:O    | 2.20                     | 0.58              |
| 22:Y:52:ARG:O     | 22:Y:56:ILE:HG13  | 2.04                     | 0.58              |
| 41:s:62:ARG:HG2   | 41:s:68:ILE:HD13  | 1.86                     | 0.57              |
| 31:h:18:MET:HE3   | 34:k:56:ALA:HA    | 1.85                     | 0.57              |
| 35:l:359:MET:O    | 35:l:436:ARG:NH2  | 2.36                     | 0.57              |
| 1:A:263:ALA:HA    | 1:A:271:SER:HB3   | 1.85                     | 0.57              |
| 3:C:154:ASP:OD1   | 3:C:154:ASP:N     | 2.35                     | 0.57              |
| 26:c:46:GLU:OE1   | 26:c:46:GLU:N     | 2.36                     | 0.57              |
| 35:l:419:THR:HA   | 35:l:422:TYR:CE2  | 2.40                     | 0.57              |
| 40:r:201:MET:HA   | 40:r:201:MET:HE2  | 1.86                     | 0.57              |
| 35:l:417:SER:OG   | 35:l:493:VAL:HG13 | 2.05                     | 0.56              |
| 33:j:22:PHE:HB3   | 48:j:202:PEE:H2   | 1.87                     | 0.56              |
| 35:l:55:MET:HE2   | 35:l:471:ASN:HB3  | 1.87                     | 0.56              |
| 41:s:7:LEU:HD23   | 41:s:10:ILE:HD11  | 1.87                     | 0.56              |
| 30:g:109:LYS:HE2  | 30:g:113:GLU:HG3  | 1.88                     | 0.56              |
| 28:e:126:VAL:O    | 28:e:130:GLU:HG2  | 2.06                     | 0.56              |
| 33:j:6:THR:HG21   | 41:s:87:VAL:HG11  | 1.86                     | 0.56              |
| 56:l:701:CDL:H601 | 56:l:701:CDL:H772 | 1.86                     | 0.56              |
| 44:w:83:LEU:HD22  | 44:w:156:GLY:HA3  | 1.87                     | 0.56              |
| 4:E:40:TYR:HB3    | 6:G:120:MET:HE1   | 1.87                     | 0.56              |
| 13:N:65:THR:O     | 13:N:73:THR:OG1   | 2.23                     | 0.56              |
| 48:j:201:PEE:H26  | 41:s:295:PRO:HB3  | 1.87                     | 0.56              |
| 35:l:562:LEU:HB3  | 35:l:563:PRO:HD3  | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:63:TYR:CD1    | 1:A:64:LYS:HG2    | 2.40                     | 0.56              |
| 16:Q:95:LEU:HB2   | 16:Q:458:PHE:CZ   | 2.41                     | 0.56              |
| 5:F:90:THR:O      | 5:F:94:VAL:HG23   | 2.06                     | 0.56              |
| 35:l:294:THR:HG22 | 56:l:702:CDL:HB61 | 1.88                     | 0.56              |
| 2:B:140:ARG:HG3   | 12:M:238:PHE:CG   | 2.41                     | 0.56              |
| 12:M:464:GLN:NE2  | 12:M:468:GLU:OE1  | 2.39                     | 0.56              |
| 41:s:101:GLY:O    | 41:s:105:MET:HG3  | 2.07                     | 0.55              |
| 44:w:132:GLN:NE2  | 44:w:166:ASP:OD2  | 2.38                     | 0.55              |
| 1:A:312:ASP:HA    | 1:A:329:LYS:HE3   | 1.88                     | 0.55              |
| 4:E:25:MET:O      | 4:E:29:LYS:HG3    | 2.07                     | 0.55              |
| 11:L:78:ARG:NH2   | 12:M:249:GLU:OE1  | 2.36                     | 0.55              |
| 15:P:43:THR:HA    | 15:P:47:ILE:HD12  | 1.87                     | 0.55              |
| 40:r:133:ILE:HD11 | 40:r:231:LEU:HD11 | 1.87                     | 0.55              |
| 6:G:140:CYS:SG    | 6:G:143:GLU:HG3   | 2.46                     | 0.55              |
| 56:V:202:CDL:H561 | 56:V:202:CDL:H731 | 1.88                     | 0.55              |
| 1:A:296:LEU:HD21  | 1:A:317:VAL:HG11  | 1.89                     | 0.55              |
| 9:J:73:LEU:HA     | 9:J:76:MET:HE2    | 1.89                     | 0.55              |
| 32:i:11:MET:HG2   | 56:i:401:CDL:H581 | 1.87                     | 0.55              |
| 41:s:146:LEU:HD12 | 41:s:188:SER:HB3  | 1.88                     | 0.55              |
| 24:a:166:GLY:O    | 24:a:170:GLN:NE2  | 2.36                     | 0.55              |
| 49:g:201:PLX:H332 | 32:i:342:ALA:HB3  | 1.87                     | 0.55              |
| 32:i:289:ASN:HA   | 32:i:292:PHE:CE2  | 2.41                     | 0.55              |
| 1:A:208:GLU:OE1   | 1:A:210:THR:OG1   | 2.25                     | 0.55              |
| 17:S:34:LYS:NZ    | 17:S:61:HIS:O     | 2.33                     | 0.55              |
| 12:M:485:ASP:HB3  | 12:M:680:LEU:HD13 | 1.90                     | 0.54              |
| 28:e:55:LEU:HD12  | 44:w:318:THR:HG22 | 1.89                     | 0.54              |
| 29:f:43:LYS:O     | 29:f:47:THR:HG23  | 2.07                     | 0.54              |
| 46:A:502:FMN:N5   | 47:A:503:NAI:H4N  | 2.22                     | 0.54              |
| 6:G:82:ARG:NE     | 6:G:125:GLU:OE2   | 2.41                     | 0.54              |
| 56:l:701:CDL:H242 | 48:l:704:PEE:H34  | 1.88                     | 0.54              |
| 36:m:61:LEU:O     | 41:s:114:TYR:OH   | 2.24                     | 0.54              |
| 11:L:99:MET:HE2   | 11:L:138:ALA:HB2  | 1.88                     | 0.54              |
| 49:e:201:PLX:H162 | 56:l:701:CDL:H822 | 1.89                     | 0.54              |
| 40:r:339:SER:HB3  | 40:r:344:LEU:HD22 | 1.89                     | 0.54              |
| 56:r:503:CDL:H271 | 56:r:503:CDL:H721 | 1.89                     | 0.54              |
| 49:J:403:PLX:H201 | 33:j:20:ILE:HD11  | 1.89                     | 0.54              |
| 33:j:18:VAL:HG23  | 41:s:222:MET:HE1  | 1.88                     | 0.54              |
| 1:A:45:LEU:HD21   | 1:A:287:THR:HG22  | 1.87                     | 0.54              |
| 26:c:70:MET:HE2   | 38:o:85:LYS:HE3   | 1.89                     | 0.54              |
| 5:F:46:LYS:HG3    | 12:M:674:LEU:HD21 | 1.89                     | 0.54              |
| 9:J:192:ARG:NH2   | 9:J:262:THR:OG1   | 2.41                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:e:143:ASP:HB3  | 28:e:146:LYS:HG3  | 1.89                     | 0.54              |
| 44:w:60:ILE:HG12  | 44:w:203:VAL:HB   | 1.90                     | 0.54              |
| 2:B:165:ASP:OD1   | 16:Q:368:ARG:NH2  | 2.39                     | 0.54              |
| 16:Q:106:VAL:HG21 | 16:Q:447:VAL:HG21 | 1.90                     | 0.54              |
| 32:i:42:PRO:HG3   | 36:m:167:VAL:HG13 | 1.90                     | 0.54              |
| 18:T:49:ASP:OD2   | 18:T:51:ARG:NH2   | 2.40                     | 0.54              |
| 20:V:120:LEU:HD21 | 49:r:502:PLX:H341 | 1.90                     | 0.54              |
| 30:g:3:MET:HG2    | 30:g:4:MET:HG3    | 1.90                     | 0.53              |
| 21:W:88:ARG:HH21  | 42:u:9:THR:HG22   | 1.72                     | 0.53              |
| 32:i:200:MET:SD   | 32:i:265:MET:HB3  | 2.49                     | 0.53              |
| 42:u:83:THR:HA    | 42:u:86:TRP:CD1   | 2.43                     | 0.53              |
| 9:J:75:ARG:NH2    | 15:P:215:GLU:OE2  | 2.41                     | 0.53              |
| 35:l:124:PHE:CE1  | 35:l:252:MET:HB2  | 2.44                     | 0.53              |
| 35:l:298:ILE:O    | 35:l:302:VAL:HG23 | 2.09                     | 0.53              |
| 40:r:325:MET:HE2  | 40:r:362:ALA:HB2  | 1.91                     | 0.53              |
| 31:h:71:LYS:HA    | 31:h:74:LYS:HG2   | 1.90                     | 0.53              |
| 12:M:137:CYS:HB3  | 12:M:140:GLN:HB2  | 1.89                     | 0.53              |
| 35:l:228:GLY:HA3  | 48:l:703:PEE:H38  | 1.91                     | 0.53              |
| 40:r:196:TRP:CD1  | 40:r:250:LEU:HB3  | 2.44                     | 0.53              |
| 1:A:89:GLY:O      | 47:A:503:NAI:H2N  | 2.09                     | 0.53              |
| 7:H:76:GLN:O      | 7:H:78:GLU:N      | 2.41                     | 0.53              |
| 21:W:98:MET:HE3   | 21:W:101:VAL:HG21 | 1.91                     | 0.53              |
| 6:X:82:ARG:O      | 6:X:86:VAL:HG23   | 2.09                     | 0.53              |
| 44:w:209:VAL:HG22 | 44:w:260:ALA:HB2  | 1.91                     | 0.53              |
| 35:l:7:LEU:HD22   | 35:l:46:LEU:HD11  | 1.89                     | 0.53              |
| 12:M:566:ILE:HD13 | 12:M:579:MET:HE3  | 1.91                     | 0.53              |
| 26:c:136:PHE:O    | 26:c:140:MET:HG2  | 2.09                     | 0.53              |
| 5:F:19:ILE:HD12   | 5:F:51:LEU:HD21   | 1.91                     | 0.53              |
| 2:B:68:ARG:NH2    | 16:Q:260:GLU:OE2  | 2.40                     | 0.52              |
| 56:V:202:CDL:H871 | 35:l:558:LEU:HD21 | 1.90                     | 0.52              |
| 56:a:201:CDL:H321 | 48:l:704:PEE:H58  | 1.91                     | 0.52              |
| 25:b:18:LEU:HD11  | 39:p:163:LEU:HD22 | 1.90                     | 0.52              |
| 6:X:87:LEU:HB3    | 6:X:98:LEU:HD21   | 1.92                     | 0.52              |
| 49:j:203:PLX:H352 | 36:m:155:ILE:HG23 | 1.90                     | 0.52              |
| 41:s:24:GLU:HA    | 41:s:271:LEU:HD13 | 1.91                     | 0.52              |
| 31:h:94:PRO:HG2   | 31:h:99:LEU:HD11  | 1.92                     | 0.52              |
| 27:d:160:LYS:NZ   | 30:g:114:ILE:O    | 2.41                     | 0.52              |
| 40:r:114:GLU:OE2  | 40:r:116:ILE:HB   | 2.09                     | 0.52              |
| 40:r:403:THR:HA   | 40:r:406:TYR:CE2  | 2.44                     | 0.52              |
| 1:A:261:TRP:O     | 1:A:264:SER:OG    | 2.28                     | 0.52              |
| 24:a:139:ILE:HG23 | 40:r:54:LEU:HD23  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 30:g:55:VAL:HG21  | 56:r:503:CDL:HB61 | 1.91                     | 0.52              |
| 42:u:80:GLU:CD    | 42:u:80:GLU:H     | 2.18                     | 0.52              |
| 1:A:132:ARG:HB3   | 1:A:165:GLU:HG3   | 1.91                     | 0.52              |
| 2:B:111:GLU:O     | 2:B:141:ARG:NH1   | 2.43                     | 0.52              |
| 27:d:163:MET:HE1  | 28:e:147:ILE:HD12 | 1.92                     | 0.52              |
| 1:A:50:ASP:OD1    | 1:A:52:ARG:NH1    | 2.42                     | 0.52              |
| 4:E:123:TYR:CZ    | 12:M:320:GLU:HG3  | 2.45                     | 0.52              |
| 30:g:19:GLU:HG2   | 42:u:158:LEU:HD22 | 1.91                     | 0.52              |
| 40:r:243:MET:HB3  | 40:r:301:ILE:HG21 | 1.92                     | 0.52              |
| 8:I:109:ASP:OD2   | 21:W:21:TYR:OH    | 2.28                     | 0.52              |
| 24:a:152:LYS:HD3  | 30:g:96:VAL:HG21  | 1.90                     | 0.52              |
| 43:v:21:ARG:O     | 43:v:21:ARG:HG2   | 2.09                     | 0.52              |
| 56:V:204:CDL:H592 | 56:V:204:CDL:H782 | 1.92                     | 0.52              |
| 40:r:198:ALA:HB2  | 48:r:501:PEE:H22  | 1.90                     | 0.52              |
| 12:M:372:PHE:H    | 12:M:532:PRO:HB2  | 1.74                     | 0.52              |
| 56:l:701:CDL:H791 | 56:l:701:CDL:H582 | 1.92                     | 0.52              |
| 7:H:58:MET:HE3    | 7:H:72:LEU:HD23   | 1.92                     | 0.51              |
| 12:M:250:SER:OG   | 12:M:251:ILE:N    | 2.42                     | 0.51              |
| 48:r:501:PEE:H29  | 48:r:501:PEE:H71  | 1.92                     | 0.51              |
| 27:d:81:ASP:O     | 27:d:85:MET:HG3   | 2.11                     | 0.51              |
| 56:l:702:CDL:H201 | 56:l:702:CDL:H861 | 1.91                     | 0.51              |
| 32:i:72:MET:HB2   | 34:k:40:LEU:HD21  | 1.91                     | 0.51              |
| 32:i:265:MET:HE3  | 32:i:340:THR:HG21 | 1.91                     | 0.51              |
| 34:k:31:LEU:HD21  | 36:m:67:VAL:HG11  | 1.92                     | 0.51              |
| 42:u:79:ALA:O     | 42:u:83:THR:OG1   | 2.27                     | 0.51              |
| 37:n:17:VAL:HG13  | 40:r:7:PRO:HB3    | 1.92                     | 0.51              |
| 13:N:78:ASP:OD2   | 13:N:80:SER:OG    | 2.27                     | 0.51              |
| 33:j:53:MET:HE1   | 36:m:70:TYR:CD1   | 2.46                     | 0.51              |
| 40:r:122:PHE:CZ   | 40:r:206:LYS:HD2  | 2.46                     | 0.51              |
| 16:Q:84:PHE:HB3   | 16:Q:97:LEU:HB3   | 1.92                     | 0.51              |
| 26:c:156:VAL:HG11 | 43:v:95:TYR:CZ    | 2.46                     | 0.51              |
| 40:r:204:MET:HG3  | 40:r:209:LEU:HB2  | 1.92                     | 0.51              |
| 12:M:299:ARG:NH1  | 12:M:703:ALA:O    | 2.42                     | 0.51              |
| 34:k:27:MET:HE1   | 36:m:70:TYR:HB3   | 1.92                     | 0.51              |
| 40:r:282:LEU:HD13 | 40:r:342:MET:HG3  | 1.91                     | 0.51              |
| 4:E:120:SER:O     | 4:E:124:VAL:HG22  | 2.11                     | 0.51              |
| 20:V:25:SER:OG    | 20:V:67:GLY:O     | 2.22                     | 0.51              |
| 56:V:204:CDL:H222 | 56:V:204:CDL:H351 | 1.92                     | 0.51              |
| 1:A:88:ARG:NH2    | 1:A:273:THR:O     | 2.44                     | 0.51              |
| 6:G:138:LEU:HD13  | 6:G:144:ILE:HA    | 1.91                     | 0.51              |
| 9:J:173:ASP:HB3   | 9:J:176:SER:HB2   | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:O:59:ASN:ND2   | 14:O:89:GLN:OE1   | 2.41                     | 0.51              |
| 56:V:202:CDL:H361 | 38:o:88:LEU:HD21  | 1.93                     | 0.51              |
| 27:d:168:LYS:O    | 27:d:172:GLU:HG2  | 2.11                     | 0.51              |
| 32:i:128:LEU:O    | 32:i:132:THR:OG1  | 2.25                     | 0.51              |
| 32:i:276:ILE:HG21 | 48:r:501:PEE:H7   | 1.93                     | 0.51              |
| 21:W:54:ASN:HD22  | 41:s:156:MET:HE3  | 1.76                     | 0.50              |
| 26:c:96:ASP:N     | 26:c:96:ASP:OD1   | 2.43                     | 0.50              |
| 32:i:75:ILE:HD12  | 34:k:40:LEU:HD22  | 1.93                     | 0.50              |
| 40:r:266:MET:O    | 40:r:269:MET:HG2  | 2.10                     | 0.50              |
| 4:E:119:LEU:HD22  | 4:E:123:TYR:CZ    | 2.46                     | 0.50              |
| 11:L:102:ASP:OD1  | 11:L:102:ASP:N    | 2.44                     | 0.50              |
| 24:a:66:ARG:HH12  | 28:e:72:ASP:HB2   | 1.76                     | 0.50              |
| 26:c:149:ILE:HG22 | 26:c:150:TYR:CD1  | 2.46                     | 0.50              |
| 33:j:68:GLU:HG3   | 33:j:98:LEU:HD13  | 1.93                     | 0.50              |
| 35:l:250:SER:HB2  | 35:l:333:ALA:HA   | 1.92                     | 0.50              |
| 1:A:122:PRO:HA    | 14:O:176:CYS:SG   | 2.50                     | 0.50              |
| 5:F:23:LEU:O      | 5:F:57:GLU:HA     | 2.11                     | 0.50              |
| 56:V:202:CDL:H861 | 38:o:98:LEU:HD11  | 1.94                     | 0.50              |
| 9:J:87:GLU:HG3    | 9:J:89:TYR:H      | 1.77                     | 0.50              |
| 20:V:67:GLY:HA2   | 56:V:201:CDL:H221 | 1.93                     | 0.50              |
| 48:V:203:PEE:H7   | 35:l:568:PHE:HE2  | 1.76                     | 0.50              |
| 56:l:701:CDL:H311 | 56:l:701:CDL:H561 | 1.93                     | 0.50              |
| 40:r:118:PHE:O    | 40:r:122:PHE:HB3  | 2.12                     | 0.50              |
| 40:r:266:MET:HB3  | 40:r:395:LEU:HD13 | 1.93                     | 0.50              |
| 9:J:135:GLU:HG2   | 9:J:140:ASP:HA    | 1.93                     | 0.50              |
| 15:P:44:ARG:HB2   | 15:P:44:ARG:CZ    | 2.41                     | 0.50              |
| 15:P:69:LEU:HD13  | 15:P:96:VAL:HG22  | 1.94                     | 0.50              |
| 24:a:147:ALA:HB2  | 40:r:173:SER:HB2  | 1.92                     | 0.50              |
| 34:k:87:THR:HG22  | 34:k:89:TYR:H     | 1.75                     | 0.50              |
| 49:j:203:PLX:H251 | 36:m:151:THR:HG21 | 1.93                     | 0.50              |
| 26:c:60:GLU:OE1   | 26:c:60:GLU:N     | 2.44                     | 0.50              |
| 32:i:108:LEU:HD11 | 32:i:191:THR:HG21 | 1.94                     | 0.50              |
| 32:i:284:MET:HE1  | 40:r:155:ALA:HA   | 1.93                     | 0.50              |
| 25:b:99:GLU:HG2   | 35:l:61:MET:HE2   | 1.93                     | 0.50              |
| 35:l:536:LEU:HB3  | 35:l:537:PRO:HD3  | 1.94                     | 0.50              |
| 2:B:84:ILE:HA     | 13:N:58:ARG:HD3   | 1.93                     | 0.50              |
| 11:L:80:PHE:HE1   | 11:L:100:GLU:HG2  | 1.76                     | 0.50              |
| 14:O:213:ILE:HD12 | 14:O:214:PRO:HD2  | 1.94                     | 0.50              |
| 17:S:19:PRO:HB3   | 41:s:9:LEU:HD12   | 1.94                     | 0.50              |
| 35:l:245:ALA:O    | 35:l:249:SER:OG   | 2.24                     | 0.50              |
| 39:p:139:GLN:NE2  | 39:p:156:PRO:O    | 2.43                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:r:203:PHE:O    | 40:r:207:MET:HG2  | 2.11                     | 0.50              |
| 56:V:202:CDL:HB4  | 38:o:82:PRO:HB2   | 1.94                     | 0.49              |
| 25:b:104:ILE:HB   | 43:v:48:ASP:HB3   | 1.92                     | 0.49              |
| 27:d:167:ARG:HH21 | 28:e:153:GLU:HG3  | 1.76                     | 0.49              |
| 38:o:83:THR:HG22  | 38:o:85:LYS:H     | 1.77                     | 0.49              |
| 1:A:210:THR:HB    | 1:A:224:ARG:H     | 1.77                     | 0.49              |
| 12:M:44:GLU:HG3   | 12:M:45:PRO:HD2   | 1.93                     | 0.49              |
| 18:T:34:THR:HG21  | 18:T:52:ARG:NH1   | 2.27                     | 0.49              |
| 20:V:106:ARG:HE   | 20:V:106:ARG:HA   | 1.77                     | 0.49              |
| 25:b:81:ILE:HD13  | 48:l:704:PEE:H64  | 1.94                     | 0.49              |
| 49:j:203:PLX:H341 | 49:j:203:PLX:H151 | 1.94                     | 0.49              |
| 1:A:210:THR:HB    | 1:A:224:ARG:HG3   | 1.94                     | 0.49              |
| 13:N:85:GLU:HG2   | 13:N:86:TRP:H     | 1.77                     | 0.49              |
| 35:l:396:ILE:HG21 | 35:l:490:ALA:HB2  | 1.95                     | 0.49              |
| 11:L:111:LEU:HD11 | 13:N:126:PRO:HG2  | 1.94                     | 0.49              |
| 12:M:340:ALA:HB3  | 12:M:366:LEU:HD13 | 1.94                     | 0.49              |
| 16:Q:210:MET:HE2  | 16:Q:247:PHE:HZ   | 1.77                     | 0.49              |
| 44:w:58:LYS:O     | 44:w:60:ILE:HG13  | 2.12                     | 0.49              |
| 27:d:160:LYS:HE2  | 28:e:147:ILE:HG23 | 1.94                     | 0.49              |
| 41:s:102:VAL:HG21 | 41:s:154:LEU:HD11 | 1.94                     | 0.49              |
| 6:G:93:ILE:HD11   | 6:G:110:LEU:HD11  | 1.94                     | 0.49              |
| 6:G:93:ILE:HG21   | 6:G:98:LEU:HD13   | 1.94                     | 0.49              |
| 11:L:131:LYS:HD2  | 11:L:147:VAL:HG11 | 1.94                     | 0.49              |
| 28:e:92:PHE:O     | 28:e:96:SER:HB2   | 2.13                     | 0.49              |
| 30:g:48:ASN:HB3   | 30:g:55:VAL:HA    | 1.94                     | 0.49              |
| 40:r:105:PHE:O    | 40:r:109:THR:OG1  | 2.24                     | 0.49              |
| 49:r:502:PLX:H6   | 49:r:502:PLX:H261 | 1.95                     | 0.49              |
| 1:A:162:PHE:HB3   | 1:A:165:GLU:HB2   | 1.94                     | 0.49              |
| 36:m:17:PHE:HA    | 36:m:20:PHE:CE2   | 2.47                     | 0.49              |
| 38:o:65:LEU:HD11  | 40:r:343:ILE:HD11 | 1.94                     | 0.49              |
| 40:r:370:PRO:HG3  | 40:r:375:LEU:HD13 | 1.94                     | 0.49              |
| 4:E:23:ARG:HB2    | 4:E:27:GLU:OE2    | 2.13                     | 0.49              |
| 11:L:112:MET:SD   | 13:N:126:PRO:HB2  | 2.52                     | 0.49              |
| 21:W:69:ILE:HA    | 21:W:72:MET:HE3   | 1.95                     | 0.49              |
| 22:Y:76:ASP:O     | 35:l:385:TYR:OH   | 2.23                     | 0.49              |
| 35:l:561:ILE:HG13 | 35:l:562:LEU:H    | 1.77                     | 0.49              |
| 1:A:128:ARG:O     | 1:A:132:ARG:HG2   | 2.12                     | 0.48              |
| 5:F:21:ILE:HG12   | 5:F:65:LEU:HD12   | 1.95                     | 0.48              |
| 44:w:50:THR:HA    | 44:w:53:LEU:HD23  | 1.93                     | 0.48              |
| 16:Q:39:PRO:HB3   | 16:Q:43:TRP:CD1   | 2.48                     | 0.48              |
| 16:Q:80:LEU:HD11  | 41:s:126:LYS:HE3  | 1.94                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:T:54:ARG:O     | 18:T:58:ARG:NH2   | 2.45                     | 0.48              |
| 20:V:38:ALA:HB2   | 56:V:204:CDL:H251 | 1.95                     | 0.48              |
| 35:l:233:LEU:HB3  | 35:l:234:PRO:HD3  | 1.94                     | 0.48              |
| 2:B:211:TYR:CZ    | 8:I:39:PRO:HG3    | 2.49                     | 0.48              |
| 9:J:179:ARG:HG2   | 9:J:179:ARG:HH11  | 1.78                     | 0.48              |
| 12:M:390:THR:HA   | 12:M:600:GLU:HG2  | 1.95                     | 0.48              |
| 13:N:144:TYR:CZ   | 13:N:145:LYS:HD2  | 2.48                     | 0.48              |
| 23:Z:18:ASP:O     | 23:Z:21:GLN:NE2   | 2.30                     | 0.48              |
| 48:j:202:PEE:H31  | 56:s:401:CDL:H222 | 1.94                     | 0.48              |
| 24:a:134:GLU:HG2  | 37:n:38:PHE:O     | 2.13                     | 0.48              |
| 26:c:58:ARG:NH1   | 26:c:61:ASP:OD1   | 2.46                     | 0.48              |
| 26:c:166:LEU:HB3  | 26:c:169:GLU:HB2  | 1.96                     | 0.48              |
| 32:i:11:MET:HE1   | 56:i:401:CDL:H771 | 1.95                     | 0.48              |
| 32:i:277:ILE:O    | 32:i:281:LEU:HG   | 2.14                     | 0.48              |
| 2:B:120:GLU:OE2   | 15:P:231:ARG:NH1  | 2.47                     | 0.48              |
| 11:L:107:TRP:HH2  | 11:L:118:ALA:HB2  | 1.79                     | 0.48              |
| 12:M:591:GLU:HG2  | 12:M:610:VAL:HG23 | 1.93                     | 0.48              |
| 19:U:66:VAL:O     | 42:u:130:LYS:HE3  | 2.13                     | 0.48              |
| 35:l:27:TYR:O     | 35:l:115:ASN:ND2  | 2.42                     | 0.48              |
| 48:C:302:PEE:H70  | 48:C:302:PEE:H36  | 1.96                     | 0.48              |
| 14:O:137:THR:HG22 | 14:O:138:THR:H    | 1.78                     | 0.48              |
| 56:l:701:CDL:H331 | 56:l:701:CDL:H142 | 1.95                     | 0.48              |
| 12:M:295:ASP:OD1  | 12:M:704:SER:OG   | 2.29                     | 0.48              |
| 23:Z:59:ASN:O     | 35:l:364:LYS:NZ   | 2.47                     | 0.48              |
| 23:Z:78:PHE:O     | 23:Z:82:VAL:HG23  | 2.13                     | 0.48              |
| 29:f:70:LYS:HE3   | 29:f:76:GLU:HB2   | 1.95                     | 0.48              |
| 32:i:95:MET:HE1   | 32:i:145:ILE:HD12 | 1.96                     | 0.48              |
| 2:B:200:GLU:HG3   | 13:N:88:ARG:HD3   | 1.95                     | 0.48              |
| 9:J:354:ARG:NH1   | 9:J:362:LEU:O     | 2.46                     | 0.48              |
| 41:s:157:ASN:OD1  | 41:s:168:THR:OG1  | 2.28                     | 0.48              |
| 48:C:302:PEE:H35  | 49:C:303:PLX:H392 | 1.96                     | 0.48              |
| 6:G:142:GLN:NE2   | 6:G:146:ASP:OD1   | 2.47                     | 0.48              |
| 9:J:38:HIS:CE1    | 13:N:132:LYS:HE3  | 2.49                     | 0.48              |
| 35:l:292:ALA:HB2  | 35:l:304:PHE:HB3  | 1.95                     | 0.48              |
| 43:v:8:ARG:NH2    | 43:v:18:ASP:OD1   | 2.46                     | 0.48              |
| 14:O:134:VAL:HG22 | 14:O:186:VAL:HG22 | 1.94                     | 0.48              |
| 35:l:505:ASN:O    | 35:l:508:THR:HG22 | 2.14                     | 0.48              |
| 15:P:125:ARG:NH2  | 15:P:201:ASP:OD1  | 2.39                     | 0.47              |
| 9:J:199:THR:OG1   | 9:J:258:ALA:O     | 2.29                     | 0.47              |
| 14:O:177:LEU:HD13 | 14:O:187:GLN:HB2  | 1.96                     | 0.47              |
| 32:i:244:MET:HE3  | 32:i:244:MET:HB2  | 1.72                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:124:MET:HE2   | 3:C:128:ARG:HB2   | 1.97                     | 0.47              |
| 7:H:96:ARG:HG2    | 7:H:96:ARG:HH11   | 1.78                     | 0.47              |
| 16:Q:84:PHE:HB2   | 16:Q:99:MET:HE2   | 1.97                     | 0.47              |
| 21:W:91:LEU:HD22  | 42:u:7:LEU:HD12   | 1.96                     | 0.47              |
| 36:m:3:MET:HE2    | 36:m:3:MET:HA     | 1.96                     | 0.47              |
| 2:B:86:TYR:CD1    | 2:B:87:PRO:HA     | 2.49                     | 0.47              |
| 35:l:331:MET:HE1  | 35:l:468:ILE:HD12 | 1.97                     | 0.47              |
| 49:r:502:PLX:H101 | 49:r:502:PLX:H72  | 1.57                     | 0.47              |
| 12:M:354:LEU:HD22 | 12:M:548:LEU:HD22 | 1.95                     | 0.47              |
| 12:M:651:PRO:O    | 12:M:654:VAL:HG22 | 2.14                     | 0.47              |
| 13:N:85:GLU:HB2   | 13:N:98:PRO:HB3   | 1.97                     | 0.47              |
| 25:b:73:THR:HA    | 25:b:77:ILE:HD12  | 1.96                     | 0.47              |
| 3:C:49:LYS:HA     | 3:C:49:LYS:HD3    | 1.70                     | 0.47              |
| 9:J:168:SER:O     | 9:J:203:PRO:HD2   | 2.14                     | 0.47              |
| 12:M:222:ILE:HA   | 12:M:225:ILE:HG12 | 1.96                     | 0.47              |
| 35:l:401:MET:HE3  | 35:l:401:MET:HB3  | 1.74                     | 0.47              |
| 40:r:233:ALA:HA   | 40:r:320:GLY:HA2  | 1.97                     | 0.47              |
| 49:J:403:PLX:H32  | 33:j:23:TRP:HZ3   | 1.79                     | 0.47              |
| 15:P:75:GLN:HB3   | 15:P:87:PHE:CD1   | 2.50                     | 0.47              |
| 16:Q:191:ALA:HB1  | 16:Q:196:ALA:HB3  | 1.97                     | 0.47              |
| 21:W:95:ALA:HA    | 21:W:106:VAL:HG21 | 1.96                     | 0.47              |
| 56:a:201:CDL:H171 | 56:a:201:CDL:H712 | 1.96                     | 0.47              |
| 26:c:85:GLU:OE2   | 38:o:13:THR:OG1   | 2.28                     | 0.47              |
| 26:c:167:TYR:CD2  | 26:c:178:PRO:HG3  | 2.50                     | 0.47              |
| 32:i:20:VAL:HG11  | 32:i:137:ALA:HB1  | 1.95                     | 0.47              |
| 49:j:203:PLX:H132 | 49:j:203:PLX:H161 | 1.44                     | 0.47              |
| 35:l:136:ASN:HA   | 35:l:197:ASP:HA   | 1.96                     | 0.47              |
| 39:p:101:GLU:OE1  | 39:p:122:ARG:NH2  | 2.41                     | 0.47              |
| 40:r:357:THR:O    | 40:r:361:VAL:HG23 | 2.14                     | 0.47              |
| 43:v:39:MET:SD    | 43:v:58:TYR:HA    | 2.55                     | 0.47              |
| 2:B:131:GLU:HG3   | 2:B:144:ARG:HD2   | 1.95                     | 0.47              |
| 7:H:44:TYR:HB2    | 15:P:68:ILE:HG23  | 1.97                     | 0.47              |
| 48:V:203:PEE:H7   | 35:l:568:PHE:CE2  | 2.50                     | 0.47              |
| 28:e:137:MET:HE3  | 28:e:137:MET:HB2  | 1.82                     | 0.47              |
| 35:l:327:LEU:O    | 35:l:331:MET:HG2  | 2.15                     | 0.47              |
| 49:J:403:PLX:H251 | 49:J:403:PLX:H282 | 1.58                     | 0.47              |
| 15:P:119:VAL:HG12 | 15:P:121:THR:HG22 | 1.97                     | 0.47              |
| 20:V:49:PHE:O     | 20:V:53:VAL:HG23  | 2.15                     | 0.47              |
| 27:d:115:GLN:HG2  | 35:l:62:ILE:HG12  | 1.97                     | 0.47              |
| 35:l:10:THR:O     | 35:l:14:ILE:HG23  | 2.14                     | 0.47              |
| 40:r:72:LEU:HD12  | 40:r:234:VAL:HG23 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:127:ASP:OD2   | 1:A:245:VAL:HB    | 2.15                     | 0.47              |
| 12:M:638:THR:O    | 12:M:642:VAL:HG23 | 2.14                     | 0.47              |
| 20:V:66:ILE:HD11  | 20:V:101:LEU:HB2  | 1.95                     | 0.47              |
| 21:W:48:TRP:CZ2   | 21:W:52:LYS:HE2   | 2.50                     | 0.47              |
| 49:e:201:PLX:H222 | 35:l:23:ASN:HB2   | 1.97                     | 0.47              |
| 40:r:104:LEU:O    | 40:r:108:MET:HG3  | 2.15                     | 0.47              |
| 16:Q:184:ILE:HG12 | 16:Q:203:MET:HE3  | 1.95                     | 0.46              |
| 22:Y:87:PRO:HG3   | 43:v:96:VAL:HG22  | 1.96                     | 0.46              |
| 24:a:95:GLU:OE1   | 56:a:201:CDL:O1   | 2.22                     | 0.46              |
| 35:l:119:LYS:NZ   | 56:l:701:CDL:OA3  | 2.48                     | 0.46              |
| 9:J:369:VAL:HG12  | 9:J:369:VAL:O     | 2.16                     | 0.46              |
| 16:Q:184:ILE:HD11 | 16:Q:251:PHE:CZ   | 2.50                     | 0.46              |
| 34:k:37:MET:HE1   | 34:k:63:LEU:HD22  | 1.96                     | 0.46              |
| 35:l:312:LEU:O    | 35:l:315:VAL:HG22 | 2.14                     | 0.46              |
| 1:A:110:PRO:O     | 1:A:238:CYS:HB3   | 2.16                     | 0.46              |
| 1:A:248:VAL:O     | 1:A:251:SER:OG    | 2.27                     | 0.46              |
| 8:I:54:TYR:CZ     | 16:Q:362:LYS:HD2  | 2.50                     | 0.46              |
| 12:M:309:ASN:OD1  | 12:M:311:LYS:N    | 2.42                     | 0.46              |
| 12:M:460:HIS:CG   | 12:M:461:PRO:HD2  | 2.50                     | 0.46              |
| 24:a:60:SER:HB2   | 39:p:107:TRP:HA   | 1.97                     | 0.46              |
| 26:c:129:MET:HB3  | 35:l:528:TYR:CG   | 2.50                     | 0.46              |
| 35:l:557:TRP:O    | 35:l:561:ILE:HG12 | 2.16                     | 0.46              |
| 40:r:94:LEU:HD21  | 56:r:503:CDL:H312 | 1.97                     | 0.46              |
| 44:w:95:ASP:OD1   | 44:w:95:ASP:N     | 2.47                     | 0.46              |
| 1:A:66:LYS:O      | 1:A:70:LEU:HG     | 2.15                     | 0.46              |
| 2:B:116:CYS:SG    | 2:B:118:LEU:HG    | 2.55                     | 0.46              |
| 8:I:70:MET:HG3    | 15:P:66:ALA:HB1   | 1.98                     | 0.46              |
| 20:V:38:ALA:HA    | 56:V:204:CDL:H201 | 1.97                     | 0.46              |
| 27:d:127:LYS:HA   | 27:d:127:LYS:HD3  | 1.76                     | 0.46              |
| 32:i:65:THR:O     | 32:i:69:MET:HG3   | 2.16                     | 0.46              |
| 32:i:311:MET:HE2  | 32:i:311:MET:HB2  | 1.78                     | 0.46              |
| 35:l:562:LEU:HD21 | 48:r:501:PEE:H45  | 1.98                     | 0.46              |
| 39:p:138:LYS:HD3  | 39:p:138:LYS:HA   | 1.65                     | 0.46              |
| 12:M:485:ASP:HA   | 12:M:677:GLN:OE1  | 2.16                     | 0.46              |
| 12:M:489:ILE:O    | 12:M:493:VAL:HG23 | 2.15                     | 0.46              |
| 15:P:44:ARG:CB    | 15:P:45:PRO:CD    | 2.36                     | 0.46              |
| 1:A:118:ASP:O     | 1:A:159:ARG:HD2   | 2.16                     | 0.46              |
| 21:W:54:ASN:ND2   | 41:s:156:MET:HE3  | 2.30                     | 0.46              |
| 26:c:129:MET:HB2  | 35:l:532:ILE:HD11 | 1.98                     | 0.46              |
| 28:e:55:LEU:HD11  | 44:w:320:GLY:HA2  | 1.98                     | 0.46              |
| 35:l:529:TYR:HB3  | 35:l:530:PRO:HD3  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:r:10:MET:HE1   | 56:r:503:CDL:H632 | 1.97                     | 0.46              |
| 5:F:61:VAL:HG23   | 5:F:62:GLN:H      | 1.81                     | 0.46              |
| 7:H:25:LYS:HE2    | 7:H:60:LYS:HG2    | 1.97                     | 0.46              |
| 12:M:547:LEU:HD11 | 12:M:579:MET:HE2  | 1.98                     | 0.46              |
| 23:Z:35:LYS:HB3   | 23:Z:35:LYS:HE2   | 1.72                     | 0.46              |
| 27:d:32:TYR:CE2   | 27:d:36:ILE:HD11  | 2.50                     | 0.46              |
| 34:k:17:ALA:O     | 34:k:21:MET:HG3   | 2.15                     | 0.46              |
| 56:l:701:CDL:H202 | 56:l:701:CDL:H231 | 1.81                     | 0.46              |
| 40:r:342:MET:HE3  | 40:r:413:THR:HG21 | 1.98                     | 0.46              |
| 41:s:207:LEU:O    | 41:s:209:SER:N    | 2.48                     | 0.46              |
| 44:w:244:THR:O    | 44:w:248:GLU:HB2  | 2.15                     | 0.46              |
| 22:Y:44:TYR:O     | 22:Y:45:ARG:HB2   | 2.16                     | 0.46              |
| 32:i:98:MET:HE2   | 32:i:98:MET:HB2   | 1.86                     | 0.46              |
| 32:i:268:GLN:O    | 32:i:271:THR:OG1  | 2.33                     | 0.46              |
| 32:i:313:MET:HE3  | 44:w:141:LEU:HD22 | 1.97                     | 0.46              |
| 42:u:77:HIS:CE1   | 42:u:115:LEU:HD21 | 2.50                     | 0.46              |
| 1:A:334:THR:O     | 1:A:334:THR:OG1   | 2.30                     | 0.46              |
| 7:H:22:GLU:OE1    | 7:H:22:GLU:N      | 2.33                     | 0.46              |
| 12:M:339:ALA:HB1  | 12:M:537:ILE:HD12 | 1.98                     | 0.46              |
| 28:e:55:LEU:CD2   | 28:e:57:GLU:HB2   | 2.46                     | 0.46              |
| 28:e:72:ASP:OD1   | 28:e:72:ASP:N     | 2.48                     | 0.46              |
| 28:e:99:LEU:HD12  | 28:e:99:LEU:HA    | 1.84                     | 0.46              |
| 32:i:54:GLU:HG3   | 34:k:93:LEU:HB3   | 1.97                     | 0.46              |
| 35:l:558:LEU:HD23 | 35:l:561:ILE:HD11 | 1.97                     | 0.46              |
| 36:m:31:LEU:HD21  | 56:s:401:CDL:H542 | 1.96                     | 0.46              |
| 41:s:20:LEU:HD12  | 41:s:20:LEU:O     | 2.15                     | 0.46              |
| 2:B:89:GLU:OE1    | 13:N:58:ARG:HD2   | 2.16                     | 0.46              |
| 9:J:370:LYS:HD2   | 9:J:370:LYS:O     | 2.16                     | 0.46              |
| 12:M:421:SER:OG   | 12:M:427:LEU:HD22 | 2.16                     | 0.46              |
| 16:Q:442:HIS:HB3  | 16:Q:446:ASP:HB2  | 1.97                     | 0.46              |
| 56:a:201:CDL:H572 | 48:l:704:PEE:H20  | 1.97                     | 0.46              |
| 28:e:76:TYR:HB2   | 28:e:83:ASP:OD1   | 2.16                     | 0.46              |
| 33:j:109:LYS:HA   | 33:j:109:LYS:HD3  | 1.66                     | 0.46              |
| 35:l:592:LEU:O    | 35:l:596:MET:HG3  | 2.16                     | 0.46              |
| 40:r:231:LEU:HD23 | 40:r:235:LEU:HD12 | 1.98                     | 0.46              |
| 44:w:68:SER:HA    | 44:w:217:ARG:HH21 | 1.81                     | 0.46              |
| 6:X:80:LYS:HE3    | 6:X:80:LYS:HB3    | 1.59                     | 0.45              |
| 26:c:84:GLN:HG2   | 26:c:114:ARG:HB2  | 1.96                     | 0.45              |
| 41:s:20:LEU:HG    | 41:s:228:TYR:CD2  | 2.51                     | 0.45              |
| 7:H:30:LYS:NZ     | 44:w:272:ASP:OD1  | 2.41                     | 0.45              |
| 15:P:132:LEU:HB2  | 15:P:141:ILE:HG22 | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:40:SER:HA    | 56:V:201:CDL:HB62 | 1.96                     | 0.45              |
| 56:a:201:CDL:H361 | 56:a:201:CDL:H392 | 1.59                     | 0.45              |
| 34:k:4:VAL:O      | 34:k:8:ILE:HG12   | 2.16                     | 0.45              |
| 3:C:188:LYS:HB2   | 3:C:188:LYS:HE3   | 1.59                     | 0.45              |
| 12:M:405:THR:HB   | 12:M:477:GLY:HA3  | 1.98                     | 0.45              |
| 16:Q:181:LEU:HD21 | 16:Q:210:MET:HB2  | 1.98                     | 0.45              |
| 40:r:281:ASP:OD1  | 40:r:340:ARG:HB3  | 2.17                     | 0.45              |
| 40:r:406:TYR:O    | 40:r:409:TYR:HB3  | 2.16                     | 0.45              |
| 42:u:19:LYS:HE3   | 42:u:19:LYS:HB3   | 1.83                     | 0.45              |
| 32:i:62:THR:HG21  | 32:i:114:TRP:CD1  | 2.51                     | 0.45              |
| 35:l:363:TYR:HD1  | 35:l:364:LYS:HG2  | 1.82                     | 0.45              |
| 41:s:186:PHE:O    | 41:s:189:THR:OG1  | 2.27                     | 0.45              |
| 1:A:62:TRP:CD2    | 1:A:181:LEU:HD13  | 2.51                     | 0.45              |
| 8:I:30:GLU:CD     | 8:I:30:GLU:H      | 2.25                     | 0.45              |
| 13:N:85:GLU:HG2   | 13:N:86:TRP:N     | 2.32                     | 0.45              |
| 40:r:185:PRO:HB3  | 40:r:252:PRO:HD3  | 1.98                     | 0.45              |
| 1:A:283:ASN:ND2   | 1:A:305:GLY:O     | 2.49                     | 0.45              |
| 49:J:403:PLX:H92  | 49:J:403:PLX:H122 | 1.66                     | 0.45              |
| 17:S:63:THR:HG23  | 42:u:21:SER:HB2   | 1.98                     | 0.45              |
| 56:V:202:CDL:H782 | 35:l:557:TRP:CD2  | 2.51                     | 0.45              |
| 26:c:46:GLU:H     | 26:c:46:GLU:CD    | 2.23                     | 0.45              |
| 35:l:338:MET:HA   | 35:l:341:MET:HE2  | 1.99                     | 0.45              |
| 56:l:701:CDL:H391 | 40:r:371:PRO:HD2  | 1.99                     | 0.45              |
| 43:v:27:PRO:O     | 43:v:34:ARG:NH1   | 2.50                     | 0.45              |
| 3:C:101:ASP:OD2   | 41:s:54:LYS:NZ    | 2.33                     | 0.45              |
| 53:J:402:UQ:HM53  | 53:J:402:UQ:H71   | 1.79                     | 0.45              |
| 12:M:306:MET:HE3  | 12:M:316:TYR:CE1  | 2.52                     | 0.45              |
| 12:M:389:THR:O    | 12:M:390:THR:OG1  | 2.28                     | 0.45              |
| 56:V:204:CDL:H362 | 56:V:204:CDL:H392 | 1.66                     | 0.45              |
| 49:a:202:PLX:H141 | 28:e:105:PHE:HB2  | 1.99                     | 0.45              |
| 27:d:101:GLU:OE1  | 28:e:119:ARG:NE   | 2.44                     | 0.45              |
| 48:j:201:PEE:H59  | 48:j:201:PEE:H64  | 1.70                     | 0.45              |
| 35:l:311:GLY:O    | 35:l:315:VAL:HG13 | 2.17                     | 0.45              |
| 35:l:332:HIS:HA   | 35:l:335:PHE:CZ   | 2.51                     | 0.45              |
| 9:J:184:LYS:O     | 9:J:188:GLU:HG2   | 2.16                     | 0.45              |
| 32:i:51:ARG:HG2   | 34:k:96:LEU:HD21  | 1.98                     | 0.45              |
| 5:F:68:ARG:NH2    | 12:M:364:ASP:OD2  | 2.50                     | 0.45              |
| 8:I:97:PRO:HD3    | 15:P:61:PHE:CE1   | 2.52                     | 0.45              |
| 9:J:370:LYS:HB3   | 9:J:370:LYS:HE3   | 1.74                     | 0.45              |
| 38:o:117:GLN:OE1  | 38:o:117:GLN:HA   | 2.16                     | 0.45              |
| 3:C:83:ARG:NH1    | 16:Q:212:GLU:OE2  | 2.31                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:103:ASP:OD1  | 21:W:103:ASP:N    | 2.50                     | 0.45              |
| 33:j:61:THR:OG1   | 33:j:105:GLU:OE2  | 2.27                     | 0.45              |
| 33:j:73:LEU:HD12  | 36:m:55:MET:HE1   | 1.98                     | 0.45              |
| 37:n:34:LYS:HE2   | 37:n:34:LYS:HB2   | 1.68                     | 0.45              |
| 41:s:149:ILE:HG21 | 41:s:185:TRP:HB2  | 1.99                     | 0.45              |
| 44:w:181:LYS:HE3  | 44:w:181:LYS:HB3  | 1.64                     | 0.45              |
| 44:w:295:ARG:HA   | 44:w:298:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:217:GLU:OE2   | 1:A:236:PHE:N     | 2.43                     | 0.44              |
| 7:H:94:MET:HE1    | 15:P:69:LEU:HD21  | 1.99                     | 0.44              |
| 9:J:36:LEU:HD23   | 9:J:41:ILE:HG12   | 1.99                     | 0.44              |
| 10:K:89:LEU:O     | 10:K:93:LEU:HG    | 2.18                     | 0.44              |
| 11:L:76:LYS:HE3   | 11:L:146:ASP:OD1  | 2.16                     | 0.44              |
| 12:M:151:SER:HB3  | 16:Q:374:SER:HB3  | 1.98                     | 0.44              |
| 6:X:105:MET:H     | 6:X:105:MET:HG2   | 1.61                     | 0.44              |
| 25:b:32:GLU:HB3   | 39:p:115:TYR:HD1  | 1.81                     | 0.44              |
| 26:c:162:PRO:HB3  | 43:v:39:MET:HG3   | 1.98                     | 0.44              |
| 32:i:245:MET:HE3  | 32:i:245:MET:HB3  | 1.92                     | 0.44              |
| 32:i:261:MET:HB2  | 32:i:337:LEU:HD12 | 1.98                     | 0.44              |
| 35:l:141:PHE:HE2  | 40:r:375:LEU:HD11 | 1.80                     | 0.44              |
| 35:l:146:GLY:O    | 35:l:150:MET:HG2  | 2.17                     | 0.44              |
| 56:l:702:CDL:H542 | 56:l:702:CDL:H511 | 1.57                     | 0.44              |
| 1:A:367:ILE:O     | 1:A:371:ILE:HG12  | 2.17                     | 0.44              |
| 47:A:503:NAI:H6N  | 47:A:503:NAI:H2D  | 1.66                     | 0.44              |
| 49:C:303:PLX:H1C3 | 49:C:303:PLX:H21  | 1.77                     | 0.44              |
| 4:E:16:SER:HA     | 11:L:52:LEU:HD13  | 2.00                     | 0.44              |
| 12:M:47:THR:O     | 12:M:96:VAL:HG12  | 2.17                     | 0.44              |
| 32:i:89:MET:HE3   | 32:i:98:MET:HE3   | 1.99                     | 0.44              |
| 35:l:358:LYS:HG3  | 39:p:80:TYR:CE1   | 2.52                     | 0.44              |
| 35:l:400:ASN:HB3  | 35:l:486:MET:SD   | 2.57                     | 0.44              |
| 35:l:530:PRO:O    | 35:l:534:HIS:HB2  | 2.17                     | 0.44              |
| 8:I:64:MET:HE2    | 15:P:80:CYS:SG    | 2.57                     | 0.44              |
| 19:U:59:ASP:OD2   | 42:u:130:LYS:HD3  | 2.17                     | 0.44              |
| 32:i:102:LEU:HD13 | 32:i:142:LEU:HG   | 2.00                     | 0.44              |
| 35:l:572:LYS:HA   | 35:l:572:LYS:HD3  | 1.82                     | 0.44              |
| 48:B:303:PEE:H59  | 41:s:277:TYR:CE2  | 2.52                     | 0.44              |
| 49:J:403:PLX:H371 | 49:J:403:PLX:H322 | 1.99                     | 0.44              |
| 12:M:219:SER:O    | 12:M:222:ILE:HG12 | 2.17                     | 0.44              |
| 56:V:202:CDL:H401 | 56:V:202:CDL:H371 | 1.57                     | 0.44              |
| 35:l:12:LEU:HD22  | 35:l:129:MET:HB3  | 1.99                     | 0.44              |
| 56:l:701:CDL:H342 | 56:l:701:CDL:H372 | 1.82                     | 0.44              |
| 1:A:384:PRO:HB2   | 1:A:423:THR:HG22  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:B:303:PEE:H14  | 48:B:303:PEE:H20  | 1.57                     | 0.44              |
| 4:E:23:ARG:HD2    | 11:L:53:ILE:HG22  | 1.99                     | 0.44              |
| 13:N:123:GLN:O    | 18:T:59:GLN:NE2   | 2.48                     | 0.44              |
| 56:V:204:CDL:H811 | 56:V:204:CDL:H632 | 2.00                     | 0.44              |
| 26:c:58:ARG:NE    | 38:o:35:GLU:OE1   | 2.46                     | 0.44              |
| 34:k:64:LEU:O     | 34:k:67:ALA:HB3   | 2.17                     | 0.44              |
| 49:r:502:PLX:H92  | 49:r:502:PLX:H121 | 1.63                     | 0.44              |
| 41:s:7:LEU:HA     | 41:s:10:ILE:HG12  | 1.99                     | 0.44              |
| 3:C:173:LEU:O     | 3:C:177:ILE:HG12  | 2.18                     | 0.44              |
| 12:M:81:GLU:OE1   | 12:M:106:SER:OG   | 2.32                     | 0.44              |
| 16:Q:178:THR:OG1  | 16:Q:214:TYR:OH   | 2.35                     | 0.44              |
| 33:j:83:ASN:OD1   | 33:j:83:ASN:N     | 2.37                     | 0.44              |
| 35:l:554:ASP:OD2  | 40:r:288:TYR:OH   | 2.21                     | 0.44              |
| 9:J:257:ASP:OD1   | 9:J:257:ASP:C     | 2.60                     | 0.44              |
| 16:Q:206:GLU:O    | 16:Q:210:MET:HG3  | 2.17                     | 0.44              |
| 19:U:27:GLY:O     | 19:U:31:ILE:HG23  | 2.18                     | 0.44              |
| 26:c:38:PRO:HG2   | 38:o:70:TYR:HD2   | 1.83                     | 0.44              |
| 35:l:332:HIS:HA   | 35:l:335:PHE:CE2  | 2.53                     | 0.44              |
| 35:l:526:LEU:HD12 | 35:l:530:PRO:HG2  | 2.00                     | 0.44              |
| 40:r:373:ILE:HD11 | 40:r:444:LEU:HD23 | 2.00                     | 0.44              |
| 44:w:345:GLU:HB3  | 44:w:352:ILE:HD12 | 2.00                     | 0.44              |
| 3:C:116:ALA:O     | 3:C:120:VAL:HG22  | 2.17                     | 0.44              |
| 9:J:157:LYS:NZ    | 9:J:197:GLU:OE1   | 2.34                     | 0.44              |
| 17:S:66:LEU:O     | 17:S:69:ILE:HG12  | 2.17                     | 0.44              |
| 56:a:201:CDL:OA4  | 25:b:89:HIS:NE2   | 2.36                     | 0.44              |
| 32:i:172:GLN:HB2  | 32:i:178:ILE:HG13 | 1.98                     | 0.44              |
| 48:j:202:PEE:P    | 41:s:62:ARG:HH12  | 2.40                     | 0.44              |
| 35:l:264:TYR:CD2  | 35:l:265:PRO:HD3  | 2.52                     | 0.44              |
| 40:r:189:SER:HA   | 49:r:502:PLX:H1B3 | 2.00                     | 0.44              |
| 53:s:402:UQ:H221  | 53:s:402:UQ:H262  | 1.67                     | 0.44              |
| 9:J:171:ASN:HA    | 9:J:327:MET:HE3   | 2.00                     | 0.44              |
| 12:M:367:CYS:HB3  | 12:M:533:GLY:O    | 2.18                     | 0.44              |
| 14:O:158:ILE:HB   | 14:O:162:GLU:HB2  | 2.00                     | 0.44              |
| 17:S:31:ASN:ND2   | 17:S:36:LYS:HB2   | 2.32                     | 0.44              |
| 20:V:63:SER:HB3   | 56:V:201:CDL:H172 | 2.00                     | 0.44              |
| 56:a:201:CDL:H342 | 56:a:201:CDL:H372 | 1.92                     | 0.44              |
| 32:i:243:LEU:HD22 | 32:i:330:ILE:HG21 | 2.00                     | 0.44              |
| 35:l:97:THR:HG21  | 35:l:125:LEU:HD22 | 2.00                     | 0.44              |
| 8:I:70:MET:O      | 8:I:70:MET:SD     | 2.76                     | 0.43              |
| 40:r:57:PHE:CD1   | 40:r:113:THR:HG22 | 2.53                     | 0.43              |
| 49:r:502:PLX:H6   | 49:r:502:PLX:H51  | 1.39                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:45:LEU:O     | 44:w:45:LEU:HD12  | 2.17                     | 0.43              |
| 44:w:215:GLN:O    | 44:w:219:GLN:NE2  | 2.51                     | 0.43              |
| 2:B:135:ARG:HD3   | 2:B:141:ARG:HG3   | 2.00                     | 0.43              |
| 5:F:46:LYS:HE3    | 5:F:46:LYS:HB2    | 1.79                     | 0.43              |
| 16:Q:198:THR:OG1  | 41:s:275:ALA:O    | 2.30                     | 0.43              |
| 26:c:164:ASN:HA   | 26:c:181:VAL:HB   | 1.99                     | 0.43              |
| 36:m:33:LEU:HD23  | 36:m:64:MET:HE3   | 2.00                     | 0.43              |
| 40:r:193:ILE:HD11 | 40:r:256:TYR:OH   | 2.18                     | 0.43              |
| 41:s:20:LEU:HG    | 41:s:228:TYR:HD2  | 1.83                     | 0.43              |
| 1:A:90:GLY:HA3    | 47:A:503:NAI:H1D  | 2.00                     | 0.43              |
| 19:U:39:THR:HG23  | 41:s:309:ILE:HG22 | 1.99                     | 0.43              |
| 25:b:123:PHE:CZ   | 43:v:61:HIS:HB2   | 2.52                     | 0.43              |
| 49:e:201:PLX:H352 | 40:r:443:PRO:HB3  | 1.99                     | 0.43              |
| 32:i:221:HIS:O    | 32:i:319:HIS:HE1  | 2.01                     | 0.43              |
| 56:r:503:CDL:H761 | 56:r:503:CDL:H791 | 1.46                     | 0.43              |
| 16:Q:412:VAL:HB   | 16:Q:421:ARG:HB3  | 1.99                     | 0.43              |
| 19:U:26:GLY:HA3   | 48:j:201:PEE:H37  | 2.00                     | 0.43              |
| 21:W:90:ASN:ND2   | 21:W:123:GLU:O    | 2.51                     | 0.43              |
| 6:X:93:ILE:HG21   | 6:X:98:LEU:HD22   | 2.01                     | 0.43              |
| 32:i:313:MET:HE1  | 44:w:138:SER:HA   | 2.00                     | 0.43              |
| 34:k:60:PRO:O     | 34:k:63:LEU:HB2   | 2.18                     | 0.43              |
| 36:m:82:VAL:HG22  | 36:m:83:TRP:H     | 1.83                     | 0.43              |
| 36:m:86:ASN:OD1   | 36:m:87:LYS:N     | 2.51                     | 0.43              |
| 40:r:202:ALA:O    | 40:r:205:VAL:HG12 | 2.18                     | 0.43              |
| 41:s:68:ILE:HG13  | 56:s:401:CDL:H121 | 2.01                     | 0.43              |
| 1:A:76:ILE:HG23   | 1:A:255:CYS:SG    | 2.59                     | 0.43              |
| 49:J:403:PLX:H1C3 | 49:J:403:PLX:H21  | 1.76                     | 0.43              |
| 14:O:193:TYR:OH   | 14:O:214:PRO:HG2  | 2.18                     | 0.43              |
| 15:P:156:SER:O    | 15:P:156:SER:OG   | 2.34                     | 0.43              |
| 33:j:73:LEU:N     | 33:j:74:PRO:HD2   | 2.34                     | 0.43              |
| 6:G:83:VAL:O      | 6:G:87:LEU:HG     | 2.18                     | 0.43              |
| 15:P:122:ARG:NH1  | 15:P:127:GLU:OE1  | 2.49                     | 0.43              |
| 15:P:187:ILE:HG23 | 15:P:188:LEU:HG   | 2.00                     | 0.43              |
| 16:Q:36:GLN:NE2   | 40:r:137:GLY:O    | 2.40                     | 0.43              |
| 18:T:104:LYS:HE2  | 18:T:104:LYS:HB2  | 1.83                     | 0.43              |
| 42:u:83:THR:HA    | 42:u:86:TRP:NE1   | 2.34                     | 0.43              |
| 1:A:322:SER:HB2   | 1:A:370:LEU:HD22  | 2.01                     | 0.43              |
| 5:F:31:GLN:HG2    | 5:F:34:ARG:NH2    | 2.33                     | 0.43              |
| 20:V:114:ALA:O    | 20:V:118:MET:HG3  | 2.19                     | 0.43              |
| 27:d:77:CYS:SG    | 27:d:84:CYS:HB3   | 2.58                     | 0.43              |
| 27:d:159:GLN:HE21 | 27:d:163:MET:HE2  | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:307:SER:OG   | 32:i:308:THR:N    | 2.52                     | 0.43              |
| 35:l:241:THR:HG21 | 35:l:344:GLY:HA3  | 2.00                     | 0.43              |
| 56:l:702:CDL:H671 | 56:l:702:CDL:H642 | 1.87                     | 0.43              |
| 41:s:179:TRP:CG   | 41:s:180:PRO:HD3  | 2.53                     | 0.43              |
| 41:s:233:MET:HB3  | 41:s:233:MET:HE3  | 1.79                     | 0.43              |
| 42:u:47:ARG:HA    | 42:u:47:ARG:HD2   | 1.79                     | 0.43              |
| 3:C:107:GLY:HA2   | 45:C:301:SF4:S1   | 2.59                     | 0.43              |
| 6:G:119:ILE:HD13  | 6:G:119:ILE:HA    | 1.87                     | 0.43              |
| 56:V:202:CDL:H242 | 56:V:202:CDL:H451 | 2.01                     | 0.43              |
| 32:i:230:LEU:HD21 | 32:i:244:MET:SD   | 2.58                     | 0.43              |
| 35:l:488:MET:HE2  | 35:l:488:MET:HA   | 2.00                     | 0.43              |
| 1:A:363:ILE:O     | 1:A:367:ILE:HG12  | 2.19                     | 0.43              |
| 8:I:69:VAL:O      | 15:P:76:VAL:HB    | 2.18                     | 0.43              |
| 9:J:375:VAL:HG23  | 9:J:375:VAL:O     | 2.18                     | 0.43              |
| 12:M:460:HIS:HA   | 12:M:461:PRO:HD3  | 1.88                     | 0.43              |
| 49:e:201:PLX:H341 | 40:r:71:TRP:CD2   | 2.54                     | 0.43              |
| 35:l:213:LEU:HB3  | 35:l:273:VAL:HG11 | 2.00                     | 0.43              |
| 48:r:501:PEE:H52  | 48:r:501:PEE:H59  | 1.76                     | 0.43              |
| 46:A:502:FMN:H9   | 46:A:502:FMN:H1'1 | 1.74                     | 0.43              |
| 4:E:119:LEU:HD12  | 12:M:628:GLU:OE1  | 2.19                     | 0.43              |
| 5:F:65:LEU:HD11   | 5:F:91:LEU:HD13   | 2.00                     | 0.43              |
| 17:S:66:LEU:HD22  | 17:S:69:ILE:HD13  | 2.01                     | 0.43              |
| 6:X:137:LYS:HA    | 25:b:3:GLY:HA2    | 2.00                     | 0.43              |
| 27:d:107:GLN:HB3  | 27:d:111:LYS:NZ   | 2.33                     | 0.43              |
| 32:i:57:THR:HA    | 34:k:77:LEU:HD13  | 2.00                     | 0.43              |
| 36:m:1:MET:SD     | 36:m:1:MET:N      | 2.91                     | 0.43              |
| 40:r:287:ALA:O    | 40:r:291:VAL:HG23 | 2.19                     | 0.43              |
| 43:v:18:ASP:OD2   | 43:v:21:ARG:NH1   | 2.42                     | 0.43              |
| 44:w:340:SER:HB2  | 44:w:343:TYR:HD2  | 1.84                     | 0.43              |
| 1:A:115:VAL:HG22  | 1:A:248:VAL:HG21  | 2.01                     | 0.42              |
| 1:A:267:ARG:NH1   | 1:A:341:ALA:HB2   | 2.33                     | 0.42              |
| 48:B:303:PEE:H61  | 48:B:303:PEE:H55  | 1.70                     | 0.42              |
| 12:M:414:PHE:CE2  | 12:M:418:ILE:HD11 | 2.54                     | 0.42              |
| 13:N:32:ASP:OD1   | 13:N:34:ARG:HD3   | 2.19                     | 0.42              |
| 16:Q:156:GLU:OE2  | 16:Q:171:ARG:NH2  | 2.46                     | 0.42              |
| 16:Q:174:PHE:O    | 16:Q:178:THR:OG1  | 2.33                     | 0.42              |
| 35:l:331:MET:SD   | 35:l:465:GLY:HA2  | 2.58                     | 0.42              |
| 3:C:86:MET:HE1    | 3:C:93:PHE:CE2    | 2.54                     | 0.42              |
| 56:V:201:CDL:H352 | 56:V:201:CDL:H322 | 1.77                     | 0.42              |
| 28:e:125:LEU:HD23 | 28:e:125:LEU:HA   | 1.88                     | 0.42              |
| 32:i:68:MET:HE2   | 32:i:68:MET:HA    | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:97:MET:HG2   | 35:l:599:MET:HE1  | 2.00                     | 0.42              |
| 48:j:201:PEE:H22  | 48:j:201:PEE:H27  | 1.87                     | 0.42              |
| 36:m:74:MET:HE2   | 36:m:74:MET:HB2   | 1.86                     | 0.42              |
| 56:V:202:CDL:H361 | 56:V:202:CDL:H331 | 1.75                     | 0.42              |
| 56:V:204:CDL:H581 | 56:V:204:CDL:H611 | 1.45                     | 0.42              |
| 25:b:32:GLU:HB2   | 25:b:33:PRO:HD3   | 2.01                     | 0.42              |
| 35:l:44:PHE:HB2   | 35:l:94:LEU:HB3   | 2.01                     | 0.42              |
| 39:p:114:MET:H    | 39:p:114:MET:HG3  | 1.67                     | 0.42              |
| 50:C:304:DCQ:H3MB | 16:Q:92:HIS:ND1   | 2.34                     | 0.42              |
| 7:H:33:ASP:OD1    | 7:H:33:ASP:C      | 2.62                     | 0.42              |
| 11:L:71:HIS:CE1   | 11:L:120:PRO:HD2  | 2.54                     | 0.42              |
| 11:L:130:THR:OG1  | 11:L:133:ASP:OD2  | 2.35                     | 0.42              |
| 20:V:36:VAL:HG22  | 56:V:201:CDL:H742 | 2.02                     | 0.42              |
| 56:V:204:CDL:H131 | 56:V:204:CDL:H161 | 1.71                     | 0.42              |
| 6:X:98:LEU:HD12   | 6:X:99:SER:H      | 1.84                     | 0.42              |
| 6:X:98:LEU:HD12   | 6:X:99:SER:N      | 2.33                     | 0.42              |
| 32:i:68:MET:HE1   | 34:k:37:MET:SD    | 2.59                     | 0.42              |
| 35:l:21:MET:HE2   | 35:l:21:MET:HB3   | 1.96                     | 0.42              |
| 41:s:55:LEU:HD13  | 41:s:221:ALA:HB2  | 2.01                     | 0.42              |
| 44:w:57:SER:HB3   | 44:w:150:LEU:HD11 | 2.01                     | 0.42              |
| 2:B:86:TYR:CE1    | 3:C:171:GLU:HG2   | 2.55                     | 0.42              |
| 12:M:148:SER:OG   | 12:M:149:ASP:N    | 2.53                     | 0.42              |
| 14:O:93:LEU:HD12  | 14:O:122:TYR:HB3  | 2.01                     | 0.42              |
| 26:c:101:TRP:CE3  | 38:o:47:TYR:HB2   | 2.55                     | 0.42              |
| 35:l:566:THR:O    | 35:l:570:GLN:HG2  | 2.20                     | 0.42              |
| 36:m:73:ALA:C     | 36:m:74:MET:HG3   | 2.44                     | 0.42              |
| 36:m:165:VAL:O    | 36:m:168:ILE:HG12 | 2.19                     | 0.42              |
| 40:r:122:PHE:CE1  | 40:r:206:LYS:HD2  | 2.54                     | 0.42              |
| 42:u:101:ARG:NH1  | 42:u:104:GLN:OE1  | 2.47                     | 0.42              |
| 7:H:87:GLU:OE1    | 15:P:104:THR:OG1  | 2.36                     | 0.42              |
| 49:g:201:PLX:H102 | 49:g:201:PLX:H71  | 1.47                     | 0.42              |
| 35:l:244:SER:O    | 35:l:249:SER:HB3  | 2.20                     | 0.42              |
| 35:l:252:MET:HE2  | 35:l:252:MET:HB3  | 1.84                     | 0.42              |
| 40:r:6:ILE:O      | 40:r:10:MET:HG2   | 2.18                     | 0.42              |
| 40:r:346:ARG:O    | 40:r:419:TYR:HA   | 2.19                     | 0.42              |
| 1:A:267:ARG:HH12  | 1:A:341:ALA:HB2   | 1.85                     | 0.42              |
| 7:H:55:LYS:HE3    | 15:P:104:THR:HG21 | 2.00                     | 0.42              |
| 7:H:77:ILE:HD12   | 7:H:78:GLU:N      | 2.35                     | 0.42              |
| 17:S:1:MET:HB2    | 17:S:3:PHE:CZ     | 2.54                     | 0.42              |
| 17:S:48:MET:HE1   | 21:W:143:TYR:CE1  | 2.55                     | 0.42              |
| 24:a:66:ARG:NH1   | 28:e:72:ASP:HB2   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:304:MET:HE3  | 40:r:135:ARG:HH22 | 1.84                     | 0.42              |
| 35:l:149:ILE:HD13 | 35:l:149:ILE:HA   | 1.85                     | 0.42              |
| 40:r:247:THR:HB   | 40:r:304:GLN:NE2  | 2.34                     | 0.42              |
| 13:N:80:SER:O     | 13:N:113:HIS:HE1  | 2.03                     | 0.42              |
| 56:V:202:CDL:H792 | 56:V:202:CDL:H761 | 1.55                     | 0.42              |
| 23:Z:36:LEU:HD12  | 23:Z:36:LEU:HA    | 1.90                     | 0.42              |
| 32:i:141:VAL:O    | 32:i:145:ILE:HG12 | 2.20                     | 0.42              |
| 32:i:222:SER:O    | 32:i:224:ALA:N    | 2.53                     | 0.42              |
| 1:A:314:LEU:HD11  | 1:A:317:VAL:HG23  | 2.01                     | 0.42              |
| 3:C:67:PHE:CZ     | 3:C:117:LEU:HD12  | 2.55                     | 0.42              |
| 16:Q:434:GLY:O    | 16:Q:438:MET:HG3  | 2.19                     | 0.42              |
| 32:i:2:ASN:HB3    | 32:i:5:ILE:HG12   | 2.01                     | 0.42              |
| 32:i:128:LEU:HD12 | 32:i:216:PHE:HB3  | 2.02                     | 0.42              |
| 32:i:168:GLY:HA3  | 32:i:181:TYR:CE1  | 2.55                     | 0.42              |
| 33:j:51:PHE:O     | 36:m:73:ALA:HA    | 2.20                     | 0.42              |
| 56:l:701:CDL:H611 | 56:l:701:CDL:H581 | 1.68                     | 0.42              |
| 36:m:71:THR:HA    | 36:m:75:ALA:HB3   | 2.01                     | 0.42              |
| 41:s:81:LEU:HD11  | 41:s:111:LEU:HG   | 2.01                     | 0.42              |
| 3:C:86:MET:HE3    | 3:C:91:VAL:HG12   | 2.02                     | 0.42              |
| 10:K:79:HIS:ND1   | 14:O:216:PRO:HD2  | 2.34                     | 0.42              |
| 12:M:277:MET:HE3  | 12:M:277:MET:HB3  | 1.98                     | 0.42              |
| 13:N:34:ARG:NH2   | 13:N:58:ARG:O     | 2.53                     | 0.42              |
| 15:P:147:THR:HB   | 15:P:153:ILE:HD11 | 2.02                     | 0.42              |
| 34:k:37:MET:CE    | 34:k:63:LEU:HD22  | 2.50                     | 0.42              |
| 35:l:49:VAL:HB    | 35:l:50:PRO:HD3   | 2.02                     | 0.42              |
| 43:v:39:MET:HE3   | 43:v:39:MET:HB3   | 1.99                     | 0.42              |
| 7:H:116:ILE:HG12  | 15:P:121:THR:HG21 | 2.01                     | 0.41              |
| 18:T:39:THR:HG22  | 18:T:62:VAL:HG22  | 2.01                     | 0.41              |
| 20:V:126:LYS:HA   | 20:V:126:LYS:HD2  | 1.91                     | 0.41              |
| 24:a:184:LYS:O    | 24:a:185:THR:OG1  | 2.36                     | 0.41              |
| 32:i:242:SER:HB3  | 56:r:503:CDL:H331 | 2.01                     | 0.41              |
| 56:l:701:CDL:H722 | 56:l:701:CDL:HA62 | 2.02                     | 0.41              |
| 40:r:328:CYS:HB2  | 40:r:437:MET:HE1  | 2.02                     | 0.41              |
| 56:r:503:CDL:H351 | 56:r:503:CDL:H201 | 2.02                     | 0.41              |
| 1:A:373:PHE:HD1   | 14:O:175:GLU:HB3  | 1.84                     | 0.41              |
| 2:B:70:LEU:HB3    | 41:s:272:TRP:CZ2  | 2.55                     | 0.41              |
| 3:C:161:ILE:HG13  | 3:C:180:LEU:HB2   | 2.02                     | 0.41              |
| 8:I:106:LEU:O     | 8:I:108:LYS:NZ    | 2.53                     | 0.41              |
| 11:L:78:ARG:NE    | 11:L:148:GLU:OE1  | 2.50                     | 0.41              |
| 19:U:38:TYR:HD1   | 19:U:41:TYR:HD2   | 1.67                     | 0.41              |
| 21:W:36:PHE:O     | 21:W:40:ILE:HG12  | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:a:69:LYS:HB2   | 24:a:69:LYS:HE2   | 1.85                     | 0.41              |
| 24:a:94:GLY:O     | 27:d:61:TYR:OH    | 2.28                     | 0.41              |
| 24:a:127:ASP:OD1  | 49:a:202:PLX:H12  | 2.20                     | 0.41              |
| 41:s:32:GLN:OE1   | 41:s:34:ARG:NH2   | 2.53                     | 0.41              |
| 2:B:144:ARG:NH1   | 11:L:112:MET:O    | 2.43                     | 0.41              |
| 8:I:18:ARG:NH2    | 21:W:24:ASN:O     | 2.45                     | 0.41              |
| 29:f:71:ARG:HG2   | 29:f:71:ARG:NH1   | 2.34                     | 0.41              |
| 35:l:341:MET:CE   | 35:l:457:LEU:HD12 | 2.50                     | 0.41              |
| 35:l:407:TRP:CZ2  | 35:l:411:MET:HE3  | 2.55                     | 0.41              |
| 40:r:267:TRP:O    | 40:r:271:MET:HG2  | 2.21                     | 0.41              |
| 5:F:24:CYS:N      | 5:F:58:CYS:SG     | 2.93                     | 0.41              |
| 10:K:83:THR:HG22  | 14:O:88:ARG:HE    | 1.85                     | 0.41              |
| 12:M:419:ARG:NH1  | 12:M:439:THR:O    | 2.52                     | 0.41              |
| 16:Q:244:ILE:HG22 | 16:Q:348:LEU:HD11 | 2.02                     | 0.41              |
| 33:j:69:ILE:HD11  | 41:s:144:VAL:HA   | 2.02                     | 0.41              |
| 35:l:304:PHE:CZ   | 35:l:526:LEU:HD22 | 2.55                     | 0.41              |
| 40:r:405:LEU:HD23 | 40:r:405:LEU:HA   | 1.90                     | 0.41              |
| 40:r:437:MET:HA   | 40:r:437:MET:HE3  | 2.01                     | 0.41              |
| 41:s:54:LYS:HD2   | 41:s:54:LYS:C     | 2.45                     | 0.41              |
| 44:w:183:CYS:HA   | 44:w:314:LEU:HD21 | 2.02                     | 0.41              |
| 2:B:39:LYS:HD2    | 16:Q:335:GLU:HG2  | 2.03                     | 0.41              |
| 6:G:84:LEU:O      | 6:G:88:LYS:HG3    | 2.20                     | 0.41              |
| 9:J:108:TRP:HA    | 9:J:115:SER:HB3   | 2.03                     | 0.41              |
| 12:M:171:THR:HG23 | 12:M:173:MET:SD   | 2.60                     | 0.41              |
| 12:M:466:LEU:HD13 | 12:M:500:ILE:HD11 | 2.02                     | 0.41              |
| 14:O:185:MET:HB2  | 14:O:185:MET:HE2  | 1.83                     | 0.41              |
| 6:X:91:ASP:OD2    | 23:Z:42:ARG:NH2   | 2.49                     | 0.41              |
| 22:Y:42:PRO:HG3   | 35:l:442:LEU:HD13 | 2.02                     | 0.41              |
| 27:d:122:ARG:HA   | 27:d:122:ARG:HD3  | 1.90                     | 0.41              |
| 28:e:89:VAL:HG21  | 40:r:25:ILE:HG23  | 2.02                     | 0.41              |
| 32:i:93:VAL:HG22  | 35:l:603:ASN:ND2  | 2.34                     | 0.41              |
| 35:l:312:LEU:O    | 35:l:316:THR:HG22 | 2.21                     | 0.41              |
| 39:p:140:LEU:HD23 | 39:p:140:LEU:HA   | 1.88                     | 0.41              |
| 44:w:65:ASN:OD1   | 44:w:66:ILE:N     | 2.42                     | 0.41              |
| 2:B:37:THR:HA     | 8:I:105:GLU:O     | 2.20                     | 0.41              |
| 3:C:62:LEU:O      | 3:C:91:VAL:HA     | 2.21                     | 0.41              |
| 12:M:487:THR:HB   | 12:M:677:GLN:HE22 | 1.85                     | 0.41              |
| 13:N:42:ASP:OD2   | 13:N:48:TYR:OH    | 2.25                     | 0.41              |
| 18:T:84:ILE:HD12  | 18:T:84:ILE:HA    | 1.91                     | 0.41              |
| 32:i:215:MET:HE1  | 32:i:244:MET:HG3  | 2.02                     | 0.41              |
| 33:j:69:ILE:HD13  | 41:s:147:ALA:HB3  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:v:51:LEU:O     | 43:v:52:MET:HG3   | 2.20                     | 0.41              |
| 1:A:224:ARG:HD2   | 11:L:164:PHE:CE1  | 2.56                     | 0.41              |
| 9:J:229:ILE:HB    | 9:J:323:HIS:CD2   | 2.55                     | 0.41              |
| 12:M:50:LEU:HD11  | 12:M:62:ARG:HE    | 1.85                     | 0.41              |
| 12:M:141:ASP:O    | 12:M:145:MET:HG2  | 2.21                     | 0.41              |
| 12:M:347:ASP:CB   | 12:M:594:ALA:HB1  | 2.50                     | 0.41              |
| 14:O:185:MET:HB3  | 14:O:194:GLU:HB3  | 2.02                     | 0.41              |
| 16:Q:457:VAL:HG12 | 16:Q:460:GLU:HG2  | 2.03                     | 0.41              |
| 44:w:129:TYR:OH   | 44:w:186:HIS:ND1  | 2.32                     | 0.41              |
| 1:A:224:ARG:HD2   | 11:L:164:PHE:CZ   | 2.55                     | 0.41              |
| 1:A:389:VAL:HA    | 1:A:392:MET:HE2   | 2.03                     | 0.41              |
| 3:C:62:LEU:HD23   | 3:C:62:LEU:HA     | 1.92                     | 0.41              |
| 48:C:302:PEE:H15  | 49:J:403:PLX:H1B1 | 2.03                     | 0.41              |
| 9:J:306:GLU:HG2   | 9:J:315:THR:HG22  | 2.02                     | 0.41              |
| 15:P:43:THR:HG22  | 15:P:47:ILE:HD12  | 2.03                     | 0.41              |
| 23:Z:53:TYR:CE2   | 35:l:434:LYS:HG3  | 2.55                     | 0.41              |
| 29:f:59:ILE:HG12  | 29:f:59:ILE:H     | 1.74                     | 0.41              |
| 32:i:228:LEU:HD23 | 32:i:228:LEU:HA   | 1.90                     | 0.41              |
| 32:i:261:MET:HE2  | 32:i:340:THR:HA   | 2.02                     | 0.41              |
| 43:v:115:ARG:HD3  | 43:v:116:GLU:N    | 2.35                     | 0.41              |
| 44:w:254:GLU:H    | 44:w:254:GLU:HG2  | 1.65                     | 0.41              |
| 1:A:118:ASP:HB3   | 46:A:502:FMN:O4   | 2.21                     | 0.41              |
| 1:A:141:GLY:HA2   | 1:A:252:PRO:HD3   | 2.03                     | 0.41              |
| 1:A:174:ARG:NH1   | 10:K:92:GLU:OE2   | 2.54                     | 0.41              |
| 4:E:14:GLY:C      | 4:E:16:SER:H      | 2.29                     | 0.41              |
| 4:E:36:TYR:CE1    | 6:G:113:LEU:HD13  | 2.56                     | 0.41              |
| 4:E:66:MET:HE3    | 4:E:106:PHE:HD1   | 1.85                     | 0.41              |
| 11:L:76:LYS:HE3   | 11:L:146:ASP:CG   | 2.46                     | 0.41              |
| 11:L:78:ARG:HH22  | 12:M:249:GLU:CD   | 2.28                     | 0.41              |
| 12:M:307:ILE:HG23 | 12:M:317:THR:HG21 | 2.02                     | 0.41              |
| 14:O:138:THR:HB   | 14:O:139:PRO:HD3  | 2.02                     | 0.41              |
| 16:Q:268:TRP:O    | 16:Q:272:THR:OG1  | 2.32                     | 0.41              |
| 26:c:123:PRO:HB2  | 35:l:525:MET:HE1  | 2.02                     | 0.41              |
| 30:g:33:LEU:HD23  | 30:g:33:LEU:HA    | 1.96                     | 0.41              |
| 56:i:401:CDL:H811 | 36:m:159:TRP:CH2  | 2.56                     | 0.41              |
| 33:j:17:LEU:HD23  | 33:j:17:LEU:HA    | 1.92                     | 0.41              |
| 33:j:71:LEU:O     | 36:m:147:TYR:OH   | 2.33                     | 0.41              |
| 35:l:486:MET:HA   | 35:l:489:THR:OG1  | 2.21                     | 0.41              |
| 35:l:561:ILE:HG13 | 35:l:562:LEU:N    | 2.36                     | 0.41              |
| 36:m:44:VAL:HG12  | 36:m:49:GLY:O     | 2.20                     | 0.41              |
| 43:v:53:LEU:HD23  | 43:v:53:LEU:HA    | 1.84                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:551:ASP:OD1  | 12:M:574:ASP:HB3  | 2.21                     | 0.41              |
| 20:V:141:VAL:HG11 | 32:i:272:LYS:HB3  | 2.03                     | 0.41              |
| 22:Y:100:LEU:HB3  | 22:Y:104:GLU:OE1  | 2.20                     | 0.41              |
| 28:e:73:SER:O     | 28:e:75:GLY:N     | 2.55                     | 0.41              |
| 32:i:294:MET:HE2  | 40:r:130:LEU:HD21 | 2.03                     | 0.41              |
| 35:l:69:MET:HE2   | 35:l:76:LEU:HD12  | 2.03                     | 0.41              |
| 35:l:264:TYR:CG   | 35:l:265:PRO:HD3  | 2.56                     | 0.41              |
| 35:l:286:LEU:HD22 | 35:l:411:MET:SD   | 2.61                     | 0.41              |
| 56:n:101:CDL:H531 | 56:n:101:CDL:H741 | 2.03                     | 0.41              |
| 40:r:455:LEU:HD23 | 40:r:455:LEU:HA   | 1.90                     | 0.41              |
| 41:s:123:SER:HB3  | 41:s:214:GLU:HG3  | 2.03                     | 0.41              |
| 44:w:110:GLY:HA2  | 44:w:134:TRP:CE2  | 2.56                     | 0.41              |
| 1:A:63:TYR:CD2    | 14:O:241:PRO:HB2  | 2.56                     | 0.40              |
| 1:A:120:GLY:HA3   | 1:A:204:TYR:HD1   | 1.85                     | 0.40              |
| 2:B:49:ASP:OD2    | 2:B:51:LYS:HB2    | 2.21                     | 0.40              |
| 48:B:303:PEE:H56  | 41:s:187:ILE:HD12 | 2.02                     | 0.40              |
| 8:I:108:LYS:HA    | 8:I:108:LYS:HD3   | 1.69                     | 0.40              |
| 9:J:204:SER:OG    | 9:J:238:GLN:O     | 2.39                     | 0.40              |
| 11:L:111:LEU:HG   | 11:L:112:MET:HG2  | 2.03                     | 0.40              |
| 15:P:197:PRO:HA   | 15:P:202:PHE:CD2  | 2.56                     | 0.40              |
| 25:b:28:LEU:HD22  | 25:b:32:GLU:HG3   | 2.02                     | 0.40              |
| 40:r:321:LEU:HD13 | 40:r:444:LEU:HG   | 2.01                     | 0.40              |
| 1:A:207:GLY:HA3   | 46:A:502:FMN:N5   | 2.36                     | 0.40              |
| 49:J:403:PLX:H32  | 33:j:23:TRP:CZ3   | 2.57                     | 0.40              |
| 14:O:143:ARG:HG3  | 14:O:183:ALA:HB3  | 2.03                     | 0.40              |
| 21:W:88:ARG:HH11  | 21:W:91:LEU:HD23  | 1.86                     | 0.40              |
| 28:e:87:MET:HE3   | 28:e:87:MET:HB3   | 1.88                     | 0.40              |
| 48:j:201:PEE:H60  | 48:j:201:PEE:H55  | 1.82                     | 0.40              |
| 35:l:169:LEU:HD12 | 35:l:169:LEU:HA   | 1.93                     | 0.40              |
| 35:l:397:GLU:HG2  | 35:l:482:MET:HE1  | 2.03                     | 0.40              |
| 37:n:50:ARG:HB3   | 37:n:51:PRO:HD2   | 2.03                     | 0.40              |
| 4:E:19:PRO:HB3    | 11:L:53:ILE:HG21  | 2.02                     | 0.40              |
| 9:J:262:THR:O     | 9:J:333:PRO:HD2   | 2.22                     | 0.40              |
| 16:Q:271:ARG:NH2  | 16:Q:445:ALA:HB1  | 2.36                     | 0.40              |
| 20:V:44:LYS:NZ    | 35:l:579:ASN:O    | 2.46                     | 0.40              |
| 26:c:65:TYR:CE2   | 26:c:77:LYS:HG3   | 2.56                     | 0.40              |
| 42:u:18:VAL:HG23  | 42:u:64:ASN:HD22  | 1.86                     | 0.40              |
| 43:v:108:LEU:HD12 | 43:v:108:LEU:HA   | 1.84                     | 0.40              |
| 48:B:303:PEE:H7   | 41:s:288:LEU:HD11 | 2.03                     | 0.40              |
| 3:C:52:ASP:HB3    | 49:C:303:PLX:H282 | 2.02                     | 0.40              |
| 16:Q:244:ILE:O    | 16:Q:248:SER:OG   | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:W:43:LEU:HG    | 41:s:179:TRP:HE1  | 1.87                     | 0.40              |
| 49:j:203:PLX:H311 | 49:j:203:PLX:H282 | 1.55                     | 0.40              |
| 35:l:338:MET:SD   | 35:l:458:LEU:HD12 | 2.61                     | 0.40              |
| 40:r:104:LEU:HD21 | 56:r:503:CDL:H861 | 2.03                     | 0.40              |
| 41:s:134:ARG:NH1  | 41:s:206:GLU:OE1  | 2.37                     | 0.40              |
| 44:w:70:LYS:NZ    | 44:w:160:GLU:OE1  | 2.54                     | 0.40              |
| 1:A:184:LYS:HB2   | 10:K:98:MET:CE    | 2.52                     | 0.40              |
| 2:B:171:PRO:HG3   | 2:B:200:GLU:HG2   | 2.03                     | 0.40              |
| 11:L:80:PHE:CE1   | 11:L:100:GLU:HG2  | 2.55                     | 0.40              |
| 12:M:144:MET:O    | 16:Q:362:LYS:HE3  | 2.22                     | 0.40              |
| 16:Q:342:ARG:HD2  | 21:W:21:TYR:CZ    | 2.56                     | 0.40              |
| 28:e:55:LEU:HD23  | 28:e:57:GLU:HB2   | 2.03                     | 0.40              |
| 35:l:152:PHE:CD1  | 35:l:168:ALA:HB1  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 431/433 (100%) | 421 (98%) | 10 (2%) | 0        | 100         | 100 |
| 2   | B     | 174/176 (99%)  | 171 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 3   | C     | 154/156 (99%)  | 149 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 4   | E     | 113/115 (98%)  | 107 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 5   | F     | 84/86 (98%)    | 80 (95%)  | 4 (5%)  | 0        | 100         | 100 |
| 6   | G     | 86/88 (98%)    | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | X     | 86/88 (98%)    | 85 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 7   | H     | 110/112 (98%)  | 105 (96%) | 4 (4%)  | 1 (1%)   | 14          | 35  |
| 8   | I     | 93/112 (83%)   | 86 (92%)  | 7 (8%)  | 0        | 100         | 100 |
| 9   | J     | 340/342 (99%)  | 327 (96%) | 12 (4%) | 1 (0%)   | 36          | 60  |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 10  | K     | 41/43 (95%)    | 41 (100%) | 0       | 0        | 100         | 100 |
| 11  | L     | 123/125 (98%)  | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 12  | M     | 688/690 (100%) | 676 (98%) | 12 (2%) | 0        | 100         | 100 |
| 13  | N     | 142/144 (99%)  | 137 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 14  | O     | 215/217 (99%)  | 198 (92%) | 17 (8%) | 0        | 100         | 100 |
| 15  | P     | 206/208 (99%)  | 200 (97%) | 5 (2%)  | 1 (0%)   | 24          | 48  |
| 16  | Q     | 427/430 (99%)  | 415 (97%) | 12 (3%) | 0        | 100         | 100 |
| 17  | S     | 68/70 (97%)    | 65 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 18  | T     | 94/96 (98%)    | 93 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 19  | U     | 81/83 (98%)    | 80 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | V     | 138/140 (99%)  | 135 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 21  | W     | 140/142 (99%)  | 135 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 22  | Y     | 65/67 (97%)    | 60 (92%)  | 5 (8%)  | 0        | 100         | 100 |
| 23  | Z     | 78/80 (98%)    | 76 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 24  | a     | 136/138 (99%)  | 133 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 25  | b     | 94/126 (75%)   | 86 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 26  | c     | 154/156 (99%)  | 144 (94%) | 10 (6%) | 0        | 100         | 100 |
| 27  | d     | 173/175 (99%)  | 170 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 28  | e     | 102/104 (98%)  | 95 (93%)  | 7 (7%)  | 0        | 100         | 100 |
| 29  | f     | 47/49 (96%)    | 44 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 30  | g     | 120/122 (98%)  | 114 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 31  | h     | 103/105 (98%)  | 101 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 32  | i     | 345/347 (99%)  | 334 (97%) | 11 (3%) | 0        | 100         | 100 |
| 33  | j     | 113/115 (98%)  | 109 (96%) | 3 (3%)  | 1 (1%)   | 14          | 35  |
| 34  | k     | 96/98 (98%)    | 95 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | l     | 604/606 (100%) | 591 (98%) | 13 (2%) | 0        | 100         | 100 |
| 36  | m     | 173/175 (99%)  | 160 (92%) | 13 (8%) | 0        | 100         | 100 |
| 37  | n     | 54/56 (96%)    | 53 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 38  | o     | 126/128 (98%)  | 123 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 39  | p     | 176/178 (99%)  | 169 (96%) | 6 (3%)  | 1 (1%)   | 21          | 44  |
| 40  | r     | 457/459 (100%) | 452 (99%) | 5 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 41  | s     | 316/318 (99%)   | 305 (96%)  | 10 (3%)  | 1 (0%)   | 36          | 60  |
| 42  | u     | 169/171 (99%)   | 165 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 43  | v     | 122/125 (98%)   | 115 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 44  | w     | 318/320 (99%)   | 309 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| All | All   | 8175/8314 (98%) | 7912 (97%) | 257 (3%) | 6 (0%)   | 49          | 73  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | P     | 44  | ARG  |
| 7   | H     | 77  | ILE  |
| 9   | J     | 38  | HIS  |
| 33  | j     | 40  | GLY  |
| 39  | p     | 174 | PRO  |
| 41  | s     | 208 | VAL  |

### 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     | 346/346 (100%) | 341 (99%)  | 5 (1%)   | 59          | 82  |
| 2   | B     | 151/151 (100%) | 151 (100%) | 0        | 100         | 100 |
| 3   | C     | 132/132 (100%) | 131 (99%)  | 1 (1%)   | 73          | 88  |
| 4   | E     | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 5   | F     | 75/76 (99%)    | 73 (97%)   | 2 (3%)   | 39          | 69  |
| 6   | G     | 75/81 (93%)    | 75 (100%)  | 0        | 100         | 100 |
| 6   | X     | 75/81 (93%)    | 74 (99%)   | 1 (1%)   | 61          | 83  |
| 7   | H     | 99/99 (100%)   | 98 (99%)   | 1 (1%)   | 68          | 86  |
| 8   | I     | 87/97 (90%)    | 86 (99%)   | 1 (1%)   | 65          | 85  |
| 9   | J     | 295/296 (100%) | 293 (99%)  | 2 (1%)   | 76          | 90  |
| 10  | K     | 42/42 (100%)   | 41 (98%)   | 1 (2%)   | 43          | 72  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 11  | L     | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 87  |
| 12  | M     | 580/580 (100%) | 571 (98%)  | 9 (2%)   | 55          | 80  |
| 13  | N     | 130/130 (100%) | 130 (100%) | 0        | 100         | 100 |
| 14  | O     | 183/183 (100%) | 183 (100%) | 0        | 100         | 100 |
| 15  | P     | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 16  | Q     | 370/370 (100%) | 364 (98%)  | 6 (2%)   | 55          | 80  |
| 17  | S     | 57/58 (98%)    | 57 (100%)  | 0        | 100         | 100 |
| 18  | T     | 79/79 (100%)   | 78 (99%)   | 1 (1%)   | 61          | 83  |
| 19  | U     | 69/69 (100%)   | 69 (100%)  | 0        | 100         | 100 |
| 20  | V     | 101/101 (100%) | 98 (97%)   | 3 (3%)   | 36          | 66  |
| 21  | W     | 121/123 (98%)  | 121 (100%) | 0        | 100         | 100 |
| 22  | Y     | 62/62 (100%)   | 62 (100%)  | 0        | 100         | 100 |
| 23  | Z     | 62/62 (100%)   | 61 (98%)   | 1 (2%)   | 55          | 80  |
| 24  | a     | 121/121 (100%) | 121 (100%) | 0        | 100         | 100 |
| 25  | b     | 90/119 (76%)   | 90 (100%)  | 0        | 100         | 100 |
| 26  | c     | 141/141 (100%) | 140 (99%)  | 1 (1%)   | 76          | 90  |
| 27  | d     | 155/155 (100%) | 152 (98%)  | 3 (2%)   | 50          | 77  |
| 28  | e     | 96/96 (100%)   | 95 (99%)   | 1 (1%)   | 68          | 86  |
| 29  | f     | 36/45 (80%)    | 36 (100%)  | 0        | 100         | 100 |
| 30  | g     | 108/109 (99%)  | 108 (100%) | 0        | 100         | 100 |
| 31  | h     | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 85  |
| 32  | i     | 311/311 (100%) | 304 (98%)  | 7 (2%)   | 44          | 73  |
| 33  | j     | 100/100 (100%) | 99 (99%)   | 1 (1%)   | 68          | 86  |
| 34  | k     | 85/85 (100%)   | 84 (99%)   | 1 (1%)   | 63          | 84  |
| 35  | l     | 537/540 (99%)  | 535 (100%) | 2 (0%)   | 84          | 93  |
| 36  | m     | 126/141 (89%)  | 124 (98%)  | 2 (2%)   | 55          | 80  |
| 37  | n     | 53/53 (100%)   | 51 (96%)   | 2 (4%)   | 29          | 58  |
| 38  | o     | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 87  |
| 39  | p     | 159/159 (100%) | 157 (99%)  | 2 (1%)   | 61          | 83  |
| 40  | r     | 410/410 (100%) | 404 (98%)  | 6 (2%)   | 57          | 81  |
| 41  | s     | 275/275 (100%) | 272 (99%)  | 3 (1%)   | 65          | 85  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 42  | u     | 153/153 (100%)  | 152 (99%)  | 1 (1%)   | 76          | 90  |
| 43  | v     | 104/111 (94%)   | 104 (100%) | 0        | 100         | 100 |
| 44  | w     | 281/283 (99%)   | 276 (98%)  | 5 (2%)   | 51          | 78  |
| All | All   | 7148/7241 (99%) | 7074 (99%) | 74 (1%)  | 65          | 86  |

All (74) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 30  | THR  |
| 1   | A     | 106 | SER  |
| 1   | A     | 149 | MET  |
| 1   | A     | 334 | THR  |
| 1   | A     | 344 | GLN  |
| 3   | C     | 71  | CYS  |
| 5   | F     | 48  | ASN  |
| 5   | F     | 88  | THR  |
| 7   | H     | 48  | THR  |
| 8   | I     | 41  | LEU  |
| 9   | J     | 174 | ILE  |
| 9   | J     | 220 | MET  |
| 10  | K     | 107 | SER  |
| 11  | L     | 154 | LYS  |
| 12  | M     | 361 | VAL  |
| 12  | M     | 364 | ASP  |
| 12  | M     | 484 | SER  |
| 12  | M     | 498 | GLN  |
| 12  | M     | 534 | VAL  |
| 12  | M     | 540 | ASN  |
| 12  | M     | 575 | VAL  |
| 12  | M     | 658 | ASP  |
| 12  | M     | 674 | LEU  |
| 16  | Q     | 182 | ASN  |
| 16  | Q     | 217 | VAL  |
| 16  | Q     | 248 | SER  |
| 16  | Q     | 258 | LEU  |
| 16  | Q     | 453 | THR  |
| 16  | Q     | 457 | VAL  |
| 18  | T     | 104 | LYS  |
| 20  | V     | 4   | THR  |
| 20  | V     | 120 | LEU  |
| 20  | V     | 141 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | X     | 100 | VAL  |
| 23  | Z     | 36  | LEU  |
| 26  | c     | 33  | THR  |
| 27  | d     | 40  | LEU  |
| 27  | d     | 52  | ILE  |
| 27  | d     | 144 | SER  |
| 28  | e     | 55  | LEU  |
| 31  | h     | 21  | GLN  |
| 32  | i     | 89  | MET  |
| 32  | i     | 147 | GLN  |
| 32  | i     | 157 | MET  |
| 32  | i     | 164 | ILE  |
| 32  | i     | 194 | LEU  |
| 32  | i     | 229 | SER  |
| 32  | i     | 336 | VAL  |
| 33  | j     | 83  | ASN  |
| 34  | k     | 3   | LEU  |
| 35  | l     | 233 | LEU  |
| 35  | l     | 507 | THR  |
| 36  | m     | 1   | MET  |
| 36  | m     | 74  | MET  |
| 37  | n     | 19  | VAL  |
| 37  | n     | 52  | ASN  |
| 38  | o     | 41  | SER  |
| 39  | p     | 85  | SER  |
| 39  | p     | 90  | SER  |
| 40  | r     | 58  | SER  |
| 40  | r     | 138 | ASN  |
| 40  | r     | 179 | ILE  |
| 40  | r     | 187 | SER  |
| 40  | r     | 343 | ILE  |
| 40  | r     | 375 | LEU  |
| 41  | s     | 24  | GLU  |
| 41  | s     | 110 | SER  |
| 41  | s     | 174 | MET  |
| 42  | u     | 37  | ASP  |
| 44  | w     | 56  | THR  |
| 44  | w     | 133 | SER  |
| 44  | w     | 152 | SER  |
| 44  | w     | 223 | ASN  |
| 44  | w     | 254 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 49  | HIS  |
| 1   | A     | 164 | ASN  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 284 | HIS  |
| 3   | C     | 111 | ASN  |
| 4   | E     | 48  | HIS  |
| 8   | I     | 29  | GLN  |
| 9   | J     | 122 | HIS  |
| 9   | J     | 128 | ASN  |
| 9   | J     | 138 | ASN  |
| 9   | J     | 295 | HIS  |
| 10  | K     | 70  | ASN  |
| 10  | K     | 106 | GLN  |
| 11  | L     | 71  | HIS  |
| 12  | M     | 498 | GLN  |
| 13  | N     | 113 | HIS  |
| 14  | O     | 90  | ASN  |
| 14  | O     | 182 | ASN  |
| 15  | P     | 82  | ASN  |
| 15  | P     | 124 | ASN  |
| 15  | P     | 196 | HIS  |
| 16  | Q     | 233 | HIS  |
| 16  | Q     | 285 | ASN  |
| 18  | T     | 120 | GLN  |
| 21  | W     | 90  | ASN  |
| 22  | Y     | 75  | HIS  |
| 24  | a     | 189 | ASN  |
| 27  | d     | 55  | GLN  |
| 28  | e     | 65  | ASN  |
| 32  | i     | 63  | GLN  |
| 32  | i     | 120 | GLN  |
| 35  | l     | 59  | GLN  |
| 35  | l     | 470 | ASN  |
| 40  | r     | 30  | HIS  |
| 40  | r     | 251 | ASN  |
| 43  | v     | 84  | GLN  |
| 44  | w     | 37  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 16  | 2MR  | Q     | 118 | 16   | 10,12,13     | 1.97 | 1 (10%)     | 5,13,15     | 5.94 | 3 (60%)     |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 16  | 2MR  | Q     | 118 | 16   | -       | 3/10/13/15 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 16  | Q     | 118 | 2MR  | CZ-NE | 5.65 | 1.46        | 1.34     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 16  | Q     | 118 | 2MR  | NE-CZ-NH2  | 12.08 | 130.55      | 119.48   |
| 16  | Q     | 118 | 2MR  | CD-NE-CZ   | 4.32  | 131.50      | 123.41   |
| 16  | Q     | 118 | 2MR  | CQ2-NH2-CZ | 3.19  | 130.91      | 123.86   |

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 16  | Q     | 118 | 2MR  | NE-CD-CG-CB |
| 16  | Q     | 118 | 2MR  | CA-CB-CG-CD |
| 16  | Q     | 118 | 2MR  | CG-CD-NE-CZ |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 2 are monoatomic - leaving 44 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 | $\# Z  > 2$ |
| 45  | SF4  | M     | 802 | 12   | 0,12,12      | -    | -           | -           |      |             |
| 49  | PLX  | j     | 203 | -    | 51,51,51     | 1.15 | 4 (7%)      | 55,59,59    | 0.61 | 1 (1%)      |
| 51  | 8Q1  | G     | 201 | -    | 31,34,34     | 1.70 | 6 (19%)     | 40,43,43    | 1.64 | 5 (12%)     |
| 56  | CDL  | V     | 201 | -    | 93,93,99     | 1.12 | 9 (9%)      | 99,105,111  | 0.89 | 5 (5%)      |
| 48  | PEE  | l     | 703 | -    | 50,50,50     | 1.16 | 6 (12%)     | 53,55,55    | 0.92 | 2 (3%)      |
| 56  | CDL  | N     | 201 | -    | 50,50,99     | 1.41 | 8 (16%)     | 56,62,111   | 1.12 | 4 (7%)      |
| 48  | PEE  | j     | 201 | -    | 50,50,50     | 1.15 | 6 (12%)     | 53,55,55    | 0.95 | 2 (3%)      |
| 56  | CDL  | i     | 401 | -    | 86,86,99     | 1.15 | 8 (9%)      | 92,98,111   | 0.89 | 4 (4%)      |
| 49  | PLX  | J     | 403 | -    | 51,51,51     | 1.16 | 4 (7%)      | 55,59,59    | 0.57 | 1 (1%)      |
| 47  | NAI  | A     | 503 | -    | 45,48,48     | 3.90 | 20 (44%)    | 60,73,73    | 1.77 | 12 (20%)    |
| 48  | PEE  | j     | 202 | -    | 40,40,50     | 1.15 | 5 (12%)     | 43,45,55    | 1.01 | 2 (4%)      |
| 56  | CDL  | a     | 201 | -    | 99,99,99     | 1.09 | 8 (8%)      | 105,111,111 | 0.84 | 4 (3%)      |
| 48  | PEE  | C     | 302 | -    | 46,46,50     | 1.20 | 6 (13%)     | 49,51,55    | 1.00 | 2 (4%)      |
| 50  | DCQ  | C     | 304 | -    | 23,23,23     | 1.31 | 4 (17%)     | 26,29,29    | 0.99 | 1 (3%)      |
| 45  | SF4  | B     | 301 | 2    | 0,12,12      | -    | -           | -           |      |             |
| 48  | PEE  | r     | 501 | -    | 50,50,50     | 1.16 | 6 (12%)     | 53,55,55    | 0.95 | 2 (3%)      |
| 48  | PEE  | l     | 704 | -    | 45,45,50     | 1.22 | 6 (13%)     | 48,50,55    | 1.00 | 2 (4%)      |
| 45  | SF4  | A     | 501 | 1    | 0,12,12      | -    | -           | -           |      |             |
| 49  | PLX  | C     | 303 | -    | 51,51,51     | 1.15 | 4 (7%)      | 55,59,59    | 0.58 | 1 (1%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 54  | FES  | O     | 301 | 14   | 0,4,4        | -    | -        | -           |      |          |
| 58  | ADP  | w     | 401 | -    | 27,29,29     | 2.97 | 8 (29%)  | 42,45,45    | 2.05 | 10 (23%) |
| 56  | CDL  | V     | 202 | -    | 99,99,99     | 1.09 | 9 (9%)   | 105,111,111 | 0.88 | 4 (3%)   |
| 48  | PEE  | B     | 303 | -    | 50,50,50     | 1.17 | 6 (12%)  | 53,55,55    | 0.97 | 2 (3%)   |
| 48  | PEE  | V     | 203 | -    | 39,39,50     | 1.31 | 6 (15%)  | 41,44,55    | 1.04 | 2 (4%)   |
| 56  | CDL  | s     | 401 | -    | 88,88,99     | 1.14 | 9 (10%)  | 94,100,111  | 0.94 | 5 (5%)   |
| 56  | CDL  | r     | 503 | -    | 99,99,99     | 1.09 | 8 (8%)   | 105,111,111 | 0.86 | 4 (3%)   |
| 45  | SF4  | B     | 302 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 46  | FMN  | A     | 502 | -    | 33,33,33     | 1.07 | 2 (6%)   | 48,50,50    | 1.23 | 9 (18%)  |
| 49  | PLX  | a     | 202 | -    | 51,51,51     | 1.15 | 4 (7%)   | 55,59,59    | 0.60 | 1 (1%)   |
| 52  | NDP  | J     | 401 | -    | 49,52,52     | 4.39 | 23 (46%) | 66,80,80    | 2.20 | 12 (18%) |
| 56  | CDL  | n     | 101 | -    | 54,54,99     | 1.37 | 8 (14%)  | 60,66,111   | 1.11 | 4 (6%)   |
| 49  | PLX  | g     | 201 | -    | 51,51,51     | 1.15 | 4 (7%)   | 55,59,59    | 0.59 | 1 (1%)   |
| 56  | CDL  | V     | 204 | -    | 99,99,99     | 1.09 | 8 (8%)   | 105,111,111 | 0.85 | 4 (3%)   |
| 45  | SF4  | M     | 801 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 54  | FES  | M     | 803 | 12   | 0,4,4        | -    | -        | -           |      |          |
| 49  | PLX  | r     | 502 | -    | 51,51,51     | 1.15 | 5 (9%)   | 55,59,59    | 0.63 | 1 (1%)   |
| 53  | UQ   | J     | 402 | -    | 33,33,63     | 3.45 | 8 (24%)  | 40,43,79    | 2.77 | 13 (32%) |
| 56  | CDL  | l     | 701 | -    | 98,98,99     | 1.09 | 8 (8%)   | 104,110,111 | 0.87 | 4 (3%)   |
| 51  | 8Q1  | X     | 201 | 6    | 31,34,34     | 1.72 | 6 (19%)  | 40,43,43    | 1.56 | 7 (17%)  |
| 48  | PEE  | W     | 201 | -    | 40,40,50     | 1.15 | 5 (12%)  | 43,45,55    | 0.98 | 2 (4%)   |
| 53  | UQ   | s     | 402 | -    | 38,38,63     | 3.56 | 11 (28%) | 46,49,79    | 2.74 | 15 (32%) |
| 49  | PLX  | e     | 201 | -    | 51,51,51     | 1.15 | 4 (7%)   | 55,59,59    | 0.52 | 0        |
| 45  | SF4  | C     | 301 | 3    | 0,12,12      | -    | -        | -           |      |          |
| 56  | CDL  | l     | 702 | -    | 91,91,99     | 1.12 | 8 (8%)   | 97,103,111  | 0.87 | 4 (4%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 45  | SF4  | M     | 802 | 12   | -       | -              | 0/6/5/5 |
| 49  | PLX  | j     | 203 | -    | -       | 30/55/55/55    | -       |
| 51  | 8Q1  | G     | 201 | -    | -       | 14/41/41/41    | -       |
| 56  | CDL  | V     | 201 | -    | -       | 62/104/104/110 | -       |
| 48  | PEE  | l     | 703 | -    | -       | 26/54/54/54    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 56  | CDL  | N     | 201 | -    | -       | 36/61/61/110   | -       |
| 48  | PEE  | j     | 201 | -    | -       | 23/54/54/54    | -       |
| 56  | CDL  | i     | 401 | -    | -       | 47/97/97/110   | -       |
| 49  | PLX  | J     | 403 | -    | -       | 30/55/55/55    | -       |
| 47  | NAI  | A     | 503 | -    | -       | 8/29/72/72     | 0/5/5/5 |
| 48  | PEE  | j     | 202 | -    | -       | 22/44/44/54    | -       |
| 56  | CDL  | a     | 201 | -    | -       | 56/110/110/110 | -       |
| 48  | PEE  | C     | 302 | -    | -       | 26/50/50/54    | -       |
| 50  | DCQ  | C     | 304 | -    | -       | 4/14/38/38     | 0/1/1/1 |
| 45  | SF4  | B     | 301 | 2    | -       | -              | 0/6/5/5 |
| 48  | PEE  | r     | 501 | -    | -       | 30/54/54/54    | -       |
| 48  | PEE  | l     | 704 | -    | -       | 24/49/49/54    | -       |
| 49  | PLX  | C     | 303 | -    | -       | 26/55/55/55    | -       |
| 45  | SF4  | A     | 501 | 1    | -       | -              | 0/6/5/5 |
| 54  | FES  | O     | 301 | 14   | -       | -              | 0/1/1/1 |
| 58  | ADP  | w     | 401 | -    | -       | 4/16/32/32     | 0/3/3/3 |
| 56  | CDL  | V     | 202 | -    | -       | 55/110/110/110 | -       |
| 48  | PEE  | B     | 303 | -    | -       | 22/54/54/54    | -       |
| 48  | PEE  | V     | 203 | -    | -       | 24/43/43/54    | -       |
| 56  | CDL  | s     | 401 | -    | -       | 52/99/99/110   | -       |
| 56  | CDL  | r     | 503 | -    | -       | 61/110/110/110 | -       |
| 45  | SF4  | B     | 302 | 2    | -       | -              | 0/6/5/5 |
| 46  | FMN  | A     | 502 | -    | -       | 7/18/18/18     | 0/3/3/3 |
| 49  | PLX  | a     | 202 | -    | -       | 28/55/55/55    | -       |
| 52  | NDP  | J     | 401 | -    | -       | 8/34/77/77     | 0/4/5/5 |
| 56  | CDL  | n     | 101 | -    | -       | 28/65/65/110   | -       |
| 49  | PLX  | g     | 201 | -    | -       | 32/55/55/55    | -       |
| 56  | CDL  | V     | 204 | -    | -       | 66/110/110/110 | -       |
| 45  | SF4  | M     | 801 | 12   | -       | -              | 0/6/5/5 |
| 54  | FES  | M     | 803 | 12   | -       | -              | 0/1/1/1 |
| 49  | PLX  | r     | 502 | -    | -       | 31/55/55/55    | -       |
| 53  | UQ   | J     | 402 | -    | -       | 13/27/51/87    | 0/1/1/1 |
| 56  | CDL  | l     | 701 | -    | -       | 58/109/109/110 | -       |
| 51  | 8Q1  | X     | 201 | 6    | -       | 7/41/41/41     | -       |
| 48  | PEE  | W     | 201 | -    | -       | 21/44/44/54    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 53  | UQ   | s     | 402 | -    | -       | 14/33/57/87    | 0/1/1/1 |
| 49  | PLX  | e     | 201 | -    | -       | 35/55/55/55    | -       |
| 45  | SF4  | C     | 301 | 3    | -       | -              | 0/6/5/5 |
| 56  | CDL  | l     | 702 | -    | -       | 56/102/102/110 | -       |

All (260) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 52  | J     | 401 | NDP  | C3B-C2B | -13.02 | 1.23        | 1.52     |
| 52  | J     | 401 | NDP  | C6N-C5N | 12.37  | 1.55        | 1.33     |
| 52  | J     | 401 | NDP  | O4D-C4D | 10.66  | 1.68        | 1.45     |
| 47  | A     | 503 | NAI  | C3D-C4D | -10.25 | 1.26        | 1.53     |
| 52  | J     | 401 | NDP  | C3D-C4D | -9.84  | 1.27        | 1.53     |
| 53  | s     | 402 | UQ   | C18-C19 | 9.64   | 1.56        | 1.33     |
| 53  | J     | 402 | UQ   | C18-C19 | 9.62   | 1.56        | 1.33     |
| 53  | s     | 402 | UQ   | C13-C14 | 9.28   | 1.55        | 1.33     |
| 53  | J     | 402 | UQ   | C13-C14 | 9.21   | 1.55        | 1.33     |
| 47  | A     | 503 | NAI  | O4B-C1B | 9.18   | 1.63        | 1.42     |
| 53  | s     | 402 | UQ   | C23-C24 | 9.13   | 1.54        | 1.33     |
| 53  | J     | 402 | UQ   | C8-C9   | 8.95   | 1.54        | 1.33     |
| 53  | s     | 402 | UQ   | C8-C9   | 8.95   | 1.54        | 1.33     |
| 58  | w     | 401 | ADP  | C3'-C4' | -8.86  | 1.30        | 1.53     |
| 47  | A     | 503 | NAI  | O4B-C4B | -8.23  | 1.26        | 1.45     |
| 53  | J     | 402 | UQ   | C23-C24 | 7.88   | 1.55        | 1.32     |
| 52  | J     | 401 | NDP  | O4B-C4B | -7.79  | 1.27        | 1.45     |
| 58  | w     | 401 | ADP  | O4'-C4' | 7.74   | 1.62        | 1.45     |
| 53  | s     | 402 | UQ   | C28-C29 | 7.63   | 1.54        | 1.32     |
| 47  | A     | 503 | NAI  | C2D-C1D | -7.57  | 1.29        | 1.53     |
| 52  | J     | 401 | NDP  | C2N-C3N | 7.43   | 1.55        | 1.34     |
| 47  | A     | 503 | NAI  | C2B-C1B | -7.22  | 1.30        | 1.53     |
| 47  | A     | 503 | NAI  | O4D-C4D | 6.99   | 1.60        | 1.45     |
| 52  | J     | 401 | NDP  | C6A-N6A | 5.94   | 1.49        | 1.34     |
| 47  | A     | 503 | NAI  | C2D-C3D | 5.87   | 1.69        | 1.53     |
| 47  | A     | 503 | NAI  | C7N-N7N | 5.76   | 1.48        | 1.33     |
| 52  | J     | 401 | NDP  | P2B-O2B | 5.71   | 1.70        | 1.59     |
| 58  | w     | 401 | ADP  | C6-N6   | 5.60   | 1.48        | 1.34     |
| 51  | X     | 201 | 8Q1  | C34-N36 | 5.49   | 1.45        | 1.33     |
| 47  | A     | 503 | NAI  | O4D-C1D | 5.46   | 1.54        | 1.42     |
| 51  | G     | 201 | 8Q1  | C39-N41 | 5.46   | 1.45        | 1.33     |
| 51  | G     | 201 | 8Q1  | C34-N36 | 5.41   | 1.45        | 1.33     |
| 51  | X     | 201 | 8Q1  | C39-N41 | 5.41   | 1.45        | 1.33     |
| 52  | J     | 401 | NDP  | C3B-C4B | 5.40   | 1.66        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | A     | 503 | NAI  | C6A-N6A | 5.19  | 1.47        | 1.34     |
| 47  | A     | 503 | NAI  | C4N-C3N | -4.97 | 1.40        | 1.49     |
| 52  | J     | 401 | NDP  | O4D-C1D | -4.89 | 1.30        | 1.42     |
| 52  | J     | 401 | NDP  | C6N-N1N | 4.88  | 1.49        | 1.37     |
| 52  | J     | 401 | NDP  | O4B-C1B | 4.64  | 1.53        | 1.42     |
| 47  | A     | 503 | NAI  | O2B-C2B | 4.56  | 1.53        | 1.43     |
| 58  | w     | 401 | ADP  | O4'-C1' | -4.50 | 1.31        | 1.42     |
| 52  | J     | 401 | NDP  | C1B-N9A | -4.43 | 1.33        | 1.46     |
| 52  | J     | 401 | NDP  | O2D-C2D | -4.15 | 1.33        | 1.43     |
| 52  | J     | 401 | NDP  | C7N-N7N | 4.14  | 1.44        | 1.33     |
| 47  | A     | 503 | NAI  | C6N-C5N | 4.05  | 1.40        | 1.33     |
| 48  | B     | 303 | PEE  | C18-C19 | 3.75  | 1.53        | 1.31     |
| 48  | j     | 201 | PEE  | C18-C19 | 3.74  | 1.53        | 1.31     |
| 48  | r     | 501 | PEE  | C18-C19 | 3.73  | 1.53        | 1.31     |
| 48  | V     | 203 | PEE  | C18-C19 | 3.73  | 1.53        | 1.31     |
| 48  | W     | 201 | PEE  | C18-C19 | 3.73  | 1.53        | 1.31     |
| 48  | C     | 302 | PEE  | C18-C19 | 3.72  | 1.53        | 1.31     |
| 48  | j     | 202 | PEE  | C18-C19 | 3.72  | 1.53        | 1.31     |
| 48  | l     | 704 | PEE  | C18-C19 | 3.72  | 1.53        | 1.31     |
| 48  | l     | 703 | PEE  | C18-C19 | 3.71  | 1.53        | 1.31     |
| 46  | A     | 502 | FMN  | C4A-N5  | 3.67  | 1.37        | 1.30     |
| 48  | B     | 303 | PEE  | C39-C38 | 3.67  | 1.53        | 1.31     |
| 48  | r     | 501 | PEE  | C39-C38 | 3.65  | 1.52        | 1.31     |
| 48  | j     | 201 | PEE  | C39-C38 | 3.65  | 1.52        | 1.31     |
| 48  | C     | 302 | PEE  | C39-C38 | 3.64  | 1.52        | 1.31     |
| 48  | V     | 203 | PEE  | C39-C38 | 3.64  | 1.52        | 1.31     |
| 48  | l     | 703 | PEE  | C39-C38 | 3.63  | 1.52        | 1.31     |
| 48  | l     | 704 | PEE  | C39-C38 | 3.63  | 1.52        | 1.31     |
| 47  | A     | 503 | NAI  | C7N-C3N | 3.60  | 1.56        | 1.48     |
| 56  | i     | 401 | CDL  | OA8-CA7 | 3.51  | 1.43        | 1.33     |
| 56  | l     | 701 | CDL  | OA8-CA7 | 3.50  | 1.43        | 1.33     |
| 56  | V     | 204 | CDL  | OA8-CA7 | 3.48  | 1.43        | 1.33     |
| 56  | n     | 101 | CDL  | OA8-CA7 | 3.46  | 1.43        | 1.33     |
| 56  | N     | 201 | CDL  | OA8-CA7 | 3.46  | 1.43        | 1.33     |
| 56  | a     | 201 | CDL  | OA8-CA7 | 3.45  | 1.43        | 1.33     |
| 56  | V     | 201 | CDL  | OA8-CA7 | 3.44  | 1.43        | 1.33     |
| 56  | l     | 702 | CDL  | OA8-CA7 | 3.44  | 1.43        | 1.33     |
| 56  | r     | 503 | CDL  | OA8-CA7 | 3.43  | 1.43        | 1.33     |
| 56  | s     | 401 | CDL  | OA8-CA7 | 3.42  | 1.43        | 1.33     |
| 56  | V     | 202 | CDL  | OA8-CA7 | 3.38  | 1.43        | 1.33     |
| 58  | w     | 401 | ADP  | O2'-C2' | -3.37 | 1.35        | 1.43     |
| 47  | A     | 503 | NAI  | C4N-C5N | -3.29 | 1.40        | 1.48     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 58  | w     | 401 | ADP  | C8-N9   | -3.17 | 1.31        | 1.37     |
| 56  | V     | 201 | CDL  | OA6-CA5 | 3.13  | 1.43        | 1.34     |
| 56  | V     | 204 | CDL  | OA6-CA5 | 3.12  | 1.43        | 1.34     |
| 58  | w     | 401 | ADP  | O3'-C3' | 3.08  | 1.50        | 1.43     |
| 56  | r     | 503 | CDL  | OB6-CB5 | 3.08  | 1.43        | 1.34     |
| 56  | i     | 401 | CDL  | OB6-CB5 | 3.07  | 1.43        | 1.34     |
| 56  | s     | 401 | CDL  | OB6-CB5 | 3.06  | 1.42        | 1.34     |
| 56  | n     | 101 | CDL  | OB8-CB7 | 3.05  | 1.42        | 1.33     |
| 56  | l     | 701 | CDL  | OB6-CB5 | 3.04  | 1.42        | 1.34     |
| 56  | N     | 201 | CDL  | OB6-CB5 | 3.04  | 1.42        | 1.34     |
| 56  | s     | 401 | CDL  | OA6-CA5 | 3.04  | 1.42        | 1.34     |
| 56  | a     | 201 | CDL  | OB6-CB5 | 3.04  | 1.42        | 1.34     |
| 52  | J     | 401 | NDP  | O3D-C3D | 3.03  | 1.50        | 1.43     |
| 56  | n     | 101 | CDL  | OB6-CB5 | 3.03  | 1.42        | 1.34     |
| 56  | N     | 201 | CDL  | OB8-CB7 | 3.02  | 1.42        | 1.33     |
| 56  | V     | 202 | CDL  | OA6-CA5 | 3.02  | 1.42        | 1.34     |
| 52  | J     | 401 | NDP  | C7N-C3N | 3.02  | 1.55        | 1.48     |
| 56  | a     | 201 | CDL  | OB8-CB7 | 3.01  | 1.42        | 1.33     |
| 56  | a     | 201 | CDL  | OA6-CA5 | 3.00  | 1.42        | 1.34     |
| 56  | V     | 201 | CDL  | OB8-CB7 | 3.00  | 1.42        | 1.33     |
| 56  | l     | 702 | CDL  | OA6-CA5 | 3.00  | 1.42        | 1.34     |
| 56  | V     | 202 | CDL  | OB8-CB7 | 3.00  | 1.42        | 1.33     |
| 56  | V     | 204 | CDL  | OB8-CB7 | 3.00  | 1.42        | 1.33     |
| 56  | i     | 401 | CDL  | OA6-CA5 | 3.00  | 1.42        | 1.34     |
| 56  | l     | 701 | CDL  | OB8-CB7 | 2.99  | 1.42        | 1.33     |
| 56  | V     | 202 | CDL  | OB6-CB5 | 2.99  | 1.42        | 1.34     |
| 56  | V     | 204 | CDL  | OB6-CB5 | 2.99  | 1.42        | 1.34     |
| 56  | V     | 201 | CDL  | OB6-CB5 | 2.99  | 1.42        | 1.34     |
| 56  | l     | 702 | CDL  | OB8-CB7 | 2.98  | 1.42        | 1.33     |
| 56  | i     | 401 | CDL  | OB8-CB7 | 2.98  | 1.42        | 1.33     |
| 56  | l     | 702 | CDL  | OB6-CB5 | 2.98  | 1.42        | 1.34     |
| 56  | r     | 503 | CDL  | OB8-CB7 | 2.97  | 1.42        | 1.33     |
| 52  | J     | 401 | NDP  | C8A-N9A | -2.96 | 1.32        | 1.37     |
| 56  | s     | 401 | CDL  | OB8-CB7 | 2.96  | 1.42        | 1.33     |
| 56  | n     | 101 | CDL  | OA6-CA5 | 2.93  | 1.42        | 1.34     |
| 56  | N     | 201 | CDL  | OA6-CA5 | 2.92  | 1.42        | 1.34     |
| 56  | r     | 503 | CDL  | OA6-CA5 | 2.90  | 1.42        | 1.34     |
| 52  | J     | 401 | NDP  | C5A-N7A | -2.89 | 1.33        | 1.39     |
| 56  | l     | 701 | CDL  | OA6-CA5 | 2.88  | 1.42        | 1.34     |
| 49  | e     | 201 | PLX  | O6-C4   | -2.78 | 1.40        | 1.44     |
| 49  | a     | 202 | PLX  | O6-C4   | -2.75 | 1.40        | 1.44     |
| 53  | J     | 402 | UQ   | C6-C1   | 2.73  | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | g     | 201 | PLX  | O6-C4   | -2.73 | 1.41        | 1.44     |
| 53  | s     | 402 | UQ   | C6-C1   | 2.71  | 1.54        | 1.46     |
| 49  | J     | 403 | PLX  | O6-C4   | -2.71 | 1.41        | 1.44     |
| 53  | s     | 402 | UQ   | C7-C8   | 2.68  | 1.54        | 1.50     |
| 49  | C     | 303 | PLX  | O6-C4   | -2.61 | 1.41        | 1.44     |
| 49  | j     | 203 | PLX  | O6-C4   | -2.57 | 1.41        | 1.44     |
| 46  | A     | 502 | FMN  | C10-N1  | 2.54  | 1.38        | 1.33     |
| 47  | A     | 503 | NAI  | C8A-N9A | -2.51 | 1.33        | 1.37     |
| 49  | r     | 502 | PLX  | O6-C4   | -2.50 | 1.41        | 1.44     |
| 51  | X     | 201 | 8Q1  | C1-S44  | 2.49  | 1.82        | 1.76     |
| 47  | A     | 503 | NAI  | O3B-C3B | -2.47 | 1.37        | 1.43     |
| 48  | B     | 303 | PEE  | O3-C30  | 2.47  | 1.40        | 1.33     |
| 48  | r     | 501 | PEE  | O2-C2   | -2.45 | 1.40        | 1.46     |
| 49  | j     | 203 | PLX  | C7-C6   | 2.44  | 1.55        | 1.50     |
| 56  | l     | 701 | CDL  | OA6-CA4 | -2.44 | 1.40        | 1.46     |
| 56  | n     | 101 | CDL  | OA6-CA4 | -2.44 | 1.40        | 1.46     |
| 48  | W     | 201 | PEE  | O2-C2   | -2.44 | 1.40        | 1.46     |
| 48  | V     | 203 | PEE  | O3-C30  | 2.43  | 1.40        | 1.33     |
| 48  | j     | 202 | PEE  | O2-C2   | -2.43 | 1.40        | 1.46     |
| 56  | a     | 201 | CDL  | OA6-CA4 | -2.43 | 1.40        | 1.46     |
| 48  | C     | 302 | PEE  | O2-C2   | -2.43 | 1.40        | 1.46     |
| 48  | j     | 201 | PEE  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 48  | l     | 703 | PEE  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 48  | j     | 202 | PEE  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 48  | W     | 201 | PEE  | O3-C30  | 2.42  | 1.40        | 1.33     |
| 56  | r     | 503 | CDL  | OA6-CA4 | -2.42 | 1.40        | 1.46     |
| 48  | l     | 704 | PEE  | O3-C30  | 2.41  | 1.40        | 1.33     |
| 51  | G     | 201 | 8Q1  | C1-S44  | 2.41  | 1.82        | 1.76     |
| 48  | B     | 303 | PEE  | O2-C2   | -2.41 | 1.40        | 1.46     |
| 56  | N     | 201 | CDL  | OA6-CA4 | -2.41 | 1.40        | 1.46     |
| 51  | X     | 201 | 8Q1  | C6-C1   | 2.41  | 1.53        | 1.50     |
| 48  | r     | 501 | PEE  | O3-C30  | 2.40  | 1.40        | 1.33     |
| 48  | C     | 302 | PEE  | O3-C30  | 2.40  | 1.40        | 1.33     |
| 56  | i     | 401 | CDL  | OA6-CA4 | -2.40 | 1.40        | 1.46     |
| 48  | j     | 201 | PEE  | O2-C2   | -2.39 | 1.40        | 1.46     |
| 52  | J     | 401 | NDP  | O2B-C2B | 2.38  | 1.52        | 1.44     |
| 49  | C     | 303 | PLX  | C7-C6   | 2.37  | 1.55        | 1.50     |
| 49  | J     | 403 | PLX  | C7-C6   | 2.37  | 1.55        | 1.50     |
| 47  | A     | 503 | NAI  | PN-O5D  | 2.36  | 1.68        | 1.59     |
| 56  | l     | 702 | CDL  | OA6-CA4 | -2.36 | 1.40        | 1.46     |
| 48  | V     | 203 | PEE  | O2-C10  | 2.36  | 1.41        | 1.34     |
| 48  | l     | 704 | PEE  | O2-C2   | -2.35 | 1.40        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56  | V     | 202 | CDL  | OA6-CA4 | -2.35 | 1.40        | 1.46     |
| 48  | l     | 703 | PEE  | O2-C2   | -2.35 | 1.40        | 1.46     |
| 56  | s     | 401 | CDL  | OA6-CA4 | -2.34 | 1.40        | 1.46     |
| 48  | l     | 703 | PEE  | O2-C10  | 2.34  | 1.40        | 1.34     |
| 52  | J     | 401 | NDP  | C2D-C3D | 2.33  | 1.59        | 1.53     |
| 53  | J     | 402 | UQ   | C7-C8   | 2.33  | 1.54        | 1.50     |
| 48  | l     | 704 | PEE  | O2-C10  | 2.32  | 1.40        | 1.34     |
| 49  | a     | 202 | PLX  | C7-C6   | 2.32  | 1.55        | 1.50     |
| 48  | V     | 203 | PEE  | O2-C2   | -2.31 | 1.40        | 1.46     |
| 48  | W     | 201 | PEE  | O2-C10  | 2.31  | 1.40        | 1.34     |
| 47  | A     | 503 | NAI  | C5B-C4B | 2.29  | 1.58        | 1.51     |
| 58  | w     | 401 | ADP  | C5-N7   | -2.29 | 1.34        | 1.39     |
| 49  | r     | 502 | PLX  | C7-C6   | 2.29  | 1.55        | 1.50     |
| 49  | e     | 201 | PLX  | C7-C6   | 2.28  | 1.55        | 1.50     |
| 50  | C     | 304 | DCQ  | C6-C5   | 2.28  | 1.53        | 1.46     |
| 51  | X     | 201 | 8Q1  | O40-C39 | -2.27 | 1.18        | 1.23     |
| 48  | B     | 303 | PEE  | O2-C10  | 2.27  | 1.40        | 1.34     |
| 51  | G     | 201 | 8Q1  | O40-C39 | -2.26 | 1.18        | 1.23     |
| 56  | l     | 702 | CDL  | OB6-CB4 | -2.26 | 1.41        | 1.46     |
| 48  | C     | 302 | PEE  | O2-C10  | 2.25  | 1.40        | 1.34     |
| 56  | V     | 201 | CDL  | PB2-OB2 | 2.25  | 1.68        | 1.59     |
| 49  | g     | 201 | PLX  | C7-C6   | 2.25  | 1.55        | 1.50     |
| 48  | j     | 201 | PEE  | O2-C10  | 2.24  | 1.40        | 1.34     |
| 48  | j     | 202 | PEE  | O2-C10  | 2.23  | 1.40        | 1.34     |
| 56  | V     | 202 | CDL  | OB6-CB4 | -2.23 | 1.41        | 1.46     |
| 51  | G     | 201 | 8Q1  | O35-C34 | -2.23 | 1.19        | 1.23     |
| 56  | n     | 101 | CDL  | PB2-OB2 | 2.23  | 1.68        | 1.59     |
| 56  | V     | 204 | CDL  | OA6-CA4 | -2.22 | 1.41        | 1.46     |
| 48  | r     | 501 | PEE  | O2-C10  | 2.22  | 1.40        | 1.34     |
| 56  | n     | 101 | CDL  | OB6-CB4 | -2.21 | 1.41        | 1.46     |
| 56  | N     | 201 | CDL  | PB2-OB5 | 2.21  | 1.68        | 1.59     |
| 56  | N     | 201 | CDL  | PB2-OB2 | 2.21  | 1.68        | 1.59     |
| 53  | s     | 402 | UQ   | O4-C4   | -2.21 | 1.18        | 1.23     |
| 56  | a     | 201 | CDL  | PB2-OB2 | 2.21  | 1.68        | 1.59     |
| 56  | i     | 401 | CDL  | PB2-OB5 | 2.20  | 1.68        | 1.59     |
| 56  | V     | 202 | CDL  | PB2-OB2 | 2.20  | 1.68        | 1.59     |
| 56  | s     | 401 | CDL  | PB2-OB2 | 2.20  | 1.68        | 1.59     |
| 56  | n     | 101 | CDL  | PB2-OB5 | 2.19  | 1.68        | 1.59     |
| 51  | X     | 201 | 8Q1  | O35-C34 | -2.19 | 1.19        | 1.23     |
| 56  | r     | 503 | CDL  | PB2-OB2 | 2.19  | 1.68        | 1.59     |
| 56  | V     | 201 | CDL  | PB2-OB5 | 2.19  | 1.68        | 1.59     |
| 50  | C     | 304 | DCQ  | O4-C4M  | -2.19 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 56  | i     | 401 | CDL  | PB2-OB2 | 2.18  | 1.68        | 1.59     |
| 49  | J     | 403 | PLX  | P1-O4   | 2.18  | 1.68        | 1.59     |
| 56  | r     | 503 | CDL  | PB2-OB5 | 2.18  | 1.68        | 1.59     |
| 56  | V     | 204 | CDL  | OB6-CB4 | -2.18 | 1.41        | 1.46     |
| 56  | l     | 702 | CDL  | PB2-OB2 | 2.18  | 1.68        | 1.59     |
| 56  | V     | 204 | CDL  | PB2-OB2 | 2.17  | 1.68        | 1.59     |
| 56  | l     | 701 | CDL  | PB2-OB5 | 2.17  | 1.68        | 1.59     |
| 53  | J     | 402 | UQ   | O4-C4   | -2.17 | 1.18        | 1.23     |
| 56  | a     | 201 | CDL  | OB6-CB4 | -2.17 | 1.41        | 1.46     |
| 56  | l     | 701 | CDL  | OB6-CB4 | -2.16 | 1.41        | 1.46     |
| 56  | l     | 701 | CDL  | PB2-OB2 | 2.16  | 1.68        | 1.59     |
| 48  | V     | 203 | PEE  | O3-C3   | -2.15 | 1.40        | 1.45     |
| 56  | s     | 401 | CDL  | OB6-CB4 | -2.15 | 1.41        | 1.46     |
| 48  | W     | 201 | PEE  | O3-C3   | -2.15 | 1.40        | 1.45     |
| 56  | V     | 201 | CDL  | OB6-CB4 | -2.15 | 1.41        | 1.46     |
| 56  | a     | 201 | CDL  | PB2-OB5 | 2.15  | 1.68        | 1.59     |
| 49  | j     | 203 | PLX  | P1-O4   | 2.14  | 1.68        | 1.59     |
| 56  | s     | 401 | CDL  | PB2-OB5 | 2.14  | 1.68        | 1.59     |
| 49  | g     | 201 | PLX  | P1-O4   | 2.13  | 1.67        | 1.59     |
| 56  | V     | 202 | CDL  | PB2-OB5 | 2.13  | 1.67        | 1.59     |
| 56  | N     | 201 | CDL  | OB6-CB4 | -2.13 | 1.41        | 1.46     |
| 56  | V     | 204 | CDL  | PB2-OB5 | 2.13  | 1.67        | 1.59     |
| 49  | C     | 303 | PLX  | P1-O4   | 2.13  | 1.67        | 1.59     |
| 53  | J     | 402 | UQ   | C21-C19 | 2.13  | 1.55        | 1.51     |
| 49  | e     | 201 | PLX  | P1-O4   | 2.13  | 1.67        | 1.59     |
| 56  | l     | 702 | CDL  | PB2-OB5 | 2.12  | 1.67        | 1.59     |
| 48  | l     | 703 | PEE  | O3-C3   | -2.12 | 1.40        | 1.45     |
| 48  | B     | 303 | PEE  | O3-C3   | -2.12 | 1.40        | 1.45     |
| 52  | J     | 401 | NDP  | O7N-C7N | -2.12 | 1.19        | 1.24     |
| 48  | C     | 302 | PEE  | O3-C3   | -2.11 | 1.40        | 1.45     |
| 48  | r     | 501 | PEE  | O3-C3   | -2.11 | 1.40        | 1.45     |
| 56  | r     | 503 | CDL  | OB6-CB4 | -2.11 | 1.41        | 1.46     |
| 49  | a     | 202 | PLX  | P1-O4   | 2.10  | 1.67        | 1.59     |
| 50  | C     | 304 | DCQ  | O3-C3M  | -2.10 | 1.40        | 1.45     |
| 49  | r     | 502 | PLX  | P1-O4   | 2.09  | 1.67        | 1.59     |
| 56  | i     | 401 | CDL  | OB6-CB4 | -2.09 | 1.41        | 1.46     |
| 49  | r     | 502 | PLX  | C25-C24 | 2.09  | 1.55        | 1.50     |
| 52  | J     | 401 | NDP  | PA-O5B  | 2.08  | 1.67        | 1.59     |
| 48  | l     | 704 | PEE  | O3-C3   | -2.08 | 1.40        | 1.45     |
| 49  | e     | 201 | PLX  | P1-O1   | 2.07  | 1.67        | 1.59     |
| 48  | j     | 202 | PEE  | O3-C3   | -2.07 | 1.40        | 1.45     |
| 48  | j     | 201 | PEE  | O3-C3   | -2.06 | 1.40        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | j     | 203 | PLX  | P1-O1   | 2.06  | 1.67        | 1.59     |
| 49  | J     | 403 | PLX  | P1-O1   | 2.06  | 1.67        | 1.59     |
| 56  | V     | 201 | CDL  | C11-CA5 | 2.05  | 1.56        | 1.50     |
| 49  | C     | 303 | PLX  | P1-O1   | 2.05  | 1.67        | 1.59     |
| 50  | C     | 304 | DCQ  | O2-C2   | -2.05 | 1.18        | 1.23     |
| 51  | G     | 201 | 8Q1  | C6-C1   | 2.05  | 1.52        | 1.50     |
| 53  | s     | 402 | UQ   | C21-C19 | 2.05  | 1.55        | 1.51     |
| 53  | s     | 402 | UQ   | O1-C1   | -2.04 | 1.18        | 1.23     |
| 56  | V     | 202 | CDL  | C11-CA5 | 2.03  | 1.56        | 1.50     |
| 53  | s     | 402 | UQ   | O3-CM3  | -2.03 | 1.40        | 1.45     |
| 49  | a     | 202 | PLX  | P1-O1   | 2.03  | 1.67        | 1.59     |
| 49  | r     | 502 | PLX  | P1-O1   | 2.03  | 1.67        | 1.59     |
| 56  | V     | 201 | CDL  | OA6-CA4 | -2.02 | 1.41        | 1.46     |
| 49  | g     | 201 | PLX  | P1-O1   | 2.02  | 1.67        | 1.59     |
| 56  | s     | 401 | CDL  | C11-CA5 | 2.01  | 1.56        | 1.50     |
| 47  | A     | 503 | NAI  | C5A-N7A | -2.00 | 1.35        | 1.39     |

All (154) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 53  | J     | 402 | UQ   | C7-C8-C9    | -8.01 | 113.45      | 126.79   |
| 52  | J     | 401 | NDP  | C3N-C2N-N1N | -7.73 | 112.06      | 123.10   |
| 52  | J     | 401 | NDP  | C1D-N1N-C2N | -7.18 | 109.16      | 121.11   |
| 53  | s     | 402 | UQ   | C7-C8-C9    | -7.02 | 115.10      | 126.79   |
| 51  | G     | 201 | 8Q1  | C6-C1-S44   | 6.63  | 121.17      | 113.46   |
| 52  | J     | 401 | NDP  | C5A-C4A-N3A | -6.02 | 118.89      | 126.75   |
| 53  | J     | 402 | UQ   | C12-C13-C14 | -6.01 | 113.19      | 127.66   |
| 53  | J     | 402 | UQ   | C17-C18-C19 | -5.92 | 113.40      | 127.66   |
| 51  | X     | 201 | 8Q1  | C6-C1-S44   | 5.87  | 120.29      | 113.46   |
| 53  | s     | 402 | UQ   | C12-C13-C14 | -5.78 | 113.74      | 127.66   |
| 58  | w     | 401 | ADP  | C5-C4-N3    | -5.73 | 119.27      | 126.75   |
| 47  | A     | 503 | NAI  | C5A-C4A-N3A | -5.69 | 119.32      | 126.75   |
| 53  | s     | 402 | UQ   | C22-C23-C24 | -5.66 | 114.02      | 127.66   |
| 53  | s     | 402 | UQ   | C17-C18-C19 | -5.60 | 114.16      | 127.66   |
| 52  | J     | 401 | NDP  | C1D-N1N-C6N | -5.51 | 108.96      | 120.83   |
| 53  | s     | 402 | UQ   | C10-C9-C8   | -4.59 | 111.89      | 123.68   |
| 58  | w     | 401 | ADP  | N3-C2-N1    | -4.53 | 121.51      | 128.60   |
| 53  | J     | 402 | UQ   | C10-C9-C8   | -4.49 | 112.16      | 123.68   |
| 58  | w     | 401 | ADP  | N3-C4-N9    | 4.48  | 134.46      | 127.08   |
| 56  | s     | 401 | CDL  | OA6-CA5-C11 | 4.39  | 120.96      | 111.50   |
| 53  | s     | 402 | UQ   | C25-C24-C23 | -4.35 | 112.51      | 123.68   |
| 47  | A     | 503 | NAI  | N3A-C2A-N1A | -4.34 | 121.81      | 128.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 53  | J     | 402 | UQ   | C16-C14-C13 | -4.32 | 112.37      | 121.12   |
| 53  | s     | 402 | UQ   | C27-C28-C29 | -4.29 | 113.08      | 127.75   |
| 53  | J     | 402 | UQ   | C15-C14-C13 | -4.24 | 112.79      | 123.68   |
| 53  | J     | 402 | UQ   | C22-C23-C24 | -4.20 | 113.40      | 127.75   |
| 52  | J     | 401 | NDP  | N3A-C4A-N9A | 4.20  | 134.00      | 127.08   |
| 56  | V     | 201 | CDL  | OB6-CB5-C51 | 4.17  | 120.48      | 111.50   |
| 53  | J     | 402 | UQ   | C20-C19-C18 | -4.13 | 113.07      | 123.68   |
| 56  | N     | 201 | CDL  | OB6-CB5-C51 | 4.11  | 120.37      | 111.50   |
| 52  | J     | 401 | NDP  | N3A-C2A-N1A | -4.07 | 122.23      | 128.60   |
| 53  | s     | 402 | UQ   | C21-C19-C18 | -4.07 | 112.88      | 121.12   |
| 48  | j     | 202 | PEE  | O2-C10-C11  | 4.06  | 120.25      | 111.50   |
| 56  | V     | 204 | CDL  | OB6-CB5-C51 | 4.05  | 120.22      | 111.50   |
| 56  | V     | 202 | CDL  | OA6-CA5-C11 | 4.04  | 120.22      | 111.50   |
| 48  | C     | 302 | PEE  | O2-C10-C11  | 4.04  | 120.20      | 111.50   |
| 53  | s     | 402 | UQ   | C11-C9-C8   | -4.04 | 112.95      | 121.12   |
| 53  | J     | 402 | UQ   | C11-C9-C8   | -4.01 | 113.00      | 121.12   |
| 48  | B     | 303 | PEE  | O2-C10-C11  | 3.98  | 120.09      | 111.50   |
| 47  | A     | 503 | NAI  | N3A-C4A-N9A | 3.98  | 133.63      | 127.08   |
| 56  | r     | 503 | CDL  | OA6-CA5-C11 | 3.97  | 120.06      | 111.50   |
| 56  | s     | 401 | CDL  | OB6-CB5-C51 | 3.97  | 120.06      | 111.50   |
| 53  | s     | 402 | UQ   | C16-C14-C13 | -3.97 | 113.08      | 121.12   |
| 51  | G     | 201 | 8Q1  | O4-C1-C6    | -3.96 | 119.31      | 123.99   |
| 48  | V     | 203 | PEE  | O2-C10-C11  | 3.96  | 120.03      | 111.50   |
| 56  | a     | 201 | CDL  | OB6-CB5-C51 | 3.95  | 120.02      | 111.50   |
| 56  | i     | 401 | CDL  | OB6-CB5-C51 | 3.95  | 120.02      | 111.50   |
| 56  | n     | 101 | CDL  | OA6-CA5-C11 | 3.94  | 120.00      | 111.50   |
| 56  | l     | 701 | CDL  | OA6-CA5-C11 | 3.93  | 119.97      | 111.50   |
| 53  | s     | 402 | UQ   | C20-C19-C18 | -3.93 | 113.61      | 123.68   |
| 56  | V     | 202 | CDL  | OB6-CB5-C51 | 3.92  | 119.95      | 111.50   |
| 56  | r     | 503 | CDL  | OB6-CB5-C51 | 3.92  | 119.95      | 111.50   |
| 48  | l     | 704 | PEE  | O2-C10-C11  | 3.91  | 119.94      | 111.50   |
| 56  | l     | 702 | CDL  | OA6-CA5-C11 | 3.91  | 119.93      | 111.50   |
| 56  | n     | 101 | CDL  | OB6-CB5-C51 | 3.90  | 119.90      | 111.50   |
| 53  | s     | 402 | UQ   | C15-C14-C13 | -3.88 | 113.74      | 123.68   |
| 48  | r     | 501 | PEE  | O2-C10-C11  | 3.86  | 119.82      | 111.50   |
| 56  | V     | 201 | CDL  | OA6-CA5-C11 | 3.85  | 119.81      | 111.50   |
| 48  | j     | 201 | PEE  | O2-C10-C11  | 3.84  | 119.79      | 111.50   |
| 56  | N     | 201 | CDL  | OA6-CA5-C11 | 3.84  | 119.78      | 111.50   |
| 47  | A     | 503 | NAI  | C2A-N3A-C4A | 3.83  | 120.80      | 111.75   |
| 52  | J     | 401 | NDP  | C2A-N3A-C4A | 3.83  | 120.80      | 111.75   |
| 56  | l     | 701 | CDL  | OB6-CB5-C51 | 3.82  | 119.73      | 111.50   |
| 53  | J     | 402 | UQ   | C21-C19-C18 | -3.80 | 113.44      | 121.12   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | i     | 401 | CDL  | OA6-CA5-C11 | 3.79  | 119.66      | 111.50   |
| 48  | W     | 201 | PEE  | O2-C10-C11  | 3.77  | 119.62      | 111.50   |
| 58  | w     | 401 | ADP  | N9-C8-N7    | -3.74 | 108.80      | 113.91   |
| 58  | w     | 401 | ADP  | C2-N3-C4    | 3.74  | 120.58      | 111.75   |
| 48  | l     | 703 | PEE  | O2-C10-C11  | 3.73  | 119.54      | 111.50   |
| 53  | s     | 402 | UQ   | C26-C24-C23 | -3.72 | 113.58      | 121.12   |
| 47  | A     | 503 | NAI  | C5A-N7A-C8A | 3.70  | 108.77      | 103.51   |
| 56  | l     | 702 | CDL  | OB6-CB5-C51 | 3.61  | 119.29      | 111.50   |
| 58  | w     | 401 | ADP  | C5-N7-C8    | 3.60  | 108.62      | 103.51   |
| 56  | a     | 201 | CDL  | OA6-CA5-C11 | 3.54  | 119.13      | 111.50   |
| 47  | A     | 503 | NAI  | N9A-C8A-N7A | -3.45 | 109.20      | 113.91   |
| 51  | X     | 201 | 8Q1  | O4-C1-C6    | -3.40 | 119.97      | 123.99   |
| 51  | G     | 201 | 8Q1  | C37-C38-C39 | 3.39  | 118.00      | 112.36   |
| 52  | J     | 401 | NDP  | C5A-N7A-C8A | 3.39  | 108.32      | 103.51   |
| 56  | V     | 204 | CDL  | OA6-CA5-C11 | 3.37  | 118.77      | 111.50   |
| 53  | s     | 402 | UQ   | C30-C29-C28 | -3.37 | 112.91      | 122.65   |
| 53  | J     | 402 | UQ   | C26-C24-C23 | -3.34 | 112.99      | 122.65   |
| 53  | s     | 402 | UQ   | C31-C29-C28 | -3.34 | 113.00      | 122.65   |
| 56  | n     | 101 | CDL  | OA8-CA7-C31 | 3.31  | 120.06      | 111.38   |
| 53  | J     | 402 | UQ   | C25-C24-C23 | -3.27 | 113.19      | 122.65   |
| 52  | J     | 401 | NDP  | N9A-C8A-N7A | -3.24 | 109.48      | 113.91   |
| 47  | A     | 503 | NAI  | C4A-C5A-N7A | -3.22 | 106.69      | 110.62   |
| 58  | w     | 401 | ADP  | C4-N9-C8    | 3.18  | 109.17      | 105.73   |
| 46  | A     | 502 | FMN  | C4-N3-C2    | -3.14 | 119.83      | 125.64   |
| 47  | A     | 503 | NAI  | C3D-C2D-C1D | 3.09  | 107.30      | 101.43   |
| 52  | J     | 401 | NDP  | C4A-C5A-N7A | -3.07 | 106.88      | 110.62   |
| 47  | A     | 503 | NAI  | C2D-C3D-C4D | 2.94  | 108.36      | 102.64   |
| 58  | w     | 401 | ADP  | C4-C5-N7    | -2.86 | 107.14      | 110.62   |
| 48  | B     | 303 | PEE  | O3-C30-C31  | 2.81  | 120.73      | 111.91   |
| 56  | V     | 204 | CDL  | OB8-CB7-C71 | 2.81  | 120.71      | 111.91   |
| 56  | l     | 701 | CDL  | OA8-CA7-C31 | 2.77  | 120.61      | 111.91   |
| 56  | V     | 204 | CDL  | OA8-CA7-C31 | 2.75  | 120.53      | 111.91   |
| 51  | X     | 201 | 8Q1  | C38-C39-N41 | 2.74  | 121.04      | 116.42   |
| 51  | X     | 201 | 8Q1  | C37-C38-C39 | 2.72  | 116.89      | 112.36   |
| 56  | N     | 201 | CDL  | OB8-CB7-C71 | 2.69  | 120.35      | 111.91   |
| 46  | A     | 502 | FMN  | C4A-C4-N3   | 2.68  | 119.99      | 113.19   |
| 56  | i     | 401 | CDL  | OA8-CA7-C31 | 2.68  | 120.31      | 111.91   |
| 56  | V     | 201 | CDL  | OB8-CB7-C71 | 2.67  | 120.30      | 111.91   |
| 56  | a     | 201 | CDL  | OB8-CB7-C71 | 2.67  | 120.28      | 111.91   |
| 56  | n     | 101 | CDL  | OB8-CB7-C71 | 2.66  | 120.27      | 111.91   |
| 56  | r     | 503 | CDL  | OB8-CB7-C71 | 2.64  | 120.20      | 111.91   |
| 48  | l     | 704 | PEE  | O3-C30-C31  | 2.64  | 120.20      | 111.91   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 48  | r     | 501 | PEE  | O3-C30-C31  | 2.63  | 120.18      | 111.91   |
| 48  | V     | 203 | PEE  | O3-C30-C31  | 2.63  | 120.15      | 111.91   |
| 58  | w     | 401 | ADP  | C4'-O4'-C1' | -2.63 | 103.68      | 109.47   |
| 48  | l     | 703 | PEE  | O3-C30-C31  | 2.62  | 120.13      | 111.91   |
| 47  | A     | 503 | NAI  | PN-O3-PA    | -2.61 | 123.86      | 132.83   |
| 56  | V     | 202 | CDL  | OB8-CB7-C71 | 2.61  | 120.10      | 111.91   |
| 56  | l     | 701 | CDL  | OB8-CB7-C71 | 2.61  | 120.09      | 111.91   |
| 56  | a     | 201 | CDL  | OA8-CA7-C31 | 2.61  | 120.09      | 111.91   |
| 58  | w     | 401 | ADP  | PA-O3A-PB   | -2.60 | 123.91      | 132.83   |
| 56  | i     | 401 | CDL  | OB8-CB7-C71 | 2.58  | 120.02      | 111.91   |
| 48  | j     | 202 | PEE  | O3-C30-C31  | 2.58  | 120.01      | 111.91   |
| 56  | r     | 503 | CDL  | OA8-CA7-C31 | 2.57  | 119.97      | 111.91   |
| 46  | A     | 502 | FMN  | O4-C4-C4A   | -2.57 | 119.79      | 126.60   |
| 50  | C     | 304 | DCQ  | C1M-C1-C6   | -2.56 | 120.22      | 124.40   |
| 56  | V     | 201 | CDL  | OA8-CA7-C31 | 2.56  | 119.93      | 111.91   |
| 56  | N     | 201 | CDL  | OA8-CA7-C31 | 2.55  | 119.90      | 111.91   |
| 56  | l     | 702 | CDL  | OB8-CB7-C71 | 2.54  | 119.88      | 111.91   |
| 56  | l     | 702 | CDL  | OA8-CA7-C31 | 2.54  | 119.88      | 111.91   |
| 48  | j     | 201 | PEE  | O3-C30-C31  | 2.54  | 119.87      | 111.91   |
| 56  | s     | 401 | CDL  | OA8-CA7-C31 | 2.53  | 119.85      | 111.91   |
| 48  | C     | 302 | PEE  | O3-C30-C31  | 2.53  | 119.84      | 111.91   |
| 53  | J     | 402 | UQ   | CM5-C5-C6   | -2.53 | 120.28      | 124.40   |
| 48  | W     | 201 | PEE  | O3-C30-C31  | 2.51  | 119.79      | 111.91   |
| 56  | s     | 401 | CDL  | OB8-CB7-C71 | 2.49  | 119.73      | 111.91   |
| 49  | r     | 502 | PLX  | C1A-N1-C1   | 2.48  | 120.08      | 109.92   |
| 56  | V     | 202 | CDL  | OA8-CA7-C31 | 2.48  | 119.70      | 111.91   |
| 52  | J     | 401 | NDP  | PN-O3-PA    | -2.47 | 124.35      | 132.83   |
| 51  | X     | 201 | 8Q1  | C43-S44-C1  | 2.47  | 109.56      | 101.87   |
| 46  | A     | 502 | FMN  | C4A-C10-N1  | -2.45 | 119.04      | 124.73   |
| 49  | a     | 202 | PLX  | C1A-N1-C1   | 2.40  | 119.74      | 109.92   |
| 51  | G     | 201 | 8Q1  | O4-C1-S44   | -2.39 | 119.52      | 122.61   |
| 47  | A     | 503 | NAI  | C4A-N9A-C8A | 2.37  | 108.30      | 105.73   |
| 49  | j     | 203 | PLX  | C1A-N1-C1   | 2.35  | 119.55      | 109.92   |
| 46  | A     | 502 | FMN  | C4A-C10-N10 | 2.35  | 119.91      | 116.48   |
| 49  | g     | 201 | PLX  | C1A-N1-C1   | 2.32  | 119.42      | 109.92   |
| 52  | J     | 401 | NDP  | C4A-N9A-C8A | 2.30  | 108.22      | 105.73   |
| 49  | J     | 403 | PLX  | C1A-N1-C1   | 2.29  | 119.30      | 109.92   |
| 49  | C     | 303 | PLX  | C1A-N1-C1   | 2.28  | 119.24      | 109.92   |
| 51  | X     | 201 | 8Q1  | O4-C1-S44   | -2.21 | 119.74      | 122.61   |
| 47  | A     | 503 | NAI  | C4D-O4D-C1D | -2.19 | 104.63      | 109.47   |
| 51  | X     | 201 | 8Q1  | C42-N41-C39 | -2.16 | 118.84      | 122.84   |
| 56  | s     | 401 | CDL  | CA4-OA6-CA5 | -2.13 | 112.54      | 117.79   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 46  | A     | 502 | FMN  | C10-C4A-N5  | -2.13 | 120.34      | 124.86   |
| 46  | A     | 502 | FMN  | C4-C4A-C10  | 2.08  | 120.28      | 116.79   |
| 46  | A     | 502 | FMN  | C9A-C5A-N5  | -2.07 | 120.18      | 122.43   |
| 56  | V     | 201 | CDL  | CB4-OB6-CB5 | -2.05 | 112.74      | 117.79   |
| 51  | G     | 201 | 8Q1  | C43-S44-C1  | 2.03  | 108.21      | 101.87   |
| 46  | A     | 502 | FMN  | C5A-C9A-N10 | 2.02  | 120.04      | 117.95   |

There are no chirality outliers.

All (1086) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 46  | A     | 502 | FMN  | N10-C1'-C2'-O2' |
| 46  | A     | 502 | FMN  | N10-C1'-C2'-C3' |
| 46  | A     | 502 | FMN  | C3'-C4'-C5'-O5' |
| 46  | A     | 502 | FMN  | O4'-C4'-C5'-O5' |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O2P   |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O3P   |
| 47  | A     | 503 | NAI  | PN-O3-PA-O5B    |
| 48  | C     | 302 | PEE  | C1-O3P-P-O1P    |
| 48  | V     | 203 | PEE  | C1-O3P-P-O2P    |
| 48  | W     | 201 | PEE  | O4P-C4-C5-N     |
| 48  | j     | 201 | PEE  | C1-O3P-P-O1P    |
| 48  | j     | 202 | PEE  | C11-C10-O2-C2   |
| 48  | j     | 202 | PEE  | C4-O4P-P-O2P    |
| 48  | j     | 202 | PEE  | C4-O4P-P-O1P    |
| 48  | l     | 703 | PEE  | C4-O4P-P-O3P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O1P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O4P    |
| 48  | r     | 501 | PEE  | C4-O4P-P-O1P    |
| 49  | C     | 303 | PLX  | O7-C6-C7-C8     |
| 49  | C     | 303 | PLX  | O6-C6-C7-C8     |
| 49  | C     | 303 | PLX  | O6-C4-C5-O8     |
| 49  | C     | 303 | PLX  | C2-O1-P1-O2     |
| 49  | C     | 303 | PLX  | C2-O1-P1-O3     |
| 49  | C     | 303 | PLX  | N1-C1-C2-O1     |
| 49  | C     | 303 | PLX  | O9-C24-O8-C5    |
| 49  | J     | 403 | PLX  | O7-C6-C7-C8     |
| 49  | J     | 403 | PLX  | C7-C6-O6-C4     |
| 49  | J     | 403 | PLX  | O7-C6-O6-C4     |
| 49  | J     | 403 | PLX  | C3-O4-P1-O1     |
| 49  | J     | 403 | PLX  | C3-O4-P1-O2     |
| 49  | J     | 403 | PLX  | C3-O4-P1-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | a     | 202 | PLX  | O7-C6-O6-C4     |
| 49  | a     | 202 | PLX  | C5-C4-O6-C6     |
| 49  | a     | 202 | PLX  | C3-O4-P1-O1     |
| 49  | a     | 202 | PLX  | C3-O4-P1-O2     |
| 49  | a     | 202 | PLX  | C3-O4-P1-O3     |
| 49  | a     | 202 | PLX  | O9-C24-C25-C26  |
| 49  | e     | 201 | PLX  | O7-C6-O6-C4     |
| 49  | e     | 201 | PLX  | O9-C24-O8-C5    |
| 49  | e     | 201 | PLX  | O9-C24-C25-C26  |
| 49  | g     | 201 | PLX  | O7-C6-O6-C4     |
| 49  | g     | 201 | PLX  | C2-O1-P1-O2     |
| 49  | g     | 201 | PLX  | C2-O1-P1-O3     |
| 49  | j     | 203 | PLX  | O7-C6-C7-C8     |
| 49  | j     | 203 | PLX  | O9-C24-O8-C5    |
| 49  | j     | 203 | PLX  | O9-C24-C25-C26  |
| 49  | r     | 502 | PLX  | O6-C6-C7-C8     |
| 49  | r     | 502 | PLX  | C5-C4-O6-C6     |
| 49  | r     | 502 | PLX  | C2-O1-P1-O2     |
| 49  | r     | 502 | PLX  | O9-C24-C25-C26  |
| 51  | G     | 201 | 8Q1  | O4-C1-S44-C43   |
| 51  | G     | 201 | 8Q1  | C6-C1-S44-C43   |
| 51  | G     | 201 | 8Q1  | O27-C28-C29-C30 |
| 51  | G     | 201 | 8Q1  | O27-C28-C29-C31 |
| 51  | G     | 201 | 8Q1  | O27-C28-C29-C32 |
| 51  | G     | 201 | 8Q1  | N41-C42-C43-S44 |
| 51  | G     | 201 | 8Q1  | C42-C43-S44-C1  |
| 51  | G     | 201 | 8Q1  | C28-O27-P24-O2  |
| 51  | G     | 201 | 8Q1  | C28-O27-P24-O1  |
| 51  | X     | 201 | 8Q1  | O33-C32-C34-O35 |
| 51  | X     | 201 | 8Q1  | C42-C43-S44-C1  |
| 53  | J     | 402 | UQ   | C7-C8-C9-C11    |
| 53  | J     | 402 | UQ   | C12-C13-C14-C15 |
| 53  | J     | 402 | UQ   | C14-C16-C17-C18 |
| 53  | J     | 402 | UQ   | C16-C17-C18-C19 |
| 53  | J     | 402 | UQ   | C17-C18-C19-C21 |
| 53  | J     | 402 | UQ   | C22-C23-C24-C26 |
| 53  | s     | 402 | UQ   | C7-C8-C9-C10    |
| 53  | s     | 402 | UQ   | C7-C8-C9-C11    |
| 53  | s     | 402 | UQ   | C22-C23-C24-C26 |
| 53  | s     | 402 | UQ   | C23-C24-C26-C27 |
| 56  | N     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | N     | 201 | CDL  | CA3-OA5-PA1-OA3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | N     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | N     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | N     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | V     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 56  | V     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 56  | V     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 56  | V     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | V     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | V     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | V     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | V     | 202 | CDL  | CB2-C1-CA2-OA2  |
| 56  | V     | 202 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | V     | 202 | CDL  | CA3-OA5-PA1-OA3 |
| 56  | V     | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | V     | 202 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | V     | 204 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | V     | 204 | CDL  | CA3-OA5-PA1-OA4 |
| 56  | V     | 204 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | V     | 204 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | V     | 204 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | a     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | a     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 56  | a     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | a     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | a     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | a     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | a     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | i     | 401 | CDL  | O1-C1-CB2-OB2   |
| 56  | i     | 401 | CDL  | CA2-C1-CB2-OB2  |
| 56  | i     | 401 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | i     | 401 | CDL  | CA2-OA2-PA1-OA4 |
| 56  | i     | 401 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | i     | 401 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | i     | 401 | CDL  | CA3-OA5-PA1-OA3 |
| 56  | i     | 401 | CDL  | OA9-CA7-OA8-CA6 |
| 56  | i     | 401 | CDL  | C31-CA7-OA8-CA6 |
| 56  | l     | 701 | CDL  | CB2-C1-CA2-OA2  |
| 56  | l     | 701 | CDL  | O1-C1-CB2-OB2   |
| 56  | l     | 701 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | l     | 701 | CDL  | CA2-OA2-PA1-OA4 |
| 56  | l     | 701 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | l     | 701 | CDL  | OA9-CA7-OA8-CA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | l     | 701 | CDL  | C31-CA7-OA8-CA6 |
| 56  | l     | 702 | CDL  | O1-C1-CA2-OA2   |
| 56  | l     | 702 | CDL  | O1-C1-CB2-OB2   |
| 56  | l     | 702 | CDL  | CA2-C1-CB2-OB2  |
| 56  | l     | 702 | CDL  | CA2-OA2-PA1-OA4 |
| 56  | l     | 702 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | l     | 702 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | l     | 702 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | l     | 702 | CDL  | OB6-CB4-CB6-OB8 |
| 56  | n     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | n     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 56  | n     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | n     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | n     | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | n     | 101 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | r     | 503 | CDL  | O1-C1-CA2-OA2   |
| 56  | r     | 503 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | r     | 503 | CDL  | CA3-OA5-PA1-OA3 |
| 56  | r     | 503 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | r     | 503 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | r     | 503 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | r     | 503 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | r     | 503 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | r     | 503 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | s     | 401 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | s     | 401 | CDL  | C31-CA7-OA8-CA6 |
| 56  | s     | 401 | CDL  | C51-CB5-OB6-CB4 |
| 58  | w     | 401 | ADP  | C5'-O5'-PA-O3A  |
| 56  | s     | 401 | CDL  | OA9-CA7-OA8-CA6 |
| 48  | B     | 303 | PEE  | O4-C10-O2-C2    |
| 48  | j     | 201 | PEE  | O4-C10-O2-C2    |
| 48  | j     | 202 | PEE  | O4-C10-O2-C2    |
| 56  | V     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 56  | s     | 401 | CDL  | OB7-CB5-OB6-CB4 |
| 50  | C     | 304 | DCQ  | C6-C7-C8-C9     |
| 48  | j     | 201 | PEE  | C11-C10-O2-C2   |
| 53  | s     | 402 | UQ   | C18-C19-C21-C22 |
| 48  | V     | 203 | PEE  | C17-C18-C19-C20 |
| 48  | W     | 201 | PEE  | C17-C18-C19-C20 |
| 48  | j     | 201 | PEE  | C17-C18-C19-C20 |
| 56  | l     | 702 | CDL  | C35-C36-C37-C38 |
| 53  | J     | 402 | UQ   | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | B     | 303 | PEE  | C11-C12-C13-C14 |
| 53  | J     | 402 | UQ   | C12-C13-C14-C16 |
| 53  | s     | 402 | UQ   | C17-C18-C19-C21 |
| 49  | r     | 502 | PLX  | C7-C8-C9-C10    |
| 56  | N     | 201 | CDL  | O1-C1-CA2-OA2   |
| 56  | N     | 201 | CDL  | O1-C1-CB2-OB2   |
| 56  | V     | 202 | CDL  | O1-C1-CA2-OA2   |
| 56  | V     | 204 | CDL  | O1-C1-CB2-OB2   |
| 56  | n     | 101 | CDL  | O1-C1-CA2-OA2   |
| 48  | B     | 303 | PEE  | C11-C10-O2-C2   |
| 48  | V     | 203 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 703 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 704 | PEE  | C11-C10-O2-C2   |
| 48  | r     | 501 | PEE  | C11-C10-O2-C2   |
| 56  | N     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 53  | J     | 402 | UQ   | C22-C23-C24-C25 |
| 53  | s     | 402 | UQ   | C27-C28-C29-C31 |
| 49  | g     | 201 | PLX  | C7-C8-C9-C10    |
| 49  | j     | 203 | PLX  | C13-C14-C15-C16 |
| 49  | J     | 403 | PLX  | C9-C10-C11-C12  |
| 49  | r     | 502 | PLX  | C9-C10-C11-C12  |
| 56  | r     | 503 | CDL  | C76-C77-C78-C79 |
| 56  | l     | 702 | CDL  | C71-C72-C73-C74 |
| 58  | w     | 401 | ADP  | O4'-C4'-C5'-O5' |
| 58  | w     | 401 | ADP  | C3'-C4'-C5'-O5' |
| 48  | V     | 203 | PEE  | O4-C10-O2-C2    |
| 56  | s     | 401 | CDL  | C14-C15-C16-C17 |
| 53  | J     | 402 | UQ   | C12-C11-C9-C8   |
| 53  | J     | 402 | UQ   | C13-C14-C16-C17 |
| 49  | j     | 203 | PLX  | C28-C29-C30-C31 |
| 53  | s     | 402 | UQ   | C14-C16-C17-C18 |
| 56  | V     | 201 | CDL  | C59-C60-C61-C62 |
| 56  | V     | 202 | CDL  | C17-C18-C19-C20 |
| 56  | V     | 202 | CDL  | C76-C77-C78-C79 |
| 56  | V     | 202 | CDL  | C37-C38-C39-C40 |
| 56  | V     | 204 | CDL  | C58-C59-C60-C61 |
| 49  | r     | 502 | PLX  | C11-C12-C13-C14 |
| 56  | V     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 56  | l     | 701 | CDL  | CA2-C1-CB2-OB2  |
| 56  | n     | 101 | CDL  | CB2-C1-CA2-OA2  |
| 56  | s     | 401 | CDL  | CA2-C1-CB2-OB2  |
| 48  | l     | 703 | PEE  | O4-C10-O2-C2    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | r     | 501 | PEE  | O4-C10-O2-C2    |
| 56  | V     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 56  | V     | 202 | CDL  | C31-CA7-OA8-CA6 |
| 49  | J     | 403 | PLX  | C25-C26-C27-C28 |
| 56  | N     | 201 | CDL  | CB5-C51-C52-C53 |
| 56  | l     | 701 | CDL  | CA5-C11-C12-C13 |
| 56  | r     | 503 | CDL  | C74-C75-C76-C77 |
| 48  | r     | 501 | PEE  | O3P-C1-C2-O2    |
| 56  | N     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | V     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 56  | s     | 401 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | V     | 204 | CDL  | O1-C1-CA2-OA2   |
| 56  | i     | 401 | CDL  | O1-C1-CA2-OA2   |
| 56  | l     | 701 | CDL  | O1-C1-CA2-OA2   |
| 56  | s     | 401 | CDL  | O1-C1-CB2-OB2   |
| 56  | i     | 401 | CDL  | OB6-CB4-CB6-OB8 |
| 49  | g     | 201 | PLX  | C9-C10-C11-C12  |
| 53  | s     | 402 | UQ   | C13-C14-C16-C17 |
| 56  | l     | 701 | CDL  | C58-C59-C60-C61 |
| 48  | l     | 704 | PEE  | O4-C10-O2-C2    |
| 56  | N     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 56  | n     | 101 | CDL  | CB5-C51-C52-C53 |
| 56  | s     | 401 | CDL  | CA5-C11-C12-C13 |
| 56  | l     | 702 | CDL  | C51-C52-C53-C54 |
| 48  | l     | 703 | PEE  | C31-C30-O3-C3   |
| 56  | V     | 204 | CDL  | C43-C44-C45-C46 |
| 56  | a     | 201 | CDL  | CB7-C71-C72-C73 |
| 56  | l     | 701 | CDL  | CB5-C51-C52-C53 |
| 48  | B     | 303 | PEE  | C17-C18-C19-C20 |
| 48  | l     | 704 | PEE  | C37-C38-C39-C40 |
| 56  | l     | 701 | CDL  | C55-C56-C57-C58 |
| 56  | V     | 204 | CDL  | C36-C37-C38-C39 |
| 56  | V     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | N     | 201 | CDL  | CA7-C31-C32-C33 |
| 56  | i     | 401 | CDL  | CB5-C51-C52-C53 |
| 56  | n     | 101 | CDL  | CB7-C71-C72-C73 |
| 56  | a     | 201 | CDL  | C83-C84-C85-C86 |
| 52  | J     | 401 | NDP  | O4B-C4B-C5B-O5B |
| 52  | J     | 401 | NDP  | O4D-C4D-C5D-O5D |
| 48  | j     | 201 | PEE  | C31-C30-O3-C3   |
| 56  | V     | 201 | CDL  | C32-C33-C34-C35 |
| 48  | B     | 303 | PEE  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | V     | 202 | CDL  | C33-C34-C35-C36 |
| 48  | V     | 203 | PEE  | C30-C31-C32-C33 |
| 56  | V     | 201 | CDL  | CA5-C11-C12-C13 |
| 56  | l     | 701 | CDL  | C16-C17-C18-C19 |
| 56  | V     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 56  | V     | 201 | CDL  | C34-C35-C36-C37 |
| 56  | V     | 202 | CDL  | OA9-CA7-OA8-CA6 |
| 49  | a     | 202 | PLX  | C34-C35-C36-C37 |
| 56  | V     | 204 | CDL  | C13-C14-C15-C16 |
| 56  | V     | 201 | CDL  | O1-C1-CB2-OB2   |
| 56  | V     | 202 | CDL  | O1-C1-CB2-OB2   |
| 56  | a     | 201 | CDL  | O1-C1-CA2-OA2   |
| 56  | r     | 503 | CDL  | O1-C1-CB2-OB2   |
| 48  | l     | 703 | PEE  | O5-C30-O3-C3    |
| 56  | V     | 201 | CDL  | C53-C54-C55-C56 |
| 48  | V     | 203 | PEE  | C1-O3P-P-O4P    |
| 48  | j     | 201 | PEE  | C1-O3P-P-O4P    |
| 48  | j     | 202 | PEE  | C4-O4P-P-O3P    |
| 49  | C     | 303 | PLX  | C2-O1-P1-O4     |
| 49  | g     | 201 | PLX  | C2-O1-P1-O4     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O1     |
| 56  | N     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | V     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | V     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | V     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | V     | 202 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | V     | 202 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | V     | 204 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | V     | 204 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | l     | 701 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | l     | 702 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | l     | 702 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | n     | 101 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | n     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | n     | 101 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | i     | 401 | CDL  | CB7-C71-C72-C73 |
| 52  | J     | 401 | NDP  | C2D-C1D-N1N-C6N |
| 56  | a     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 56  | n     | 101 | CDL  | C75-C76-C77-C78 |
| 56  | s     | 401 | CDL  | CB7-C71-C72-C73 |
| 56  | N     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 56  | V     | 202 | CDL  | CA2-C1-CB2-OB2  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | V     | 204 | CDL  | CB2-C1-CA2-OA2  |
| 56  | a     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 56  | i     | 401 | CDL  | CB2-C1-CA2-OA2  |
| 56  | l     | 702 | CDL  | CB2-C1-CA2-OA2  |
| 56  | r     | 503 | CDL  | CB2-C1-CA2-OA2  |
| 56  | V     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 56  | l     | 701 | CDL  | C71-CB7-OB8-CB6 |
| 48  | j     | 201 | PEE  | O5-C30-O3-C3    |
| 49  | j     | 203 | PLX  | O6-C6-C7-C8     |
| 56  | l     | 701 | CDL  | C75-C76-C77-C78 |
| 56  | n     | 101 | CDL  | C74-C75-C76-C77 |
| 56  | V     | 204 | CDL  | C11-CA5-OA6-CA4 |
| 56  | r     | 503 | CDL  | C51-CB5-OB6-CB4 |
| 48  | B     | 303 | PEE  | C20-C21-C22-C23 |
| 48  | B     | 303 | PEE  | C13-C14-C15-C16 |
| 48  | j     | 202 | PEE  | C23-C24-C25-C26 |
| 49  | a     | 202 | PLX  | C10-C11-C12-C13 |
| 49  | g     | 201 | PLX  | C28-C29-C30-C31 |
| 49  | j     | 203 | PLX  | C7-C8-C9-C10    |
| 49  | j     | 203 | PLX  | C27-C28-C29-C30 |
| 56  | V     | 204 | CDL  | C11-C12-C13-C14 |
| 56  | V     | 204 | CDL  | C55-C56-C57-C58 |
| 56  | V     | 204 | CDL  | C59-C60-C61-C62 |
| 56  | V     | 204 | CDL  | C71-C72-C73-C74 |
| 56  | V     | 204 | CDL  | C73-C74-C75-C76 |
| 56  | V     | 204 | CDL  | C76-C77-C78-C79 |
| 56  | i     | 401 | CDL  | C37-C38-C39-C40 |
| 56  | i     | 401 | CDL  | C76-C77-C78-C79 |
| 56  | s     | 401 | CDL  | C73-C74-C75-C76 |
| 48  | r     | 501 | PEE  | C11-C12-C13-C14 |
| 49  | J     | 403 | PLX  | C12-C13-C14-C15 |
| 49  | a     | 202 | PLX  | C13-C14-C15-C16 |
| 49  | g     | 201 | PLX  | C27-C28-C29-C30 |
| 49  | r     | 502 | PLX  | C11-C10-C9-C8   |
| 49  | r     | 502 | PLX  | C28-C29-C30-C31 |
| 56  | V     | 201 | CDL  | C37-C38-C39-C40 |
| 56  | V     | 202 | CDL  | C34-C35-C36-C37 |
| 56  | V     | 204 | CDL  | C32-C33-C34-C35 |
| 56  | V     | 204 | CDL  | C56-C57-C58-C59 |
| 56  | l     | 701 | CDL  | C52-C53-C54-C55 |
| 56  | s     | 401 | CDL  | C18-C19-C20-C21 |
| 56  | s     | 401 | CDL  | C52-C53-C54-C55 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | V     | 204 | CDL  | OA7-CA5-OA6-CA4 |
| 56  | r     | 503 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | j     | 202 | PEE  | C11-C12-C13-C14 |
| 48  | r     | 501 | PEE  | C31-C32-C33-C34 |
| 49  | J     | 403 | PLX  | C27-C28-C29-C30 |
| 49  | j     | 203 | PLX  | C25-C26-C27-C28 |
| 56  | V     | 202 | CDL  | C15-C16-C17-C18 |
| 48  | r     | 501 | PEE  | C17-C18-C19-C20 |
| 49  | a     | 202 | PLX  | C9-C10-C11-C12  |
| 49  | e     | 201 | PLX  | C25-C26-C27-C28 |
| 49  | r     | 502 | PLX  | C27-C28-C29-C30 |
| 49  | r     | 502 | PLX  | C33-C34-C35-C36 |
| 56  | V     | 202 | CDL  | C56-C57-C58-C59 |
| 56  | l     | 701 | CDL  | C62-C63-C64-C65 |
| 56  | n     | 101 | CDL  | C71-C72-C73-C74 |
| 56  | r     | 503 | CDL  | C59-C60-C61-C62 |
| 56  | r     | 503 | CDL  | C75-C76-C77-C78 |
| 49  | C     | 303 | PLX  | C9-C10-C11-C12  |
| 49  | g     | 201 | PLX  | C13-C14-C15-C16 |
| 56  | r     | 503 | CDL  | C71-C72-C73-C74 |
| 48  | W     | 201 | PEE  | C31-C30-O3-C3   |
| 48  | j     | 202 | PEE  | C14-C15-C16-C17 |
| 49  | a     | 202 | PLX  | C12-C13-C14-C15 |
| 49  | e     | 201 | PLX  | C13-C14-C15-C16 |
| 56  | V     | 201 | CDL  | C71-C72-C73-C74 |
| 56  | V     | 204 | CDL  | C78-C79-C80-C81 |
| 56  | l     | 702 | CDL  | C15-C16-C17-C18 |
| 56  | r     | 503 | CDL  | C43-C44-C45-C46 |
| 56  | s     | 401 | CDL  | C15-C16-C17-C18 |
| 56  | s     | 401 | CDL  | C71-C72-C73-C74 |
| 48  | W     | 201 | PEE  | C12-C13-C14-C15 |
| 49  | j     | 203 | PLX  | C16-C17-C18-C19 |
| 56  | V     | 201 | CDL  | C56-C57-C58-C59 |
| 56  | l     | 701 | CDL  | C31-C32-C33-C34 |
| 56  | l     | 702 | CDL  | C75-C76-C77-C78 |
| 56  | r     | 503 | CDL  | C33-C34-C35-C36 |
| 56  | r     | 503 | CDL  | C62-C63-C64-C65 |
| 56  | V     | 204 | CDL  | CA7-C31-C32-C33 |
| 49  | g     | 201 | PLX  | C10-C11-C12-C13 |
| 49  | j     | 203 | PLX  | C12-C13-C14-C15 |
| 51  | X     | 201 | 8Q1  | C12-C13-C14-C15 |
| 56  | V     | 201 | CDL  | C54-C55-C56-C57 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | i     | 401 | CDL  | C14-C15-C16-C17 |
| 56  | l     | 701 | CDL  | C51-C52-C53-C54 |
| 56  | r     | 503 | CDL  | C15-C16-C17-C18 |
| 56  | r     | 503 | CDL  | C55-C56-C57-C58 |
| 56  | s     | 401 | CDL  | C35-C36-C37-C38 |
| 48  | V     | 203 | PEE  | C32-C33-C34-C35 |
| 48  | l     | 704 | PEE  | C14-C15-C16-C17 |
| 56  | V     | 202 | CDL  | C55-C56-C57-C58 |
| 56  | a     | 201 | CDL  | C35-C36-C37-C38 |
| 56  | a     | 201 | CDL  | C36-C37-C38-C39 |
| 56  | l     | 701 | CDL  | C56-C57-C58-C59 |
| 56  | l     | 702 | CDL  | C51-CB5-OB6-CB4 |
| 48  | W     | 201 | PEE  | C13-C14-C15-C16 |
| 49  | a     | 202 | PLX  | C7-C8-C9-C10    |
| 49  | j     | 203 | PLX  | C14-C15-C16-C17 |
| 56  | V     | 202 | CDL  | C59-C60-C61-C62 |
| 56  | V     | 202 | CDL  | C75-C76-C77-C78 |
| 56  | s     | 401 | CDL  | C34-C35-C36-C37 |
| 48  | B     | 303 | PEE  | C35-C36-C37-C38 |
| 48  | j     | 201 | PEE  | C21-C22-C23-C24 |
| 49  | j     | 203 | PLX  | C11-C12-C13-C14 |
| 49  | j     | 203 | PLX  | C9-C10-C11-C12  |
| 49  | r     | 502 | PLX  | C13-C14-C15-C16 |
| 49  | r     | 502 | PLX  | C30-C31-C32-C33 |
| 50  | C     | 304 | DCQ  | C7-C8-C9-C10    |
| 56  | V     | 201 | CDL  | C52-C53-C54-C55 |
| 56  | V     | 204 | CDL  | C39-C40-C41-C42 |
| 56  | a     | 201 | CDL  | C21-C22-C23-C24 |
| 56  | i     | 401 | CDL  | C59-C60-C61-C62 |
| 56  | i     | 401 | CDL  | C81-C82-C83-C84 |
| 56  | l     | 702 | CDL  | C21-C22-C23-C24 |
| 56  | n     | 101 | CDL  | C73-C74-C75-C76 |
| 56  | r     | 503 | CDL  | C82-C83-C84-C85 |
| 49  | g     | 201 | PLX  | C2-C1-N1-C1A    |
| 48  | C     | 302 | PEE  | C11-C12-C13-C14 |
| 49  | J     | 403 | PLX  | C10-C11-C12-C13 |
| 49  | e     | 201 | PLX  | C11-C10-C9-C8   |
| 49  | g     | 201 | PLX  | C25-C26-C27-C28 |
| 56  | V     | 202 | CDL  | C74-C75-C76-C77 |
| 56  | n     | 101 | CDL  | C54-C55-C56-C57 |
| 56  | r     | 503 | CDL  | C41-C42-C43-C44 |
| 49  | a     | 202 | PLX  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | e     | 201 | PLX  | C17-C18-C19-C20 |
| 49  | g     | 201 | PLX  | C12-C13-C14-C15 |
| 49  | j     | 203 | PLX  | C33-C34-C35-C36 |
| 49  | r     | 502 | PLX  | C12-C13-C14-C15 |
| 56  | V     | 202 | CDL  | C52-C53-C54-C55 |
| 56  | l     | 701 | CDL  | C59-C60-C61-C62 |
| 56  | V     | 204 | CDL  | C81-C82-C83-C84 |
| 56  | l     | 702 | CDL  | C55-C56-C57-C58 |
| 56  | n     | 101 | CDL  | C51-C52-C53-C54 |
| 56  | r     | 503 | CDL  | C16-C17-C18-C19 |
| 48  | j     | 202 | PEE  | C31-C30-O3-C3   |
| 48  | j     | 201 | PEE  | C22-C23-C24-C25 |
| 49  | g     | 201 | PLX  | C30-C31-C32-C33 |
| 49  | g     | 201 | PLX  | C32-C33-C34-C35 |
| 49  | j     | 203 | PLX  | C30-C31-C32-C33 |
| 56  | s     | 401 | CDL  | C59-C60-C61-C62 |
| 48  | r     | 501 | PEE  | C33-C34-C35-C36 |
| 49  | g     | 201 | PLX  | C33-C34-C35-C36 |
| 49  | r     | 502 | PLX  | C31-C32-C33-C34 |
| 51  | G     | 201 | 8Q1  | C11-C12-C13-C14 |
| 56  | V     | 202 | CDL  | C83-C84-C85-C86 |
| 56  | V     | 204 | CDL  | C14-C15-C16-C17 |
| 56  | V     | 204 | CDL  | C18-C19-C20-C21 |
| 56  | a     | 201 | CDL  | C34-C35-C36-C37 |
| 56  | a     | 201 | CDL  | C62-C63-C64-C65 |
| 56  | s     | 401 | CDL  | C32-C33-C34-C35 |
| 56  | V     | 202 | CDL  | C41-C42-C43-C44 |
| 56  | V     | 204 | CDL  | C51-C52-C53-C54 |
| 56  | l     | 702 | CDL  | C74-C75-C76-C77 |
| 56  | l     | 702 | CDL  | OB7-CB5-OB6-CB4 |
| 56  | l     | 701 | CDL  | C72-C73-C74-C75 |
| 48  | r     | 501 | PEE  | C30-C31-C32-C33 |
| 56  | l     | 701 | CDL  | CA7-C31-C32-C33 |
| 56  | V     | 204 | CDL  | C37-C38-C39-C40 |
| 56  | l     | 702 | CDL  | C59-C60-C61-C62 |
| 56  | a     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 48  | C     | 302 | PEE  | C11-C10-O2-C2   |
| 56  | V     | 201 | CDL  | C14-C15-C16-C17 |
| 49  | C     | 303 | PLX  | O9-C24-C25-C26  |
| 49  | J     | 403 | PLX  | O9-C24-C25-C26  |
| 49  | r     | 502 | PLX  | O7-C6-C7-C8     |
| 49  | C     | 303 | PLX  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | J     | 403 | PLX  | C28-C29-C30-C31 |
| 49  | g     | 201 | PLX  | C11-C12-C13-C14 |
| 56  | V     | 201 | CDL  | C21-C22-C23-C24 |
| 56  | V     | 201 | CDL  | C76-C77-C78-C79 |
| 56  | r     | 503 | CDL  | C34-C35-C36-C37 |
| 48  | j     | 202 | PEE  | C15-C16-C17-C18 |
| 56  | l     | 701 | CDL  | OB9-CB7-OB8-CB6 |
| 48  | B     | 303 | PEE  | C23-C24-C25-C26 |
| 56  | l     | 701 | CDL  | C35-C36-C37-C38 |
| 52  | J     | 401 | NDP  | C3D-C4D-C5D-O5D |
| 49  | e     | 201 | PLX  | C26-C27-C28-C29 |
| 56  | i     | 401 | CDL  | C73-C74-C75-C76 |
| 56  | r     | 503 | CDL  | C32-C33-C34-C35 |
| 48  | r     | 501 | PEE  | C23-C24-C25-C26 |
| 56  | V     | 201 | CDL  | C75-C76-C77-C78 |
| 56  | a     | 201 | CDL  | C20-C21-C22-C23 |
| 56  | i     | 401 | CDL  | C75-C76-C77-C78 |
| 48  | C     | 302 | PEE  | O4-C10-O2-C2    |
| 49  | r     | 502 | PLX  | C25-C26-C27-C28 |
| 56  | i     | 401 | CDL  | C55-C56-C57-C58 |
| 56  | r     | 503 | CDL  | C81-C82-C83-C84 |
| 48  | j     | 202 | PEE  | C22-C23-C24-C25 |
| 48  | l     | 703 | PEE  | C13-C14-C15-C16 |
| 49  | a     | 202 | PLX  | C31-C32-C33-C34 |
| 49  | C     | 303 | PLX  | C17-C18-C19-C20 |
| 56  | N     | 201 | CDL  | C11-C12-C13-C14 |
| 56  | l     | 701 | CDL  | C36-C37-C38-C39 |
| 56  | l     | 702 | CDL  | C11-C12-C13-C14 |
| 48  | B     | 303 | PEE  | C31-C30-O3-C3   |
| 56  | l     | 702 | CDL  | C71-CB7-OB8-CB6 |
| 56  | a     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 56  | s     | 401 | CDL  | C37-C38-C39-C40 |
| 48  | W     | 201 | PEE  | O5-C30-O3-C3    |
| 56  | s     | 401 | CDL  | CA7-C31-C32-C33 |
| 48  | C     | 302 | PEE  | C41-C42-C43-C44 |
| 49  | e     | 201 | PLX  | C27-C28-C29-C30 |
| 56  | V     | 201 | CDL  | C35-C36-C37-C38 |
| 56  | V     | 202 | CDL  | C19-C20-C21-C22 |
| 56  | l     | 702 | CDL  | C62-C63-C64-C65 |
| 56  | r     | 503 | CDL  | C37-C38-C39-C40 |
| 56  | s     | 401 | CDL  | C19-C20-C21-C22 |
| 48  | j     | 202 | PEE  | O5-C30-O3-C3    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | r     | 502 | PLX  | C14-C15-C16-C17 |
| 56  | r     | 503 | CDL  | C14-C15-C16-C17 |
| 48  | B     | 303 | PEE  | C10-C11-C12-C13 |
| 48  | V     | 203 | PEE  | C31-C30-O3-C3   |
| 56  | N     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 56  | V     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 51  | G     | 201 | 8Q1  | C12-C13-C14-C15 |
| 56  | V     | 204 | CDL  | C64-C65-C66-C67 |
| 56  | l     | 701 | CDL  | C11-C12-C13-C14 |
| 56  | s     | 401 | CDL  | C54-C55-C56-C57 |
| 48  | C     | 302 | PEE  | C12-C13-C14-C15 |
| 56  | V     | 201 | CDL  | C73-C74-C75-C76 |
| 49  | J     | 403 | PLX  | C33-C34-C35-C36 |
| 56  | l     | 702 | CDL  | C14-C15-C16-C17 |
| 48  | V     | 203 | PEE  | C10-C11-C12-C13 |
| 48  | W     | 201 | PEE  | C21-C22-C23-C24 |
| 49  | r     | 502 | PLX  | C16-C17-C18-C19 |
| 49  | J     | 403 | PLX  | C11-C10-C9-C8   |
| 49  | J     | 403 | PLX  | C32-C33-C34-C35 |
| 56  | V     | 201 | CDL  | C41-C42-C43-C44 |
| 56  | V     | 201 | CDL  | C63-C64-C65-C66 |
| 56  | i     | 401 | CDL  | C77-C78-C79-C80 |
| 56  | s     | 401 | CDL  | C75-C76-C77-C78 |
| 56  | V     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 48  | l     | 703 | PEE  | O3P-C1-C2-O2    |
| 48  | l     | 703 | PEE  | C11-C12-C13-C14 |
| 56  | a     | 201 | CDL  | C61-C62-C63-C64 |
| 56  | s     | 401 | CDL  | C55-C56-C57-C58 |
| 56  | V     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 56  | a     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 49  | C     | 303 | PLX  | C13-C14-C15-C16 |
| 56  | V     | 202 | CDL  | C39-C40-C41-C42 |
| 49  | g     | 201 | PLX  | O6-C4-C5-O8     |
| 56  | V     | 202 | CDL  | OB6-CB4-CB6-OB8 |
| 56  | l     | 701 | CDL  | OA6-CA4-CA6-OA8 |
| 56  | r     | 503 | CDL  | OB6-CB4-CB6-OB8 |
| 56  | n     | 101 | CDL  | C55-C56-C57-C58 |
| 56  | s     | 401 | CDL  | C82-C83-C84-C85 |
| 49  | g     | 201 | PLX  | C2-C1-N1-C1B    |
| 48  | r     | 501 | PEE  | C15-C16-C17-C18 |
| 56  | V     | 202 | CDL  | CA7-C31-C32-C33 |
| 48  | j     | 202 | PEE  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 47  | A     | 503 | NAI  | O4B-C4B-C5B-O5B |
| 52  | J     | 401 | NDP  | C3B-C4B-C5B-O5B |
| 48  | l     | 704 | PEE  | C31-C32-C33-C34 |
| 56  | i     | 401 | CDL  | C62-C63-C64-C65 |
| 49  | C     | 303 | PLX  | C33-C34-C35-C36 |
| 56  | l     | 702 | CDL  | C52-C53-C54-C55 |
| 48  | B     | 303 | PEE  | O5-C30-O3-C3    |
| 56  | l     | 702 | CDL  | OB9-CB7-OB8-CB6 |
| 48  | j     | 201 | PEE  | C36-C37-C38-C39 |
| 48  | C     | 302 | PEE  | C1-O3P-P-O4P    |
| 49  | r     | 502 | PLX  | C2-O1-P1-O4     |
| 56  | N     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | V     | 202 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | l     | 701 | CDL  | CA2-OA2-PA1-OA5 |
| 47  | A     | 503 | NAI  | C2D-C1D-N1N-C2N |
| 48  | j     | 202 | PEE  | C31-C32-C33-C34 |
| 51  | G     | 201 | 8Q1  | C6-C7-C8-C9     |
| 56  | a     | 201 | CDL  | C11-C12-C13-C14 |
| 56  | a     | 201 | CDL  | C60-C61-C62-C63 |
| 56  | i     | 401 | CDL  | C12-C13-C14-C15 |
| 48  | r     | 501 | PEE  | O3P-C1-C2-C3    |
| 56  | V     | 204 | CDL  | OA5-CA3-CA4-CA6 |
| 56  | a     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | s     | 401 | CDL  | OA5-CA3-CA4-CA6 |
| 56  | V     | 201 | CDL  | CA7-C31-C32-C33 |
| 56  | l     | 702 | CDL  | CA7-C31-C32-C33 |
| 48  | C     | 302 | PEE  | C44-C45-C46-C47 |
| 56  | r     | 503 | CDL  | C58-C59-C60-C61 |
| 48  | V     | 203 | PEE  | C33-C34-C35-C36 |
| 49  | a     | 202 | PLX  | C25-C26-C27-C28 |
| 49  | C     | 303 | PLX  | C11-C10-C9-C8   |
| 56  | V     | 202 | CDL  | C60-C61-C62-C63 |
| 48  | l     | 703 | PEE  | C32-C33-C34-C35 |
| 56  | V     | 204 | CDL  | C53-C54-C55-C56 |
| 48  | l     | 704 | PEE  | C21-C22-C23-C24 |
| 56  | l     | 701 | CDL  | C37-C38-C39-C40 |
| 49  | J     | 403 | PLX  | C34-C35-C36-C37 |
| 56  | V     | 202 | CDL  | C62-C63-C64-C65 |
| 48  | V     | 203 | PEE  | O5-C30-O3-C3    |
| 56  | N     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 48  | C     | 302 | PEE  | C1-C2-C3-O3     |
| 48  | W     | 201 | PEE  | C1-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | j     | 202 | PEE  | C1-C2-C3-O3     |
| 48  | r     | 501 | PEE  | C1-C2-C3-O3     |
| 49  | C     | 303 | PLX  | C14-C15-C16-C17 |
| 49  | C     | 303 | PLX  | C3-C4-C5-O8     |
| 49  | e     | 201 | PLX  | C3-C4-C5-O8     |
| 49  | g     | 201 | PLX  | C3-C4-C5-O8     |
| 56  | N     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 56  | V     | 202 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | s     | 401 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | a     | 201 | CDL  | C84-C85-C86-C87 |
| 48  | j     | 202 | PEE  | C12-C13-C14-C15 |
| 48  | l     | 703 | PEE  | C21-C22-C23-C24 |
| 48  | r     | 501 | PEE  | C24-C25-C26-C27 |
| 56  | V     | 204 | CDL  | C52-C53-C54-C55 |
| 56  | l     | 702 | CDL  | C73-C74-C75-C76 |
| 56  | V     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 49  | J     | 403 | PLX  | O8-C24-C25-C26  |
| 48  | C     | 302 | PEE  | C42-C43-C44-C45 |
| 56  | V     | 204 | CDL  | C84-C85-C86-C87 |
| 56  | r     | 503 | CDL  | C13-C14-C15-C16 |
| 56  | r     | 503 | CDL  | C17-C18-C19-C20 |
| 48  | W     | 201 | PEE  | C22-C23-C24-C25 |
| 48  | j     | 202 | PEE  | C24-C25-C26-C27 |
| 49  | a     | 202 | PLX  | C16-C17-C18-C19 |
| 48  | l     | 703 | PEE  | C15-C16-C17-C18 |
| 56  | V     | 204 | CDL  | C17-C18-C19-C20 |
| 49  | J     | 403 | PLX  | C11-C12-C13-C14 |
| 49  | g     | 201 | PLX  | C36-C37-C38-C39 |
| 56  | l     | 701 | CDL  | C82-C83-C84-C85 |
| 48  | j     | 202 | PEE  | C30-C31-C32-C33 |
| 56  | r     | 503 | CDL  | C71-CB7-OB8-CB6 |
| 48  | j     | 201 | PEE  | C44-C45-C46-C47 |
| 49  | C     | 303 | PLX  | C28-C29-C30-C31 |
| 56  | i     | 401 | CDL  | C35-C36-C37-C38 |
| 56  | s     | 401 | CDL  | C39-C40-C41-C42 |
| 49  | C     | 303 | PLX  | C26-C27-C28-C29 |
| 56  | l     | 701 | CDL  | CB7-C71-C72-C73 |
| 49  | e     | 201 | PLX  | C30-C31-C32-C33 |
| 56  | V     | 202 | CDL  | C54-C55-C56-C57 |
| 56  | l     | 701 | CDL  | C74-C75-C76-C77 |
| 48  | B     | 303 | PEE  | C38-C39-C40-C41 |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O1P   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | V     | 202 | CDL  | OB5-CB3-CB4-OB6 |
| 49  | g     | 201 | PLX  | C2-C1-N1-C1C    |
| 56  | s     | 401 | CDL  | C40-C41-C42-C43 |
| 49  | C     | 303 | PLX  | C7-C8-C9-C10    |
| 49  | a     | 202 | PLX  | C11-C10-C9-C8   |
| 56  | a     | 201 | CDL  | C14-C15-C16-C17 |
| 56  | i     | 401 | CDL  | CA5-C11-C12-C13 |
| 56  | V     | 201 | CDL  | C44-C45-C46-C47 |
| 56  | l     | 702 | CDL  | C36-C37-C38-C39 |
| 56  | r     | 503 | CDL  | C84-C85-C86-C87 |
| 56  | V     | 204 | CDL  | C34-C35-C36-C37 |
| 56  | a     | 201 | CDL  | C12-C13-C14-C15 |
| 56  | a     | 201 | CDL  | CA5-C11-C12-C13 |
| 48  | l     | 704 | PEE  | C12-C13-C14-C15 |
| 56  | l     | 701 | CDL  | C81-C82-C83-C84 |
| 56  | V     | 204 | CDL  | C71-CB7-OB8-CB6 |
| 48  | C     | 302 | PEE  | C32-C33-C34-C35 |
| 48  | r     | 501 | PEE  | C12-C13-C14-C15 |
| 56  | s     | 401 | CDL  | C17-C18-C19-C20 |
| 56  | r     | 503 | CDL  | CA5-C11-C12-C13 |
| 49  | e     | 201 | PLX  | C11-C12-C13-C14 |
| 56  | N     | 201 | CDL  | C52-C53-C54-C55 |
| 47  | A     | 503 | NAI  | C3B-C4B-C5B-O5B |
| 48  | l     | 703 | PEE  | O3P-C1-C2-C3    |
| 49  | J     | 403 | PLX  | O4-C3-C4-C5     |
| 56  | N     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 56  | N     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | V     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | i     | 401 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | l     | 702 | CDL  | OA5-CA3-CA4-CA6 |
| 56  | a     | 201 | CDL  | C71-C72-C73-C74 |
| 48  | W     | 201 | PEE  | C10-C11-C12-C13 |
| 56  | V     | 202 | CDL  | C73-C74-C75-C76 |
| 56  | V     | 204 | CDL  | C21-C22-C23-C24 |
| 56  | V     | 204 | CDL  | C75-C76-C77-C78 |
| 56  | r     | 503 | CDL  | CA7-C31-C32-C33 |
| 49  | j     | 203 | PLX  | C17-C18-C19-C20 |
| 48  | l     | 703 | PEE  | C31-C32-C33-C34 |
| 49  | g     | 201 | PLX  | C14-C15-C16-C17 |
| 49  | a     | 202 | PLX  | C15-C16-C17-C18 |
| 49  | e     | 201 | PLX  | C15-C16-C17-C18 |
| 56  | l     | 701 | CDL  | C14-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | r     | 503 | CDL  | C64-C65-C66-C67 |
| 49  | e     | 201 | PLX  | C16-C17-C18-C19 |
| 56  | l     | 702 | CDL  | C12-C13-C14-C15 |
| 56  | a     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 56  | i     | 401 | CDL  | C71-CB7-OB8-CB6 |
| 56  | i     | 401 | CDL  | C64-C65-C66-C67 |
| 48  | l     | 704 | PEE  | C1-C2-C3-O3     |
| 49  | a     | 202 | PLX  | C3-C4-C5-O8     |
| 49  | r     | 502 | PLX  | C3-C4-C5-O8     |
| 56  | V     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 56  | V     | 204 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | i     | 401 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | l     | 701 | CDL  | CA3-CA4-CA6-OA8 |
| 56  | r     | 503 | CDL  | CB3-CB4-CB6-OB8 |
| 48  | C     | 302 | PEE  | C34-C35-C36-C37 |
| 56  | r     | 503 | CDL  | C73-C74-C75-C76 |
| 51  | X     | 201 | 8Q1  | C9-C10-C11-C12  |
| 49  | a     | 202 | PLX  | C28-C29-C30-C31 |
| 56  | a     | 201 | CDL  | C72-C73-C74-C75 |
| 56  | r     | 503 | CDL  | OB9-CB7-OB8-CB6 |
| 53  | s     | 402 | UQ   | C12-C11-C9-C10  |
| 56  | V     | 202 | CDL  | C78-C79-C80-C81 |
| 56  | V     | 204 | CDL  | C33-C34-C35-C36 |
| 48  | r     | 501 | PEE  | C4-O4P-P-O3P    |
| 49  | a     | 202 | PLX  | C2-O1-P1-O4     |
| 49  | e     | 201 | PLX  | C5-C4-O6-C6     |
| 56  | a     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 49  | g     | 201 | PLX  | O7-C6-C7-C8     |
| 49  | J     | 403 | PLX  | C30-C31-C32-C33 |
| 49  | e     | 201 | PLX  | O4-C3-C4-O6     |
| 56  | i     | 401 | CDL  | OB5-CB3-CB4-OB6 |
| 56  | l     | 701 | CDL  | OB5-CB3-CB4-OB6 |
| 56  | n     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | l     | 701 | CDL  | C21-C22-C23-C24 |
| 56  | l     | 702 | CDL  | C32-C33-C34-C35 |
| 48  | l     | 704 | PEE  | C24-C25-C26-C27 |
| 48  | C     | 302 | PEE  | O2-C2-C3-O3     |
| 48  | W     | 201 | PEE  | O2-C2-C3-O3     |
| 49  | e     | 201 | PLX  | O6-C4-C5-O8     |
| 49  | r     | 502 | PLX  | O6-C4-C5-O8     |
| 56  | V     | 204 | CDL  | OB6-CB4-CB6-OB8 |
| 56  | l     | 701 | CDL  | OB6-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | s     | 401 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | l     | 703 | PEE  | C44-C45-C46-C47 |
| 56  | l     | 702 | CDL  | C72-C73-C74-C75 |
| 53  | J     | 402 | UQ   | C9-C11-C12-C13  |
| 56  | N     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 56  | V     | 204 | CDL  | CA2-C1-CB2-OB2  |
| 56  | a     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 49  | J     | 403 | PLX  | C14-C15-C16-C17 |
| 56  | a     | 201 | CDL  | C31-C32-C33-C34 |
| 56  | r     | 503 | CDL  | C12-C13-C14-C15 |
| 56  | l     | 701 | CDL  | C71-C72-C73-C74 |
| 56  | r     | 503 | CDL  | C1-CB2-OB2-PB2  |
| 48  | C     | 302 | PEE  | C19-C20-C21-C22 |
| 56  | V     | 204 | CDL  | C82-C83-C84-C85 |
| 56  | a     | 201 | CDL  | C38-C39-C40-C41 |
| 56  | s     | 401 | CDL  | C56-C57-C58-C59 |
| 56  | a     | 201 | CDL  | CB5-C51-C52-C53 |
| 56  | V     | 202 | CDL  | C84-C85-C86-C87 |
| 56  | l     | 702 | CDL  | C52-C51-CB5-OB6 |
| 49  | J     | 403 | PLX  | C36-C37-C38-C39 |
| 56  | V     | 204 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | V     | 201 | CDL  | C36-C37-C38-C39 |
| 56  | a     | 201 | CDL  | C44-C45-C46-C47 |
| 56  | l     | 701 | CDL  | C80-C81-C82-C83 |
| 48  | j     | 201 | PEE  | C30-C31-C32-C33 |
| 47  | A     | 503 | NAI  | C2D-C1D-N1N-C6N |
| 56  | s     | 401 | CDL  | C84-C85-C86-C87 |
| 48  | V     | 203 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C24-C25-C26-C27 |
| 49  | J     | 403 | PLX  | O6-C6-C7-C8     |
| 49  | a     | 202 | PLX  | O8-C24-C25-C26  |
| 49  | e     | 201 | PLX  | O8-C24-C25-C26  |
| 49  | r     | 502 | PLX  | O8-C24-C25-C26  |
| 49  | a     | 202 | PLX  | C27-C28-C29-C30 |
| 56  | V     | 202 | CDL  | C64-C65-C66-C67 |
| 49  | e     | 201 | PLX  | O4-C3-C4-C5     |
| 56  | n     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 48  | j     | 201 | PEE  | C38-C39-C40-C41 |
| 48  | r     | 501 | PEE  | C36-C37-C38-C39 |
| 48  | j     | 202 | PEE  | C19-C20-C21-C22 |
| 56  | i     | 401 | CDL  | C71-C72-C73-C74 |
| 48  | W     | 201 | PEE  | C30-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 51  | X     | 201 | 8Q1  | O33-C32-C34-N36 |
| 48  | l     | 704 | PEE  | C31-C30-O3-C3   |
| 56  | s     | 401 | CDL  | C71-CB7-OB8-CB6 |
| 48  | W     | 201 | PEE  | C23-C24-C25-C26 |
| 56  | a     | 201 | CDL  | C37-C38-C39-C40 |
| 56  | V     | 201 | CDL  | C11-C12-C13-C14 |
| 56  | V     | 204 | CDL  | CA6-CA4-OA6-CA5 |
| 56  | l     | 702 | CDL  | C12-C11-CA5-OA6 |
| 56  | l     | 701 | CDL  | C24-C25-C26-C27 |
| 48  | V     | 203 | PEE  | C1-C2-C3-O3     |
| 56  | i     | 401 | CDL  | CA3-CA4-CA6-OA8 |
| 56  | l     | 701 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | l     | 702 | CDL  | CA4-CA3-OA5-PA1 |
| 56  | l     | 702 | CDL  | CB3-CB4-CB6-OB8 |
| 56  | s     | 401 | CDL  | C11-CA5-OA6-CA4 |
| 48  | C     | 302 | PEE  | C14-C15-C16-C17 |
| 49  | J     | 403 | PLX  | O4-C3-C4-O6     |
| 56  | V     | 202 | CDL  | OA5-CA3-CA4-OA6 |
| 56  | l     | 702 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | V     | 203 | PEE  | C13-C14-C15-C16 |
| 56  | V     | 201 | CDL  | C51-C52-C53-C54 |
| 56  | l     | 702 | CDL  | C64-C65-C66-C67 |
| 48  | l     | 704 | PEE  | C13-C14-C15-C16 |
| 56  | a     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 56  | i     | 401 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | s     | 401 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | s     | 401 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | J     | 401 | NDP  | C2B-O2B-P2B-O2X |
| 56  | r     | 503 | CDL  | C44-C45-C46-C47 |
| 49  | e     | 201 | PLX  | C35-C36-C37-C38 |
| 49  | g     | 201 | PLX  | C11-C10-C9-C8   |
| 56  | s     | 401 | CDL  | OA7-CA5-OA6-CA4 |
| 49  | e     | 201 | PLX  | C24-C25-C26-C27 |
| 49  | g     | 201 | PLX  | C6-C7-C8-C9     |
| 48  | W     | 201 | PEE  | C34-C35-C36-C37 |
| 56  | l     | 702 | CDL  | C31-C32-C33-C34 |
| 48  | l     | 704 | PEE  | O5-C30-O3-C3    |
| 56  | l     | 701 | CDL  | C20-C21-C22-C23 |
| 48  | r     | 501 | PEE  | C41-C42-C43-C44 |
| 56  | l     | 702 | CDL  | CB7-C71-C72-C73 |
| 49  | r     | 502 | PLX  | C32-C33-C34-C35 |
| 56  | V     | 202 | CDL  | C38-C39-C40-C41 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | J     | 403 | PLX  | C24-C25-C26-C27 |
| 47  | A     | 503 | NAI  | O4D-C1D-N1N-C2N |
| 49  | e     | 201 | PLX  | C3-O4-P1-O1     |
| 56  | V     | 201 | CDL  | CB4-CB3-OB5-PB2 |
| 56  | V     | 204 | CDL  | CA4-CA3-OA5-PA1 |
| 56  | i     | 401 | CDL  | C1-CB2-OB2-PB2  |
| 56  | r     | 503 | CDL  | CB4-CB3-OB5-PB2 |
| 56  | i     | 401 | CDL  | C34-C35-C36-C37 |
| 56  | s     | 401 | CDL  | C74-C75-C76-C77 |
| 48  | C     | 302 | PEE  | C1-O3P-P-O2P    |
| 48  | j     | 201 | PEE  | C1-O3P-P-O2P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O2P    |
| 48  | r     | 501 | PEE  | C4-O4P-P-O2P    |
| 49  | e     | 201 | PLX  | C3-O4-P1-O3     |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1B    |
| 49  | j     | 203 | PLX  | C3-O4-P1-O3     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O2     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O3     |
| 49  | r     | 502 | PLX  | C2-O1-P1-O3     |
| 53  | s     | 402 | UQ   | C6-C7-C8-C9     |
| 56  | N     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | V     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 56  | V     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | V     | 202 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | V     | 202 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | i     | 401 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | l     | 701 | CDL  | CB2-OB2-PB2-OB4 |
| 56  | l     | 701 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | l     | 702 | CDL  | CB3-OB5-PB2-OB3 |
| 56  | l     | 702 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | n     | 101 | CDL  | CA2-OA2-PA1-OA4 |
| 58  | w     | 401 | ADP  | C5'-O5'-PA-O2A  |
| 56  | V     | 204 | CDL  | CB5-C51-C52-C53 |
| 56  | V     | 204 | CDL  | C79-C80-C81-C82 |
| 56  | l     | 702 | CDL  | C78-C79-C80-C81 |
| 48  | B     | 303 | PEE  | O3P-C1-C2-C3    |
| 56  | V     | 202 | CDL  | OA5-CA3-CA4-CA6 |
| 56  | l     | 701 | CDL  | OA5-CA3-CA4-CA6 |
| 49  | C     | 303 | PLX  | C11-C12-C13-C14 |
| 48  | l     | 703 | PEE  | C10-C11-C12-C13 |
| 56  | V     | 204 | CDL  | C44-C45-C46-C47 |
| 49  | e     | 201 | PLX  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | J     | 403 | PLX  | C25-C24-O8-C5   |
| 49  | a     | 202 | PLX  | C25-C24-O8-C5   |
| 49  | g     | 201 | PLX  | C25-C24-O8-C5   |
| 49  | j     | 203 | PLX  | C25-C24-O8-C5   |
| 49  | j     | 203 | PLX  | C24-C25-C26-C27 |
| 56  | V     | 202 | CDL  | CB7-C71-C72-C73 |
| 48  | r     | 501 | PEE  | C31-C30-O3-C3   |
| 48  | B     | 303 | PEE  | O3P-C1-C2-O2    |
| 56  | N     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 56  | a     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 56  | V     | 204 | CDL  | C77-C78-C79-C80 |
| 49  | e     | 201 | PLX  | C18-C19-C20-C21 |
| 49  | j     | 203 | PLX  | C29-C30-C31-C32 |
| 52  | J     | 401 | NDP  | O4D-C1D-N1N-C6N |
| 56  | s     | 401 | CDL  | CB5-C51-C52-C53 |
| 48  | j     | 201 | PEE  | C24-C25-C26-C27 |
| 56  | a     | 201 | CDL  | O1-C1-CB2-OB2   |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1C    |
| 48  | B     | 303 | PEE  | C44-C45-C46-C47 |
| 56  | s     | 401 | CDL  | C31-C32-C33-C34 |
| 49  | J     | 403 | PLX  | N1-C1-C2-O1     |
| 56  | V     | 204 | CDL  | C19-C20-C21-C22 |
| 48  | j     | 202 | PEE  | O2-C2-C3-O3     |
| 48  | l     | 704 | PEE  | O2-C2-C3-O3     |
| 56  | N     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 56  | i     | 401 | CDL  | OA6-CA4-CA6-OA8 |
| 56  | a     | 201 | CDL  | C82-C83-C84-C85 |
| 56  | r     | 503 | CDL  | C60-C61-C62-C63 |
| 48  | W     | 201 | PEE  | C24-C25-C26-C27 |
| 49  | j     | 203 | PLX  | C32-C33-C34-C35 |
| 56  | V     | 201 | CDL  | C72-C73-C74-C75 |
| 56  | a     | 201 | CDL  | C76-C77-C78-C79 |
| 48  | r     | 501 | PEE  | O5-C30-O3-C3    |
| 49  | g     | 201 | PLX  | O8-C24-C25-C26  |
| 49  | g     | 201 | PLX  | O9-C24-C25-C26  |
| 48  | j     | 201 | PEE  | C40-C41-C42-C43 |
| 56  | V     | 204 | CDL  | C35-C36-C37-C38 |
| 56  | V     | 201 | CDL  | C31-C32-C33-C34 |
| 48  | V     | 203 | PEE  | C34-C35-C36-C37 |
| 49  | a     | 202 | PLX  | C30-C31-C32-C33 |
| 56  | V     | 202 | CDL  | C36-C37-C38-C39 |
| 48  | j     | 201 | PEE  | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 703 | PEE  | C3-C2-O2-C10    |
| 56  | a     | 201 | CDL  | CA3-CA4-OA6-CA5 |
| 56  | V     | 202 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | V     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 49  | e     | 201 | PLX  | C9-C10-C11-C12  |
| 56  | a     | 201 | CDL  | C24-C25-C26-C27 |
| 56  | V     | 204 | CDL  | C54-C55-C56-C57 |
| 53  | s     | 402 | UQ   | C24-C26-C27-C28 |
| 48  | r     | 501 | PEE  | O2-C2-C3-O3     |
| 49  | a     | 202 | PLX  | O6-C4-C5-O8     |
| 48  | V     | 203 | PEE  | C4-O4P-P-O3P    |
| 48  | W     | 201 | PEE  | C1-O3P-P-O4P    |
| 48  | j     | 201 | PEE  | C4-O4P-P-O3P    |
| 49  | C     | 303 | PLX  | C3-O4-P1-O1     |
| 49  | e     | 201 | PLX  | C2-O1-P1-O4     |
| 56  | V     | 204 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | s     | 401 | CDL  | CA2-OA2-PA1-OA5 |
| 56  | s     | 401 | CDL  | CB3-OB5-PB2-OB2 |
| 56  | r     | 503 | CDL  | C57-C58-C59-C60 |
| 48  | B     | 303 | PEE  | C39-C40-C41-C42 |
| 56  | l     | 701 | CDL  | C78-C79-C80-C81 |
| 49  | e     | 201 | PLX  | C10-C11-C12-C13 |
| 49  | e     | 201 | PLX  | C28-C29-C30-C31 |
| 56  | i     | 401 | CDL  | C36-C37-C38-C39 |
| 56  | i     | 401 | CDL  | CA4-CA3-OA5-PA1 |
| 48  | C     | 302 | PEE  | C16-C17-C18-C19 |
| 49  | r     | 502 | PLX  | C18-C19-C20-C21 |
| 49  | e     | 201 | PLX  | C7-C8-C9-C10    |
| 48  | W     | 201 | PEE  | C15-C16-C17-C18 |
| 48  | l     | 703 | PEE  | C19-C20-C21-C22 |
| 48  | j     | 201 | PEE  | C41-C42-C43-C44 |
| 48  | l     | 704 | PEE  | C18-C19-C20-C21 |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1A    |
| 56  | i     | 401 | CDL  | C13-C14-C15-C16 |
| 56  | V     | 201 | CDL  | C40-C41-C42-C43 |
| 56  | n     | 101 | CDL  | C56-C57-C58-C59 |
| 56  | N     | 201 | CDL  | CB7-C71-C72-C73 |
| 56  | V     | 201 | CDL  | C64-C65-C66-C67 |
| 56  | V     | 204 | CDL  | C60-C61-C62-C63 |
| 48  | r     | 501 | PEE  | C16-C17-C18-C19 |
| 56  | V     | 204 | CDL  | C63-C64-C65-C66 |
| 56  | V     | 204 | CDL  | C52-C51-CB5-OB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | s     | 402 | UQ   | C22-C23-C24-C25 |
| 56  | l     | 702 | CDL  | C82-C83-C84-C85 |
| 49  | g     | 201 | PLX  | O6-C6-C7-C8     |
| 49  | j     | 203 | PLX  | O8-C24-C25-C26  |
| 56  | r     | 503 | CDL  | C52-C53-C54-C55 |
| 56  | r     | 503 | CDL  | C72-C71-CB7-OB8 |
| 48  | l     | 703 | PEE  | C30-C31-C32-C33 |
| 49  | r     | 502 | PLX  | C4-C3-O4-P1     |
| 48  | B     | 303 | PEE  | C21-C22-C23-C24 |
| 56  | s     | 401 | CDL  | C77-C78-C79-C80 |
| 48  | B     | 303 | PEE  | C22-C23-C24-C25 |
| 49  | J     | 403 | PLX  | C6-C7-C8-C9     |
| 51  | X     | 201 | 8Q1  | C43-C42-N41-C39 |
| 48  | l     | 704 | PEE  | C30-C31-C32-C33 |
| 56  | r     | 503 | CDL  | CA2-C1-CB2-OB2  |
| 49  | e     | 201 | PLX  | C12-C13-C14-C15 |
| 50  | C     | 304 | DCQ  | C10-C11-C12-C13 |
| 56  | V     | 202 | CDL  | C77-C78-C79-C80 |
| 56  | V     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 56  | V     | 202 | CDL  | C44-C45-C46-C47 |
| 48  | r     | 501 | PEE  | C20-C21-C22-C23 |
| 56  | V     | 204 | CDL  | C15-C16-C17-C18 |
| 47  | A     | 503 | NAI  | O4D-C1D-N1N-C6N |
| 49  | j     | 203 | PLX  | C3-O4-P1-O1     |
| 56  | i     | 401 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | i     | 401 | CDL  | C12-C11-CA5-OA6 |
| 56  | r     | 503 | CDL  | C53-C54-C55-C56 |
| 48  | V     | 203 | PEE  | C2-C1-O3P-P     |
| 56  | V     | 201 | CDL  | C38-C39-C40-C41 |
| 56  | r     | 503 | CDL  | C21-C22-C23-C24 |
| 56  | n     | 101 | CDL  | C52-C53-C54-C55 |
| 48  | V     | 203 | PEE  | C35-C36-C37-C38 |
| 48  | C     | 302 | PEE  | O3P-C1-C2-C3    |
| 56  | l     | 701 | CDL  | C18-C19-C20-C21 |
| 49  | a     | 202 | PLX  | C33-C34-C35-C36 |
| 56  | r     | 503 | CDL  | C77-C78-C79-C80 |
| 56  | i     | 401 | CDL  | C33-C34-C35-C36 |
| 48  | V     | 203 | PEE  | C37-C38-C39-C40 |
| 56  | a     | 201 | CDL  | C54-C55-C56-C57 |
| 48  | C     | 302 | PEE  | O5-C30-O3-C3    |
| 48  | r     | 501 | PEE  | C21-C22-C23-C24 |
| 52  | J     | 401 | NDP  | PN-O3-PA-O1A    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 51  | X     | 201 | 8Q1  | C11-C12-C13-C14 |
| 48  | j     | 202 | PEE  | C18-C19-C20-C21 |
| 56  | s     | 401 | CDL  | CA3-CA4-CA6-OA8 |
| 48  | C     | 302 | PEE  | C17-C18-C19-C20 |
| 56  | V     | 201 | CDL  | C43-C44-C45-C46 |
| 56  | V     | 202 | CDL  | C32-C31-CA7-OA8 |
| 49  | j     | 203 | PLX  | C4-C5-O8-C24    |
| 49  | C     | 303 | PLX  | C25-C26-C27-C28 |
| 49  | g     | 201 | PLX  | C20-C21-C22-C23 |
| 56  | l     | 701 | CDL  | C34-C35-C36-C37 |
| 56  | l     | 702 | CDL  | C18-C19-C20-C21 |
| 49  | C     | 303 | PLX  | C31-C32-C33-C34 |
| 48  | V     | 203 | PEE  | C31-C32-C33-C34 |
| 56  | l     | 701 | CDL  | OB5-CB3-CB4-CB6 |
| 53  | J     | 402 | UQ   | C19-C21-C22-C23 |
| 56  | V     | 201 | CDL  | C57-C58-C59-C60 |
| 48  | C     | 302 | PEE  | C31-C30-O3-C3   |
| 48  | V     | 203 | PEE  | O4P-C4-C5-N     |
| 48  | l     | 704 | PEE  | O4P-C4-C5-N     |
| 56  | r     | 503 | CDL  | C54-C55-C56-C57 |
| 48  | C     | 302 | PEE  | C38-C39-C40-C41 |
| 56  | N     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | a     | 201 | CDL  | C80-C81-C82-C83 |
| 51  | G     | 201 | 8Q1  | C1-C6-C7-C8     |
| 56  | n     | 101 | CDL  | C32-C31-CA7-OA8 |
| 48  | l     | 703 | PEE  | O2-C2-C3-O3     |
| 56  | r     | 503 | CDL  | OA6-CA4-CA6-OA8 |
| 56  | N     | 201 | CDL  | C52-C51-CB5-OB6 |
| 56  | N     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 56  | n     | 101 | CDL  | C32-C31-CA7-OA9 |
| 48  | j     | 201 | PEE  | C43-C44-C45-C46 |
| 56  | s     | 401 | CDL  | C72-C71-CB7-OB8 |
| 48  | B     | 303 | PEE  | C18-C19-C20-C21 |
| 48  | C     | 302 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C36-C37-C38-C39 |
| 48  | l     | 703 | PEE  | C38-C39-C40-C41 |
| 48  | r     | 501 | PEE  | C18-C19-C20-C21 |
| 49  | j     | 203 | PLX  | C10-C11-C12-C13 |
| 48  | B     | 303 | PEE  | C16-C17-C18-C19 |
| 48  | C     | 302 | PEE  | C36-C37-C38-C39 |
| 48  | j     | 201 | PEE  | C16-C17-C18-C19 |
| 48  | j     | 202 | PEE  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | V     | 204 | CDL  | C57-C58-C59-C60 |
| 48  | l     | 703 | PEE  | C1-C2-C3-O3     |
| 49  | j     | 203 | PLX  | C7-C6-O6-C4     |
| 49  | j     | 203 | PLX  | C3-C4-C5-O8     |
| 56  | r     | 503 | CDL  | C56-C57-C58-C59 |
| 56  | N     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 51  | G     | 201 | 8Q1  | C9-C10-C11-C12  |
| 48  | C     | 302 | PEE  | O3-C30-C31-C32  |
| 56  | V     | 201 | CDL  | C12-C11-CA5-OA6 |
| 56  | V     | 204 | CDL  | C12-C11-CA5-OA6 |
| 48  | W     | 201 | PEE  | C33-C34-C35-C36 |
| 56  | V     | 202 | CDL  | C80-C81-C82-C83 |
| 49  | e     | 201 | PLX  | C34-C35-C36-C37 |
| 48  | l     | 704 | PEE  | C20-C21-C22-C23 |
| 56  | a     | 201 | CDL  | C32-C33-C34-C35 |
| 48  | V     | 203 | PEE  | C38-C39-C40-C41 |
| 48  | W     | 201 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C16-C17-C18-C19 |
| 48  | l     | 704 | PEE  | C38-C39-C40-C41 |
| 49  | j     | 203 | PLX  | C19-C20-C21-C22 |
| 50  | C     | 304 | DCQ  | C11-C10-C9-C8   |
| 56  | a     | 201 | CDL  | C57-C58-C59-C60 |
| 49  | C     | 303 | PLX  | C18-C19-C20-C21 |
| 56  | l     | 702 | CDL  | OB5-CB3-CB4-CB6 |
| 56  | r     | 503 | CDL  | C79-C80-C81-C82 |
| 49  | j     | 203 | PLX  | O6-C4-C5-O8     |
| 56  | V     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 56  | s     | 401 | CDL  | C72-C73-C74-C75 |
| 56  | N     | 201 | CDL  | C12-C11-CA5-OA6 |
| 56  | i     | 401 | CDL  | C79-C80-C81-C82 |
| 56  | N     | 201 | CDL  | C72-C71-CB7-OB8 |
| 56  | s     | 401 | CDL  | C12-C11-CA5-OA6 |
| 56  | l     | 702 | CDL  | C61-C62-C63-C64 |
| 48  | W     | 201 | PEE  | C16-C17-C18-C19 |
| 48  | l     | 704 | PEE  | C36-C37-C38-C39 |
| 56  | l     | 702 | CDL  | C77-C78-C79-C80 |
| 48  | W     | 201 | PEE  | C14-C15-C16-C17 |
| 56  | l     | 701 | CDL  | C12-C11-CA5-OA6 |
| 56  | a     | 201 | CDL  | C12-C11-CA5-OA6 |
| 48  | V     | 203 | PEE  | C16-C17-C18-C19 |
| 48  | j     | 201 | PEE  | C19-C20-C21-C22 |
| 56  | r     | 503 | CDL  | C32-C31-CA7-OA8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | s     | 402 | UQ   | C12-C13-C14-C15 |
| 56  | V     | 201 | CDL  | C55-C56-C57-C58 |
| 48  | C     | 302 | PEE  | O5-C30-C31-C32  |
| 56  | a     | 201 | CDL  | C73-C74-C75-C76 |
| 56  | V     | 201 | CDL  | C12-C11-CA5-OA7 |
| 56  | s     | 401 | CDL  | C33-C34-C35-C36 |
| 48  | r     | 501 | PEE  | C1-O3P-P-O4P    |
| 56  | V     | 202 | CDL  | C71-C72-C73-C74 |
| 56  | N     | 201 | CDL  | C52-C51-CB5-OB7 |
| 48  | j     | 201 | PEE  | C11-C12-C13-C14 |
| 56  | l     | 701 | CDL  | C60-C61-C62-C63 |
| 47  | A     | 503 | NAI  | C5B-O5B-PA-O2A  |
| 48  | l     | 703 | PEE  | C1-O3P-P-O1P    |
| 48  | l     | 703 | PEE  | C4-O4P-P-O2P    |
| 48  | l     | 704 | PEE  | C4-O4P-P-O1P    |
| 49  | C     | 303 | PLX  | C3-O4-P1-O2     |
| 56  | V     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 56  | i     | 401 | CDL  | CB3-OB5-PB2-OB4 |
| 56  | l     | 701 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | N     | 201 | CDL  | C12-C11-CA5-OA7 |
| 56  | V     | 204 | CDL  | C12-C11-CA5-OA7 |
| 56  | l     | 702 | CDL  | C33-C34-C35-C36 |
| 56  | n     | 101 | CDL  | C52-C51-CB5-OB6 |
| 56  | a     | 201 | CDL  | C52-C53-C54-C55 |
| 49  | g     | 201 | PLX  | C15-C16-C17-C18 |
| 56  | l     | 702 | CDL  | C52-C51-CB5-OB7 |
| 48  | r     | 501 | PEE  | C5-C4-O4P-P     |
| 56  | N     | 201 | CDL  | C72-C71-CB7-OB9 |
| 56  | l     | 702 | CDL  | C12-C11-CA5-OA7 |
| 56  | l     | 702 | CDL  | C54-C55-C56-C57 |
| 56  | r     | 503 | CDL  | C32-C31-CA7-OA9 |
| 48  | V     | 203 | PEE  | C11-C12-C13-C14 |
| 56  | V     | 204 | CDL  | C20-C21-C22-C23 |
| 56  | a     | 201 | CDL  | C40-C41-C42-C43 |
| 48  | r     | 501 | PEE  | O2-C10-C11-C12  |
| 56  | l     | 701 | CDL  | C72-C71-CB7-OB8 |
| 49  | J     | 403 | PLX  | C31-C32-C33-C34 |
| 49  | a     | 202 | PLX  | C24-C25-C26-C27 |
| 56  | l     | 702 | CDL  | OB5-CB3-CB4-OB6 |
| 48  | l     | 704 | PEE  | C16-C17-C18-C19 |
| 56  | a     | 201 | CDL  | C12-C11-CA5-OA7 |
| 56  | s     | 401 | CDL  | C12-C11-CA5-OA7 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | r     | 502 | PLX  | C34-C35-C36-C37 |
| 48  | B     | 303 | PEE  | C12-C13-C14-C15 |
| 56  | l     | 701 | CDL  | C12-C11-CA5-OA7 |
| 48  | r     | 501 | PEE  | O4-C10-C11-C12  |
| 56  | a     | 201 | CDL  | C64-C65-C66-C67 |

There are no ring outliers.

34 monomers are involved in 150 short contacts:

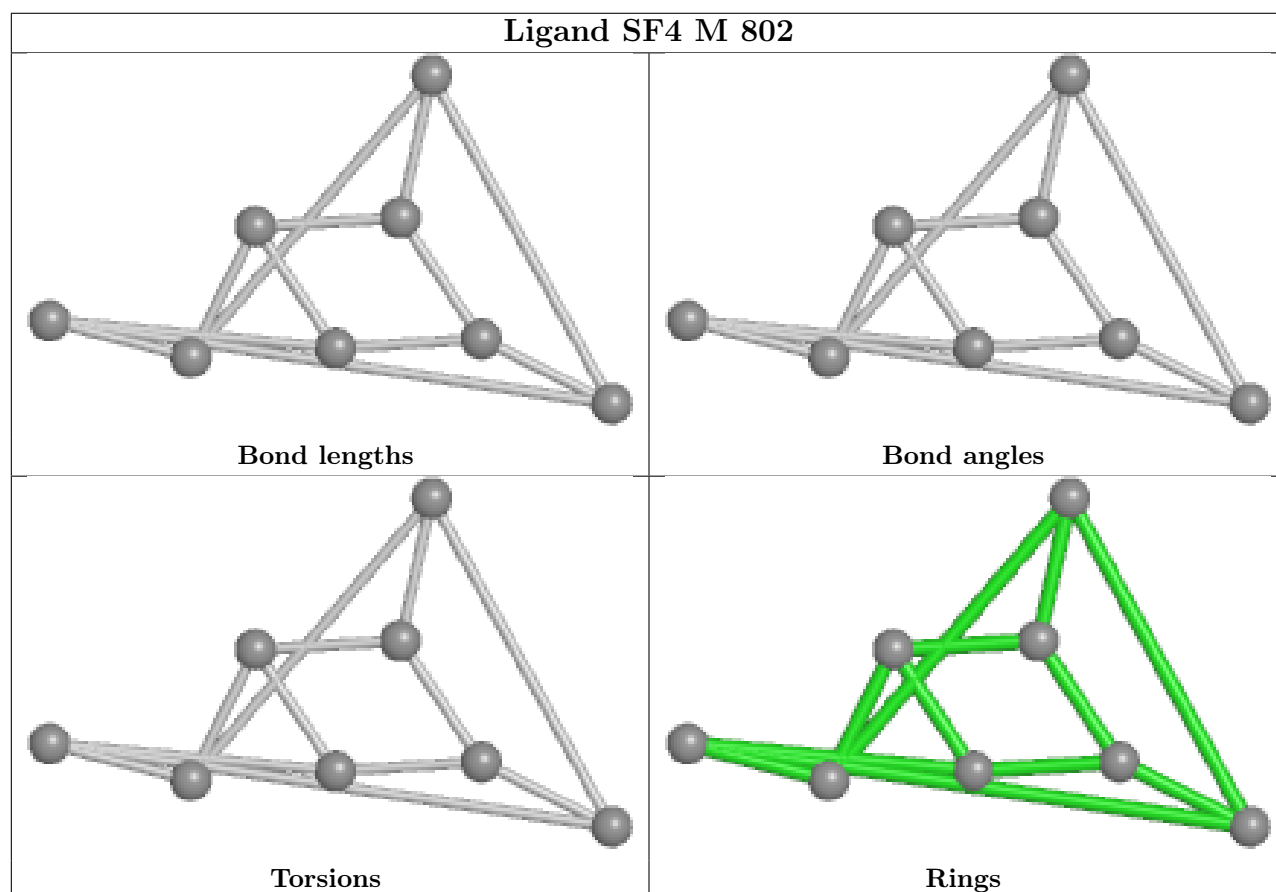
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 49  | j     | 203 | PLX  | 5       | 0            |
| 56  | V     | 201 | CDL  | 5       | 0            |
| 48  | l     | 703 | PEE  | 2       | 0            |
| 48  | j     | 201 | PEE  | 5       | 0            |
| 56  | i     | 401 | CDL  | 4       | 0            |
| 49  | J     | 403 | PLX  | 8       | 0            |
| 47  | A     | 503 | NAI  | 7       | 0            |
| 48  | j     | 202 | PEE  | 3       | 0            |
| 56  | a     | 201 | CDL  | 7       | 0            |
| 48  | C     | 302 | PEE  | 3       | 0            |
| 50  | C     | 304 | DCQ  | 2       | 0            |
| 48  | r     | 501 | PEE  | 8       | 0            |
| 48  | l     | 704 | PEE  | 4       | 0            |
| 45  | A     | 501 | SF4  | 1       | 0            |
| 49  | C     | 303 | PLX  | 4       | 0            |
| 58  | w     | 401 | ADP  | 2       | 0            |
| 56  | V     | 202 | CDL  | 10      | 0            |
| 48  | B     | 303 | PEE  | 5       | 0            |
| 48  | V     | 203 | PEE  | 2       | 0            |
| 56  | s     | 401 | CDL  | 5       | 0            |
| 56  | r     | 503 | CDL  | 10      | 0            |
| 46  | A     | 502 | FMN  | 5       | 0            |
| 49  | a     | 202 | PLX  | 2       | 0            |
| 52  | J     | 401 | NDP  | 2       | 0            |
| 56  | n     | 101 | CDL  | 1       | 0            |
| 49  | g     | 201 | PLX  | 3       | 0            |
| 56  | V     | 204 | CDL  | 10      | 0            |
| 49  | r     | 502 | PLX  | 6       | 0            |
| 53  | J     | 402 | UQ   | 1       | 0            |
| 56  | l     | 701 | CDL  | 14      | 0            |
| 53  | s     | 402 | UQ   | 2       | 0            |
| 49  | e     | 201 | PLX  | 5       | 0            |

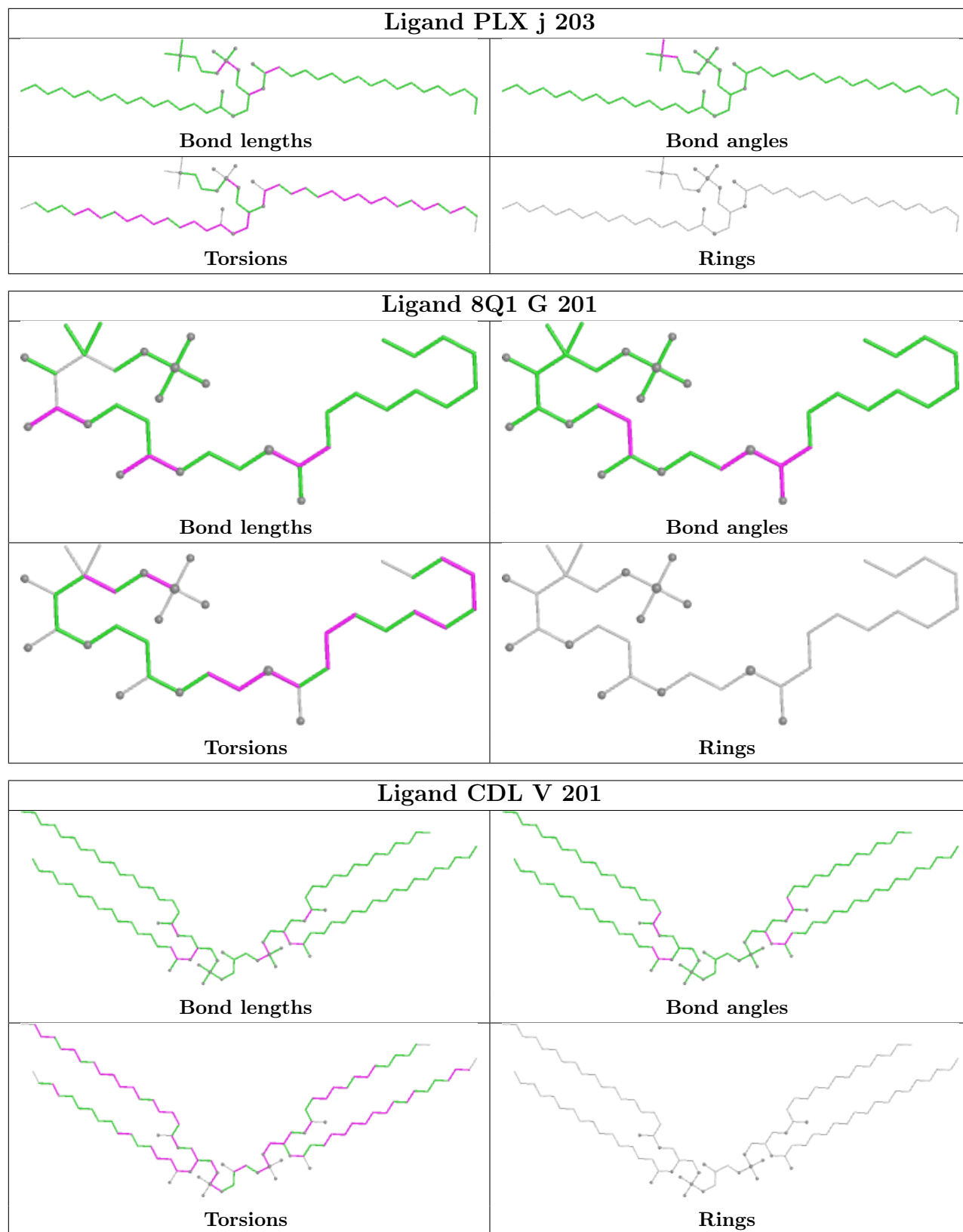
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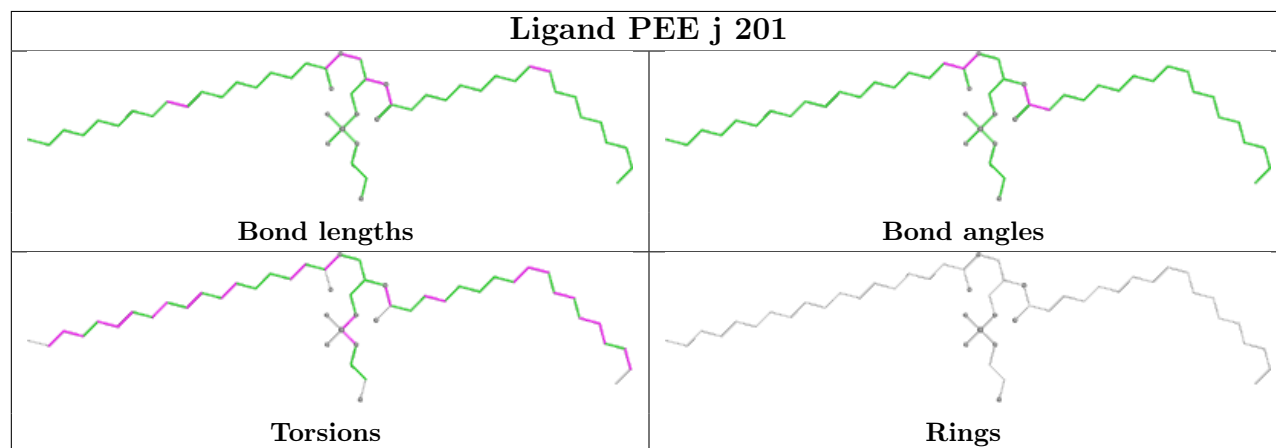
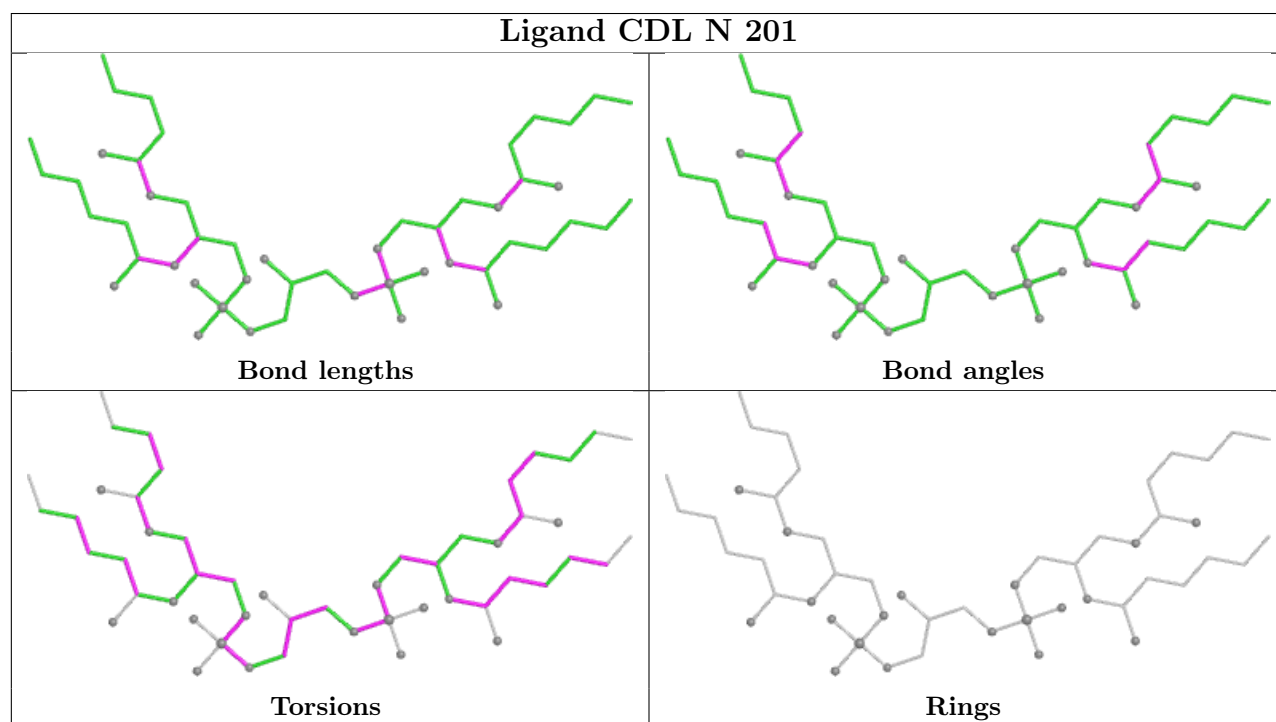
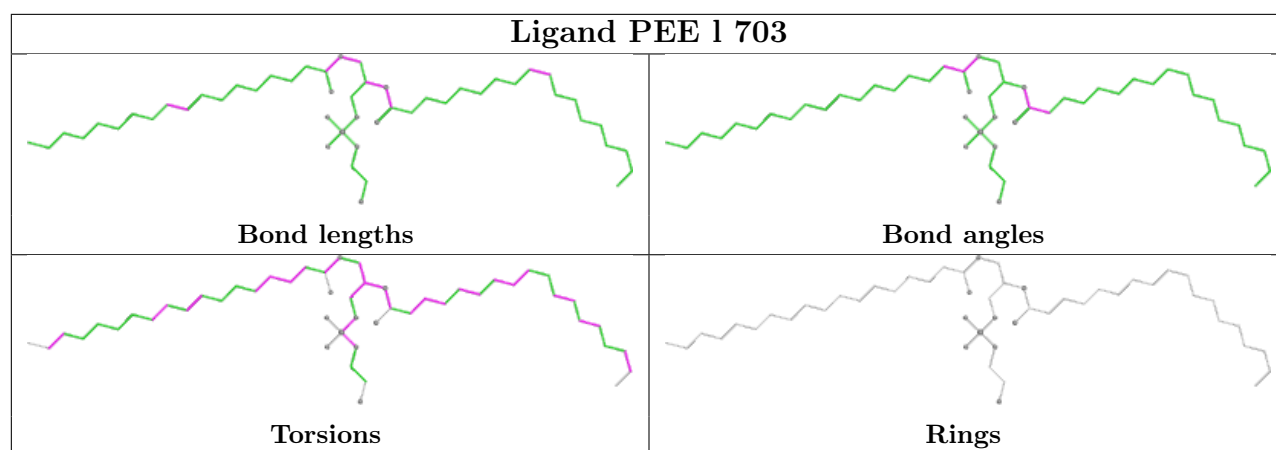
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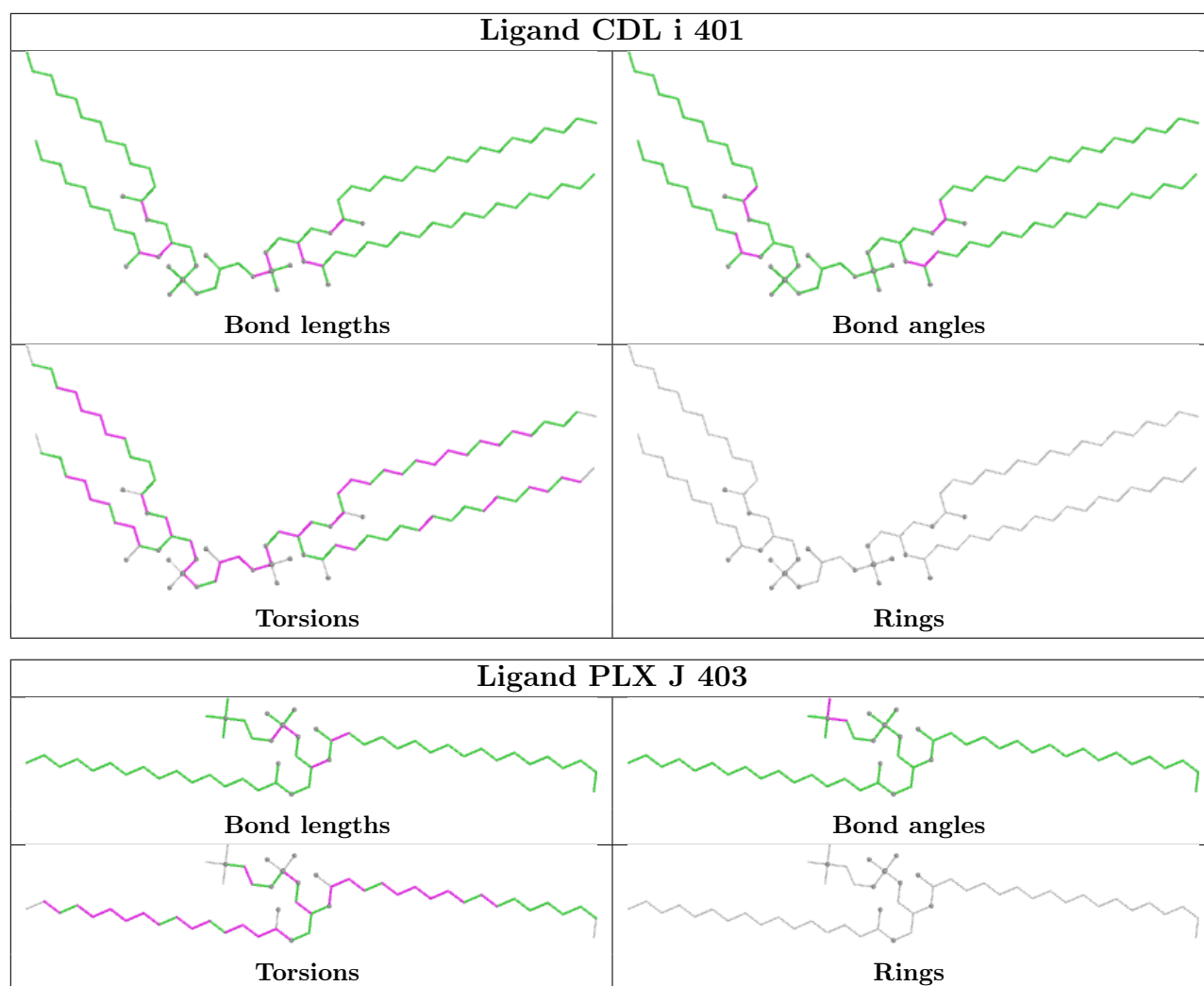
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 45  | C     | 301 | SF4  | 1       | 0            |
| 56  | 1     | 702 | CDL  | 5       | 0            |

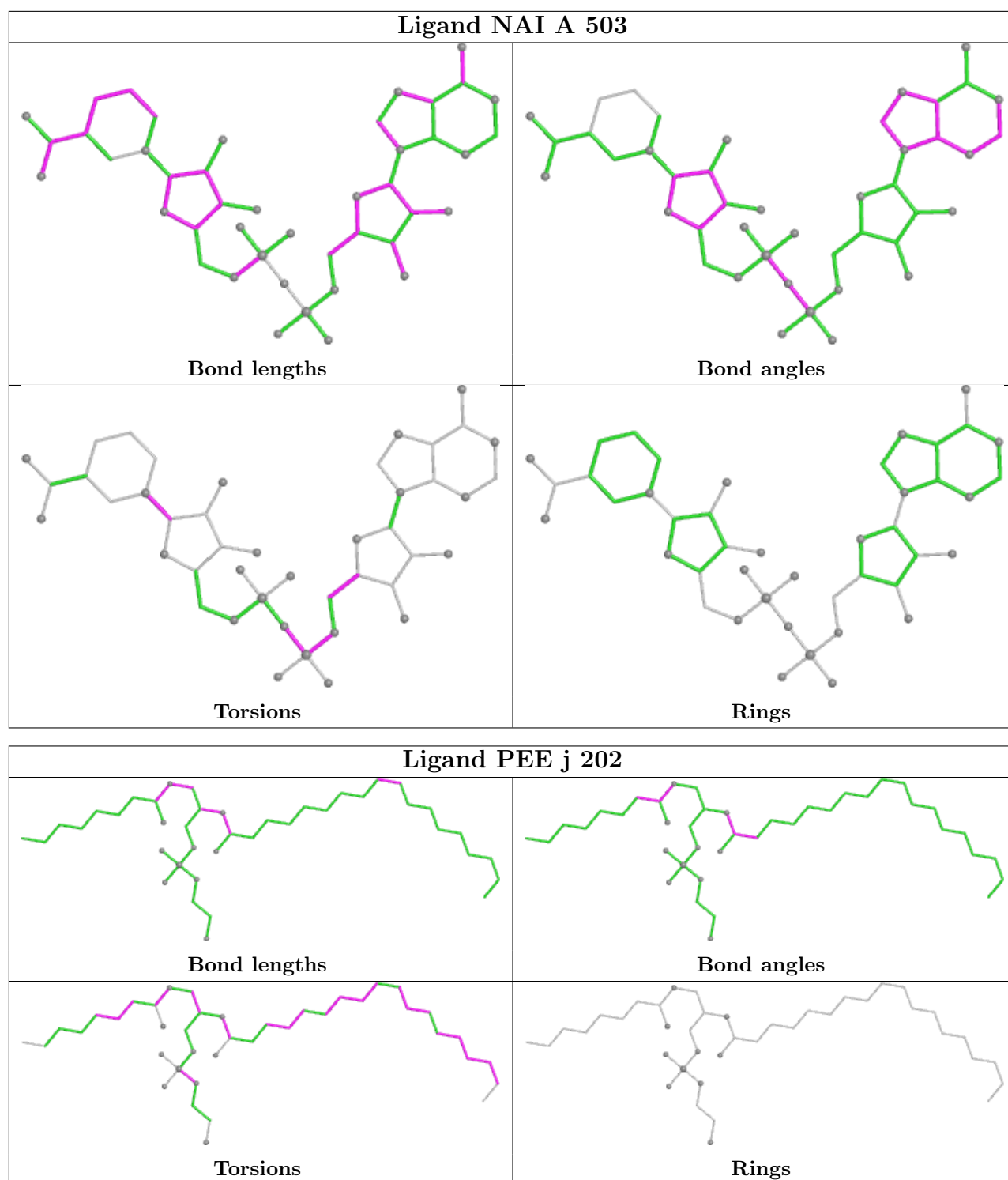
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

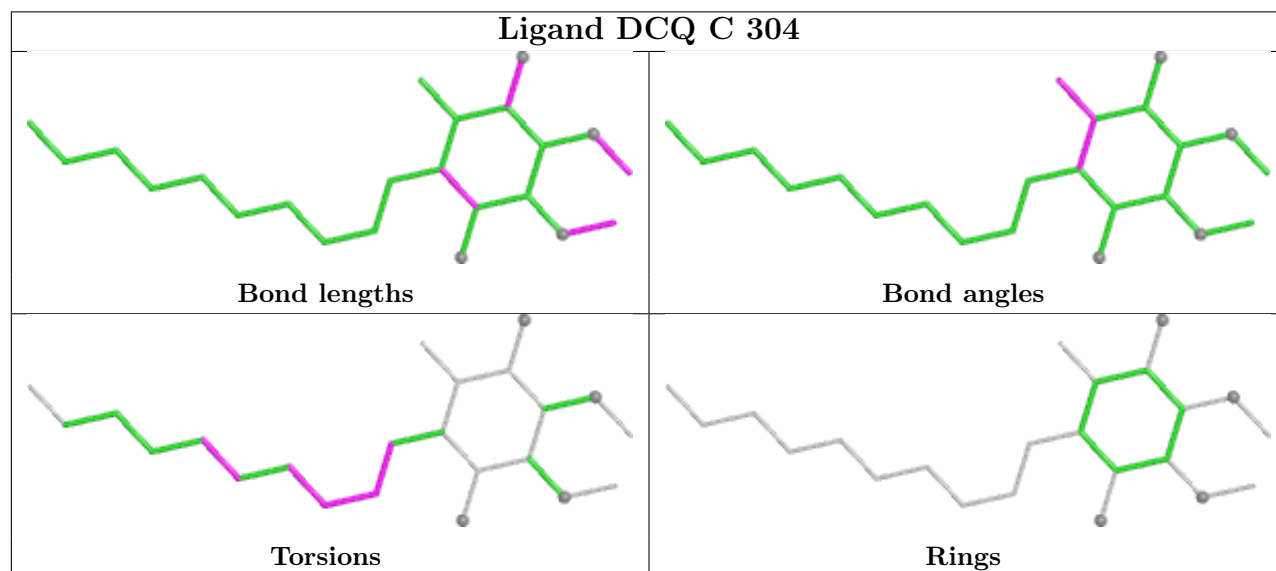
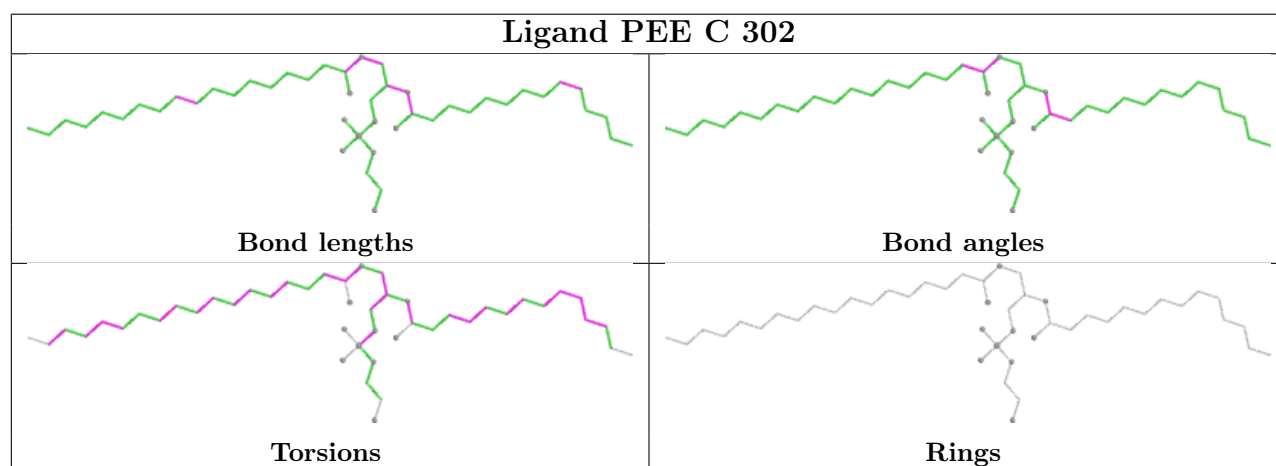
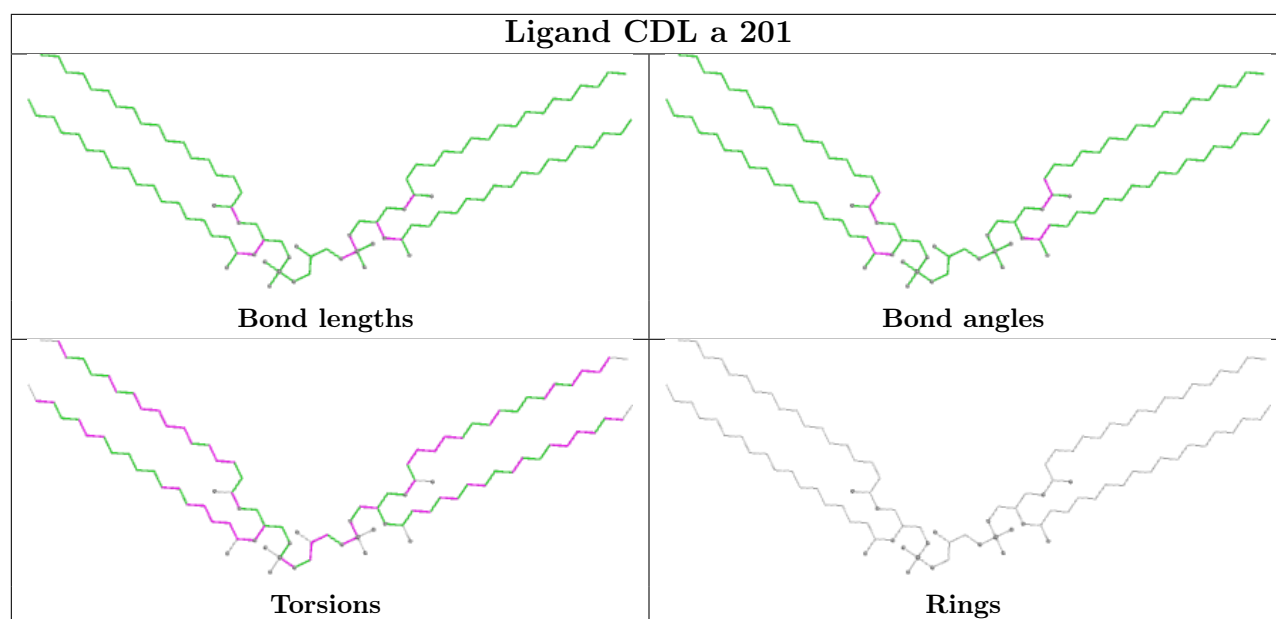


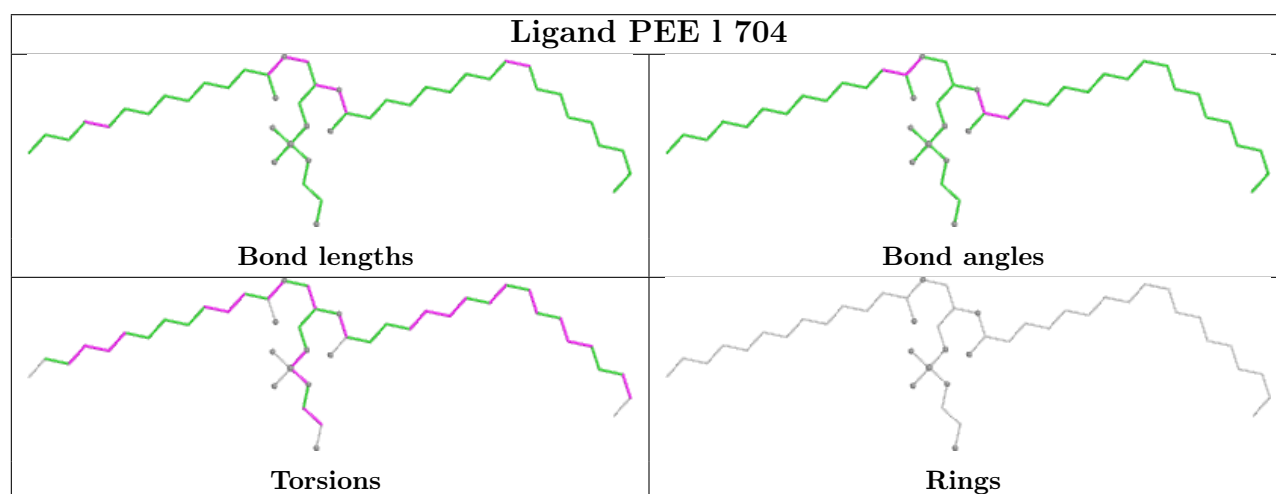
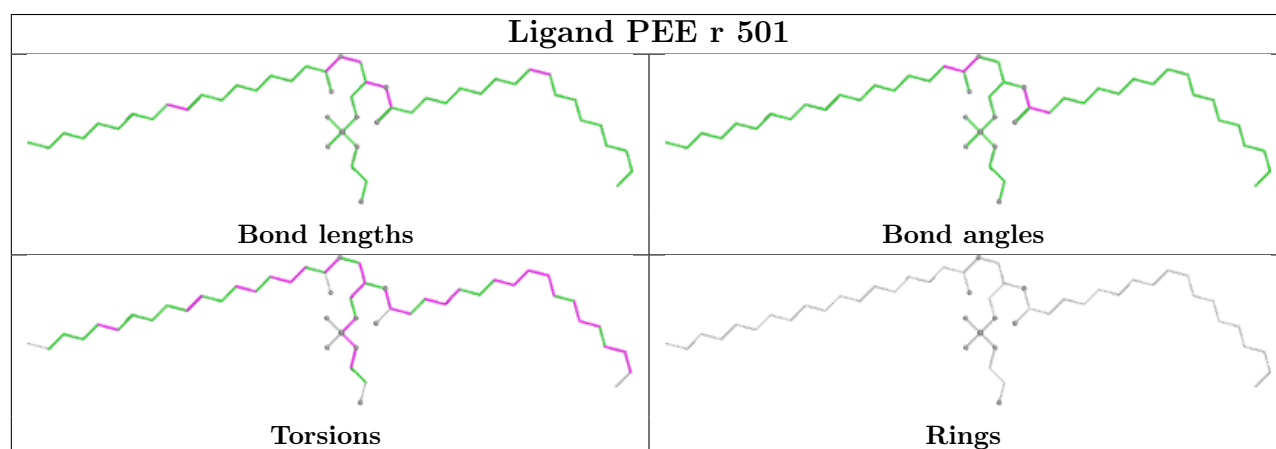
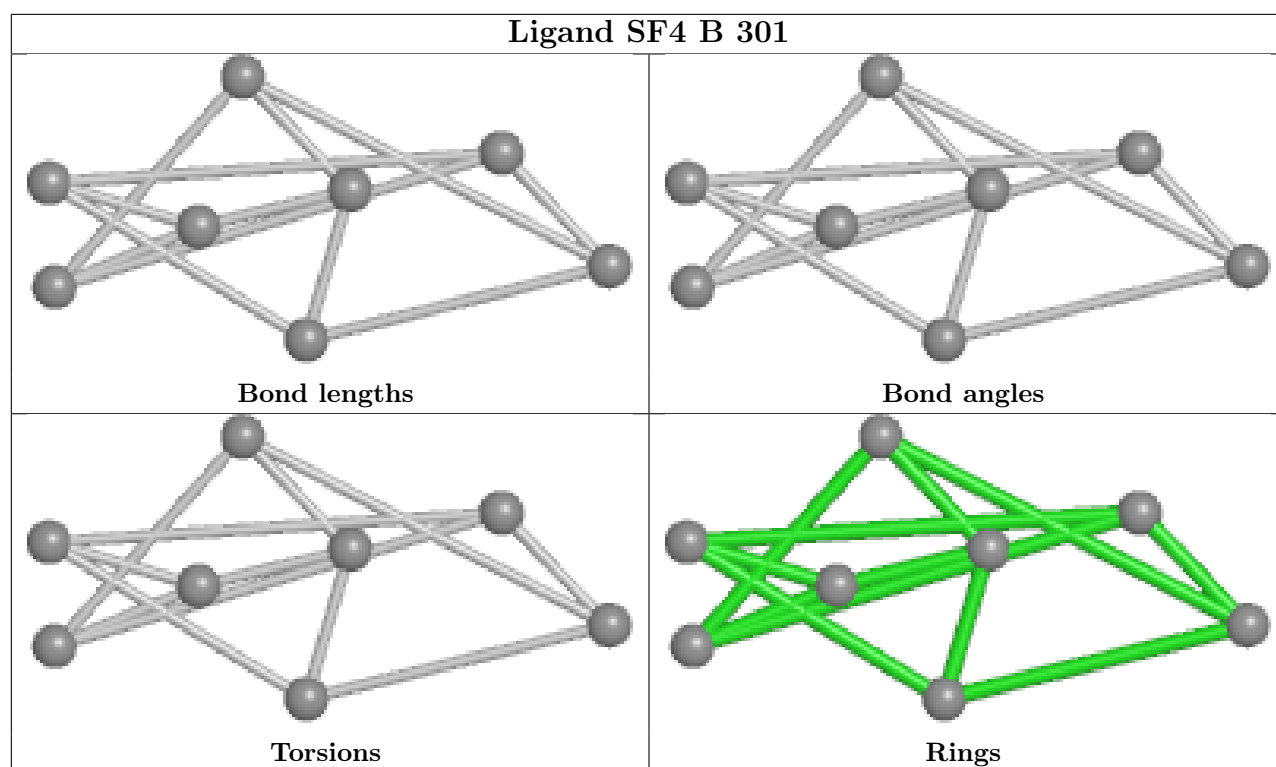


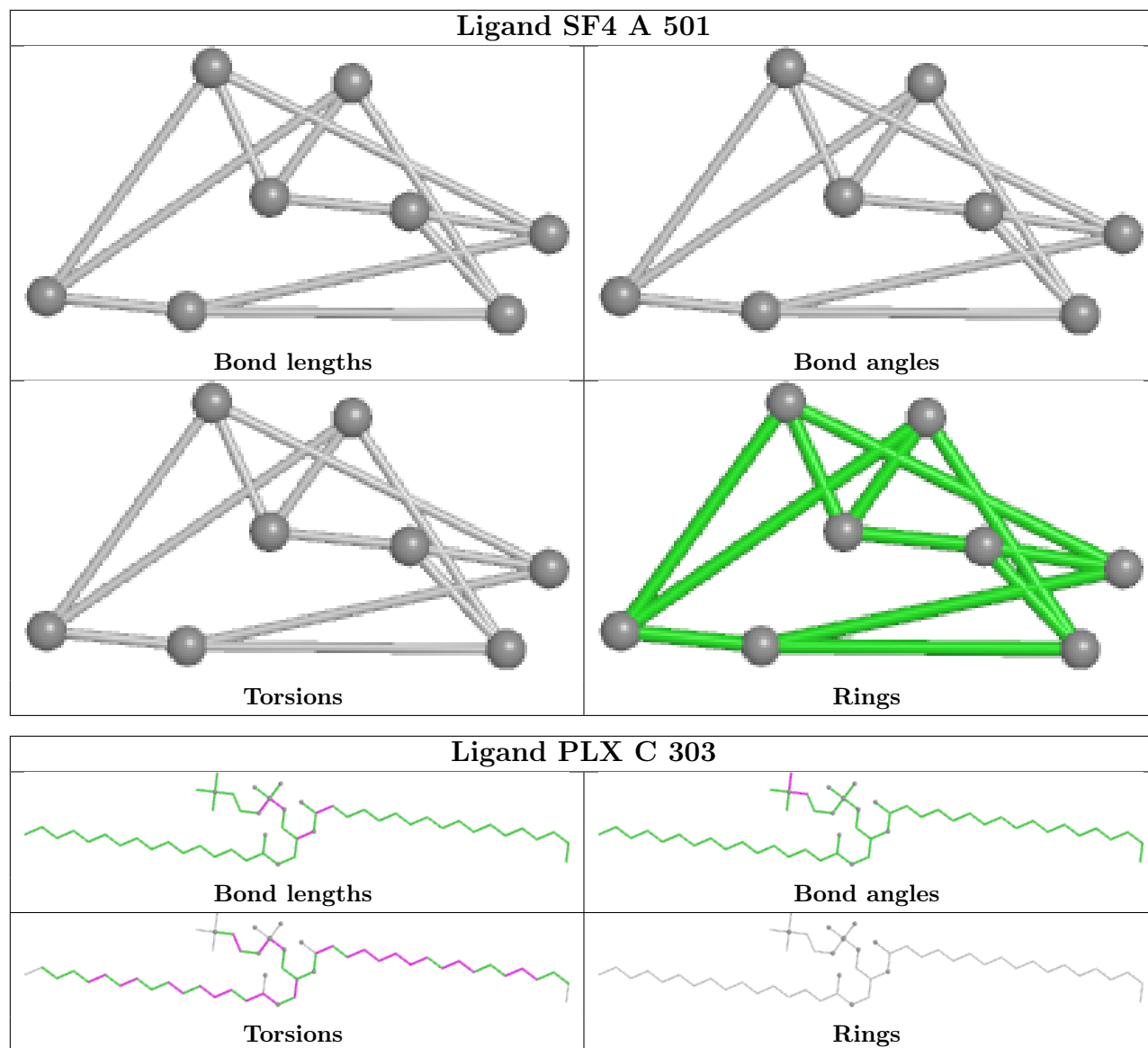


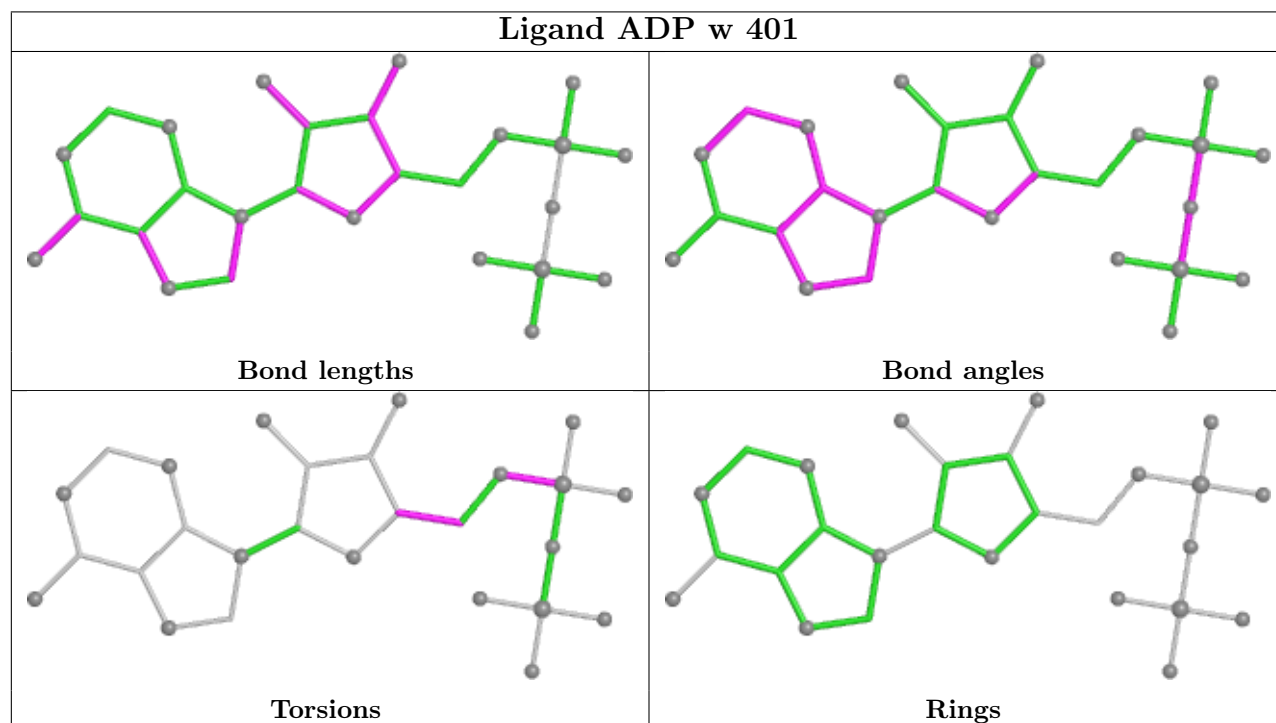
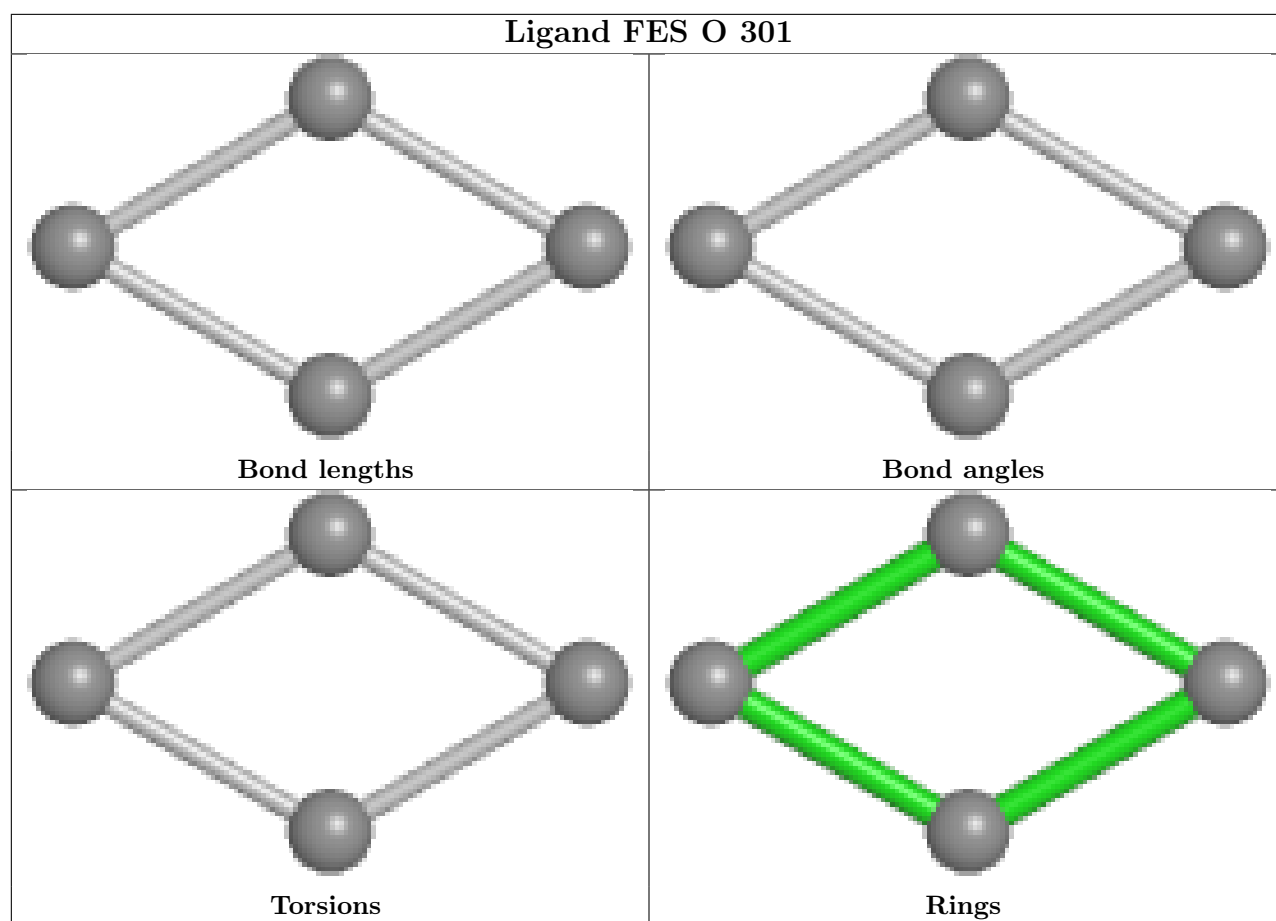


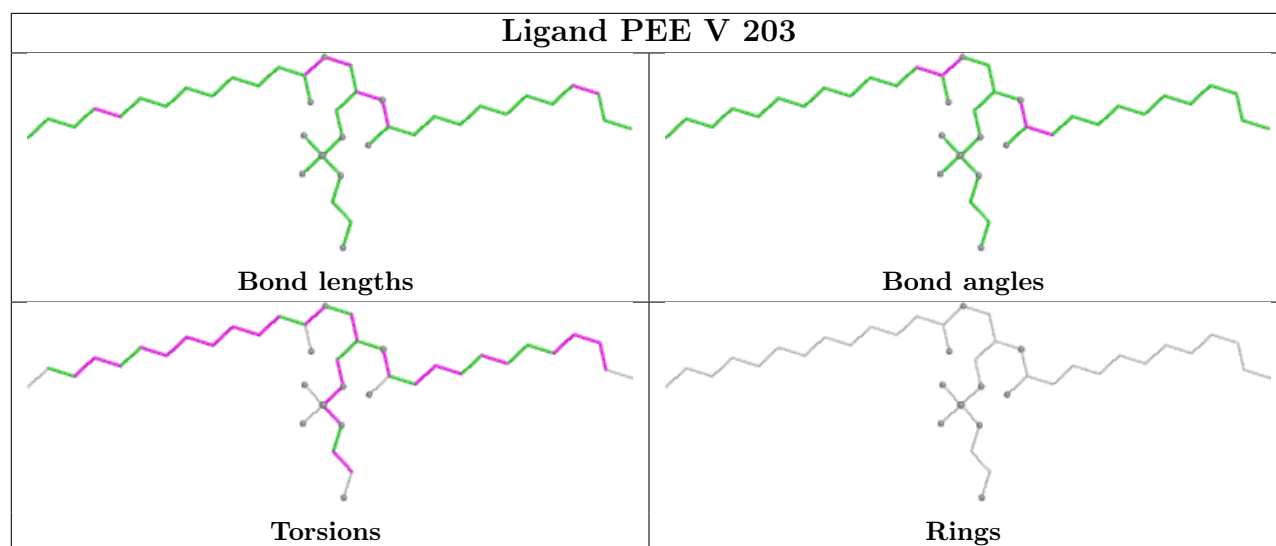
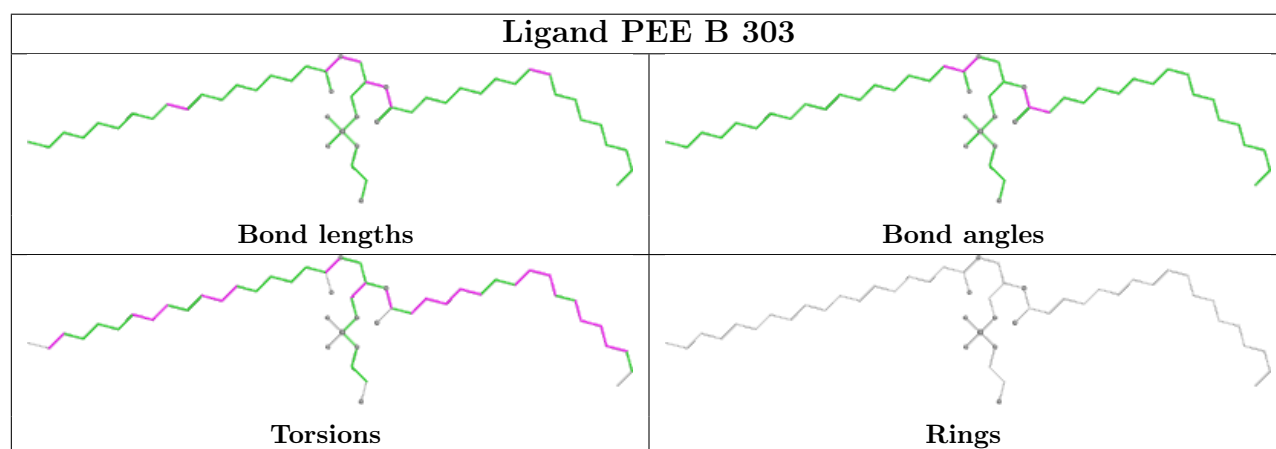
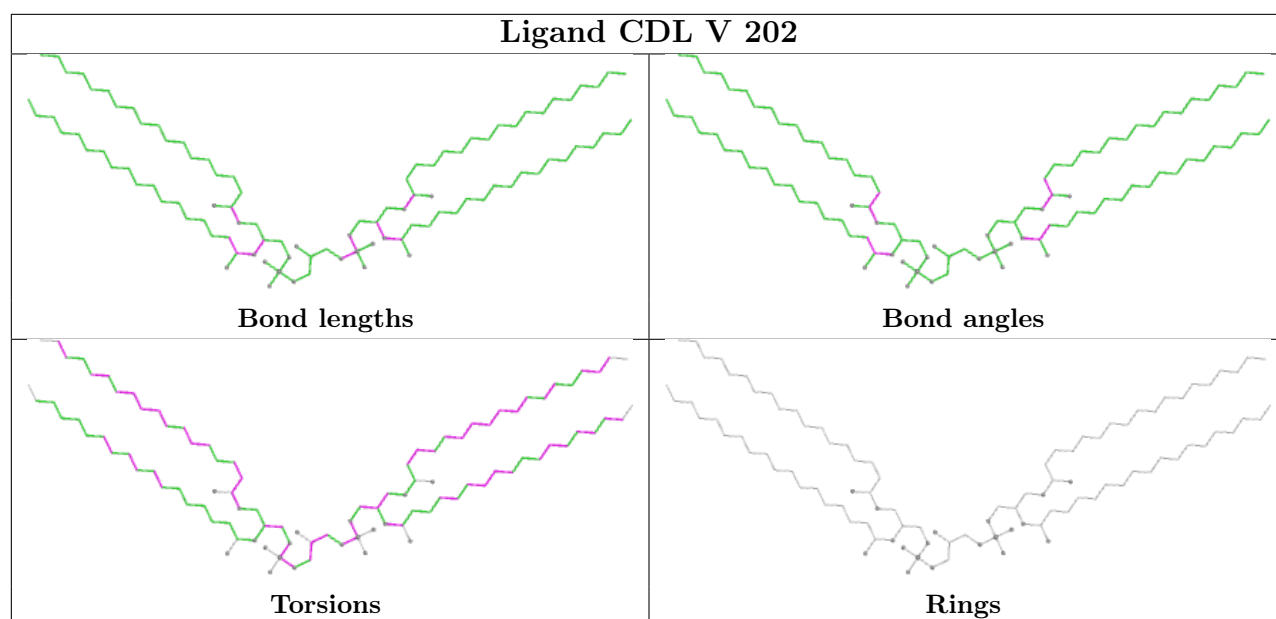


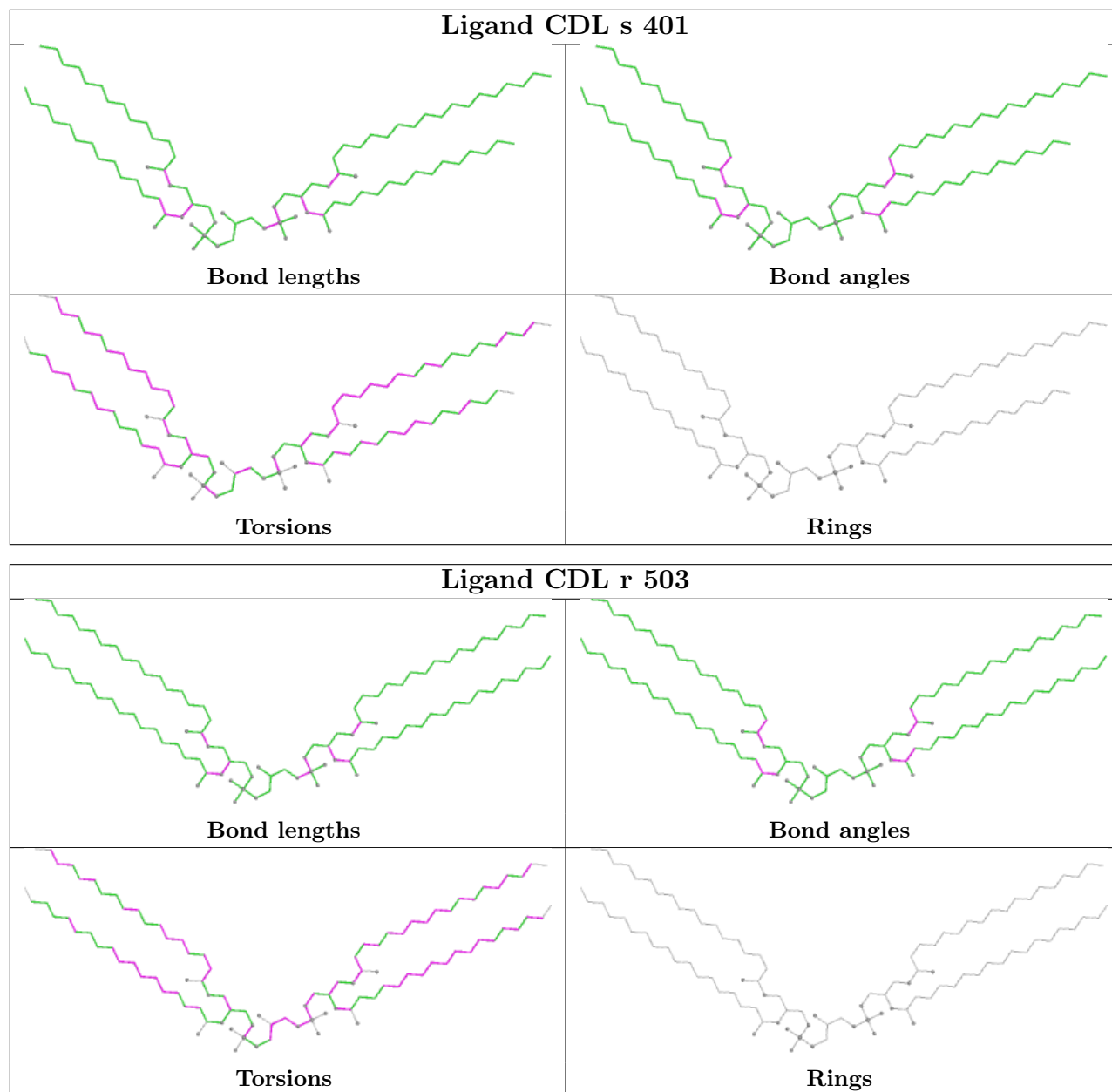


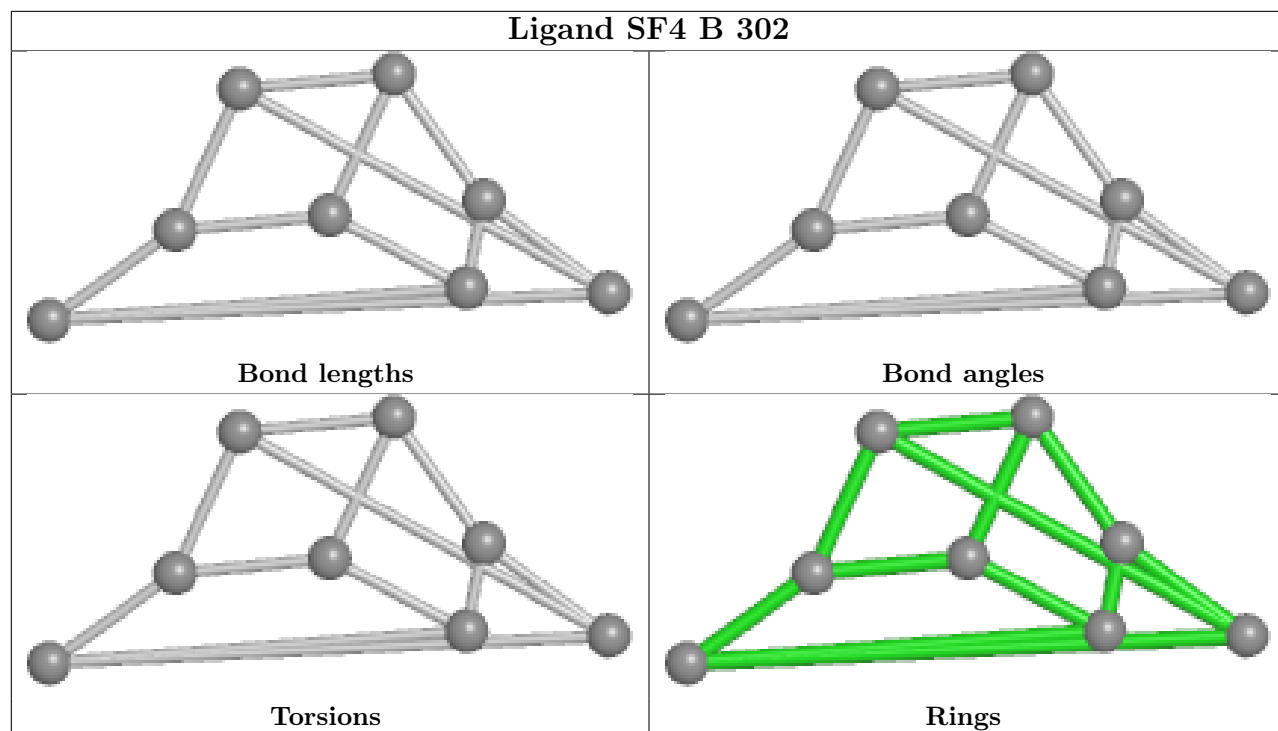


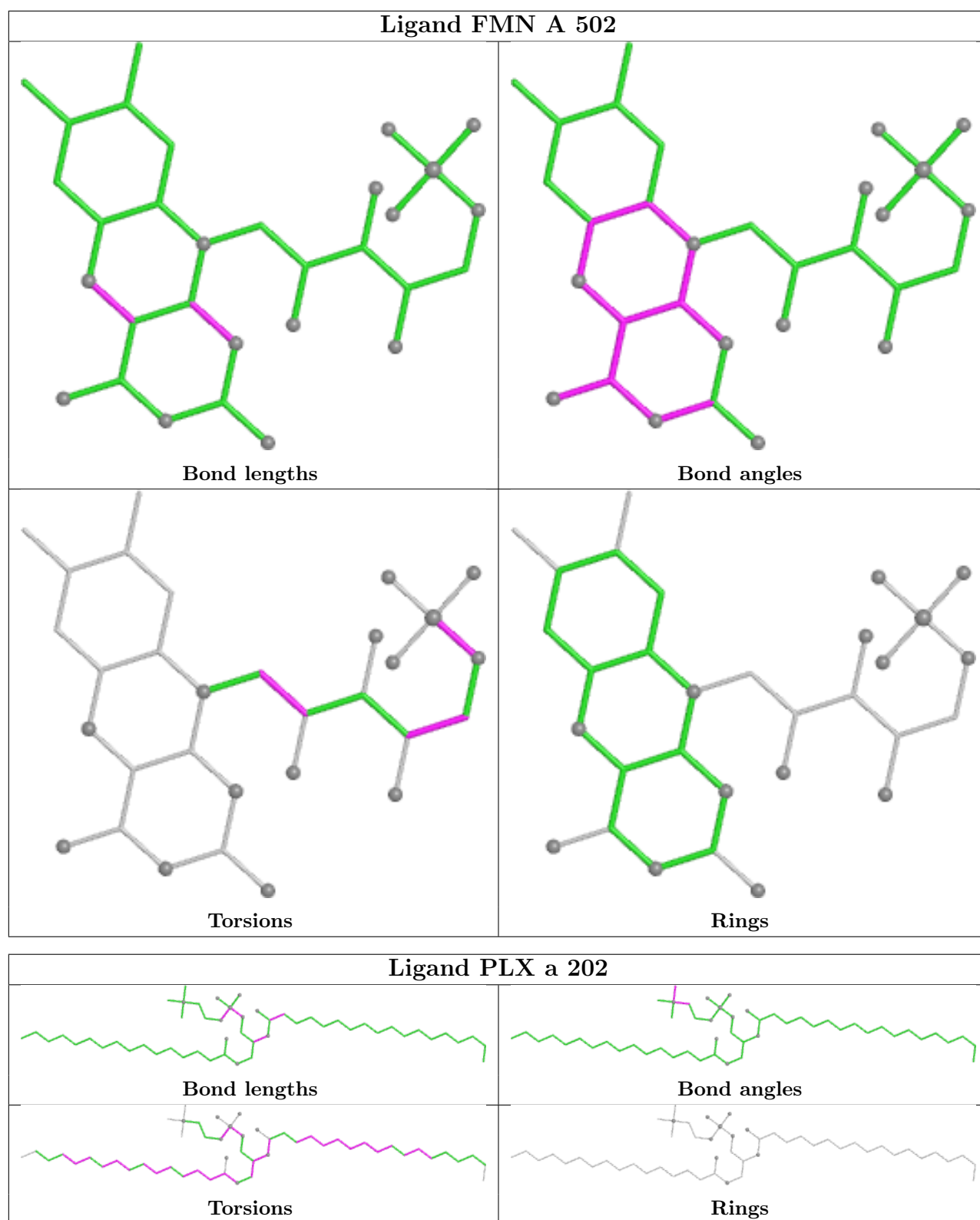


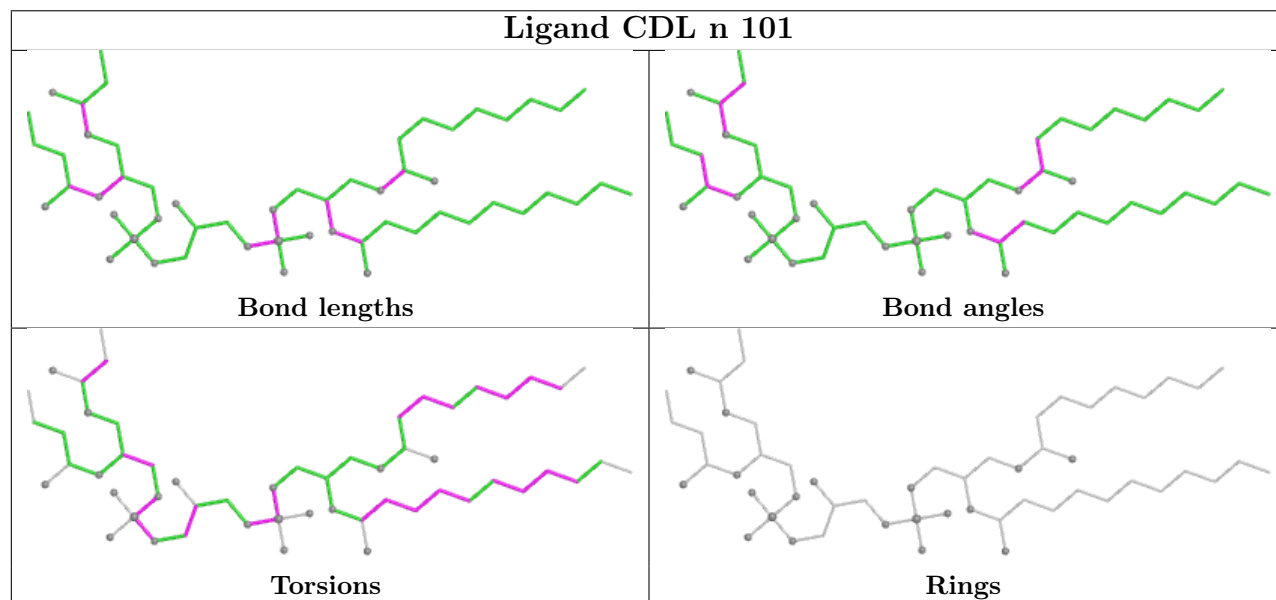
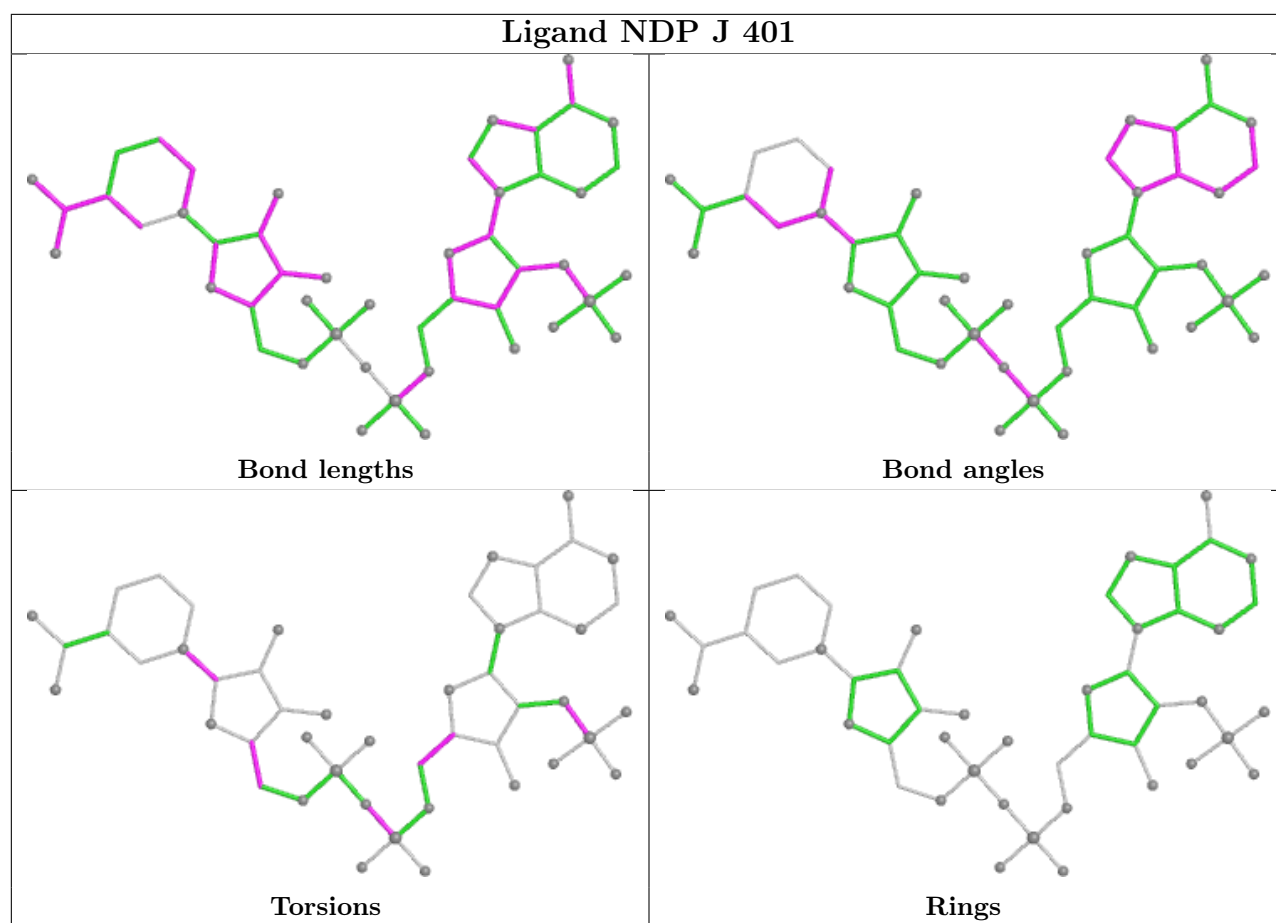


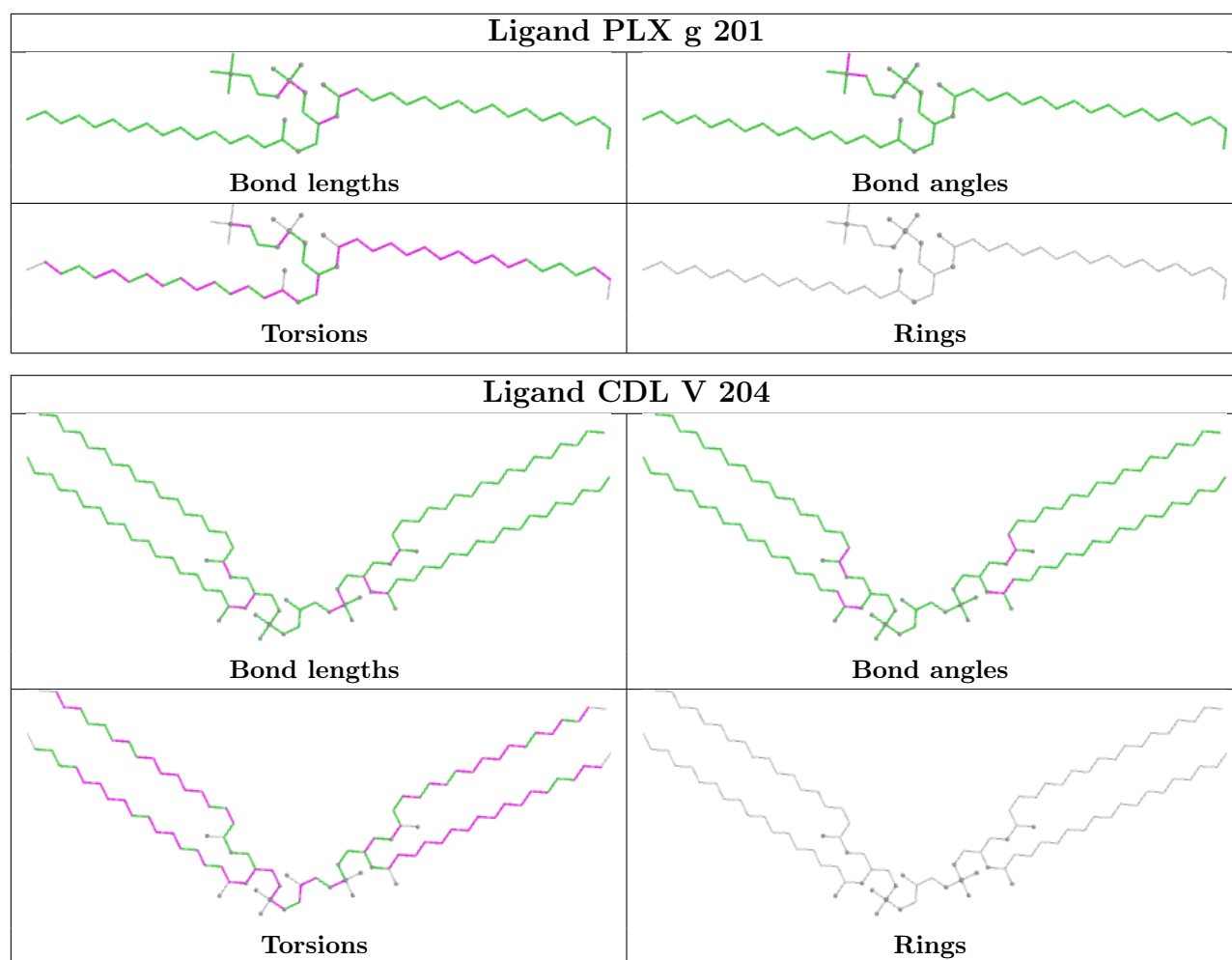


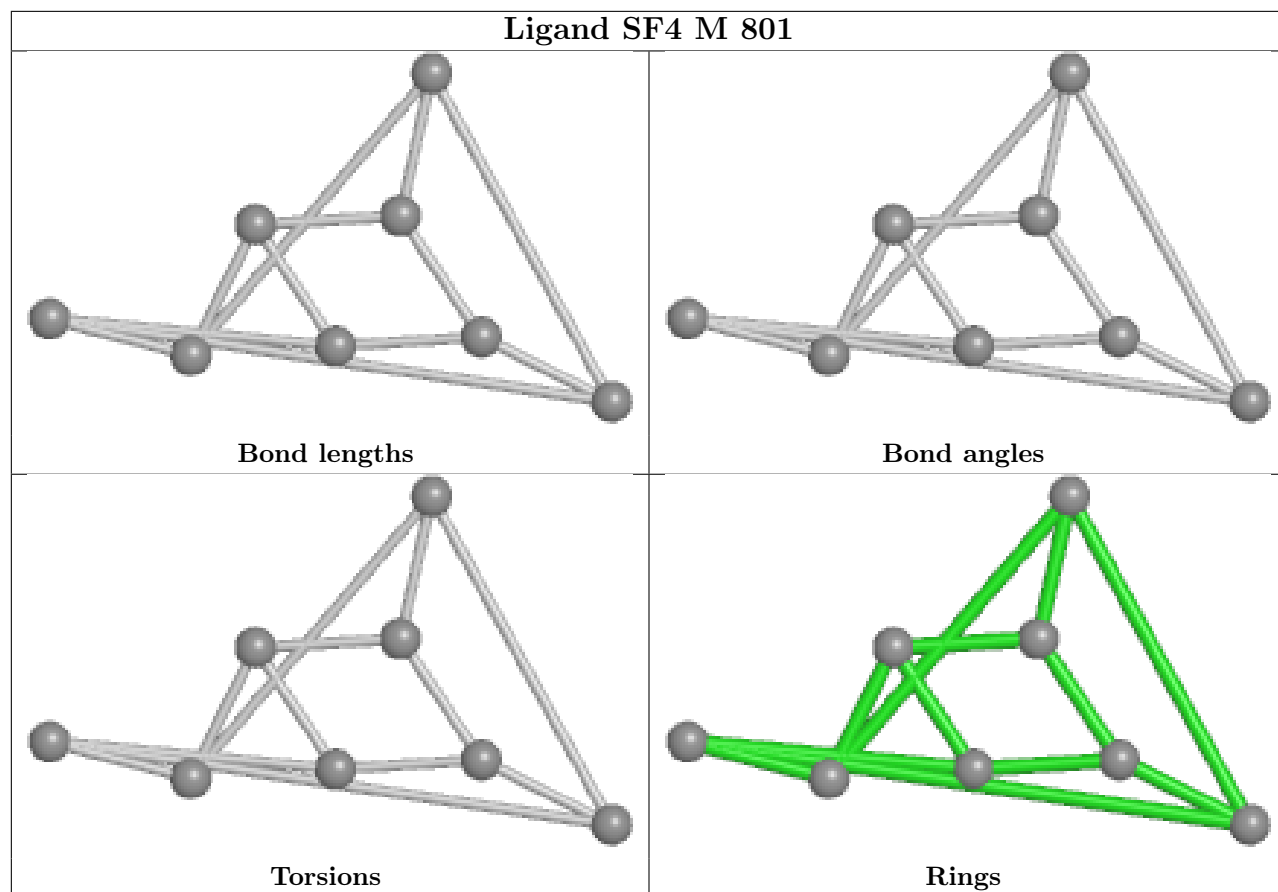


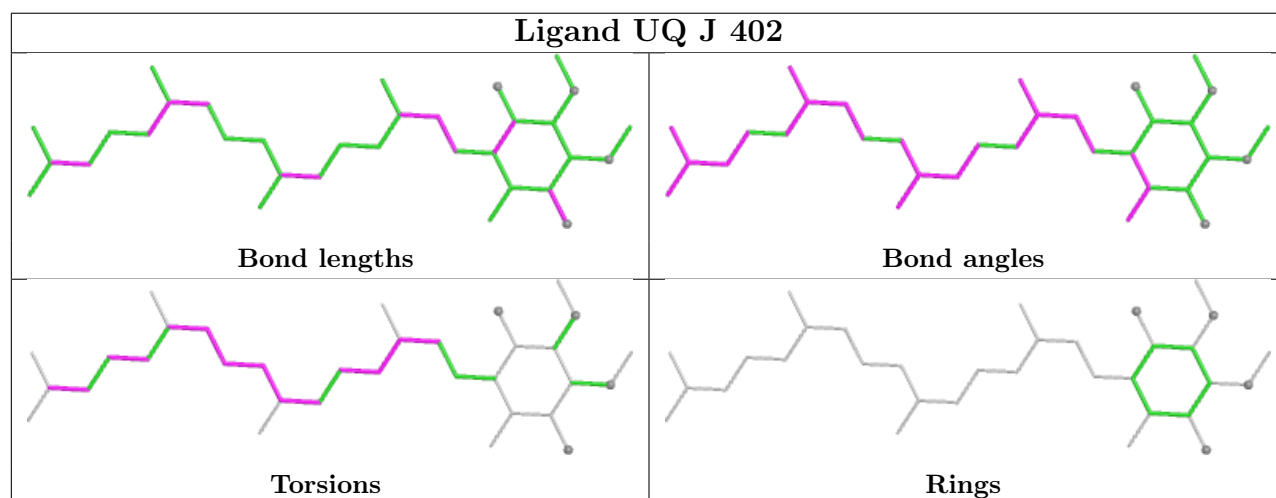
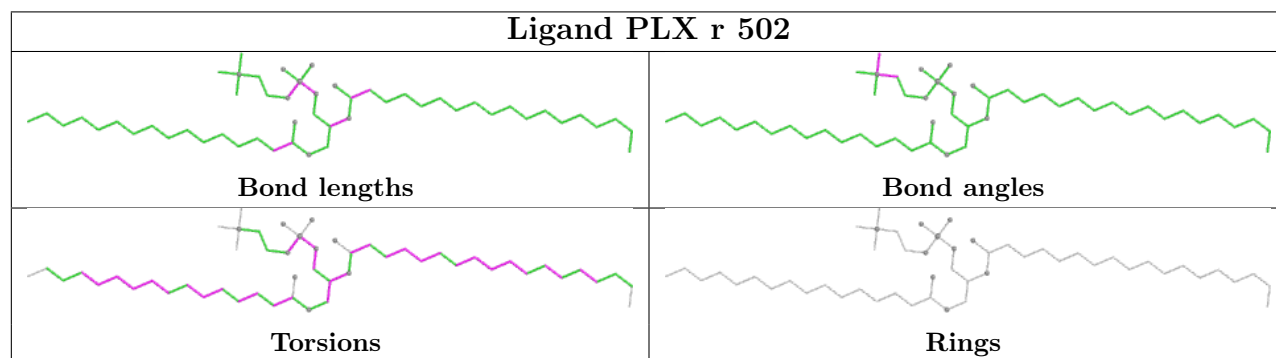
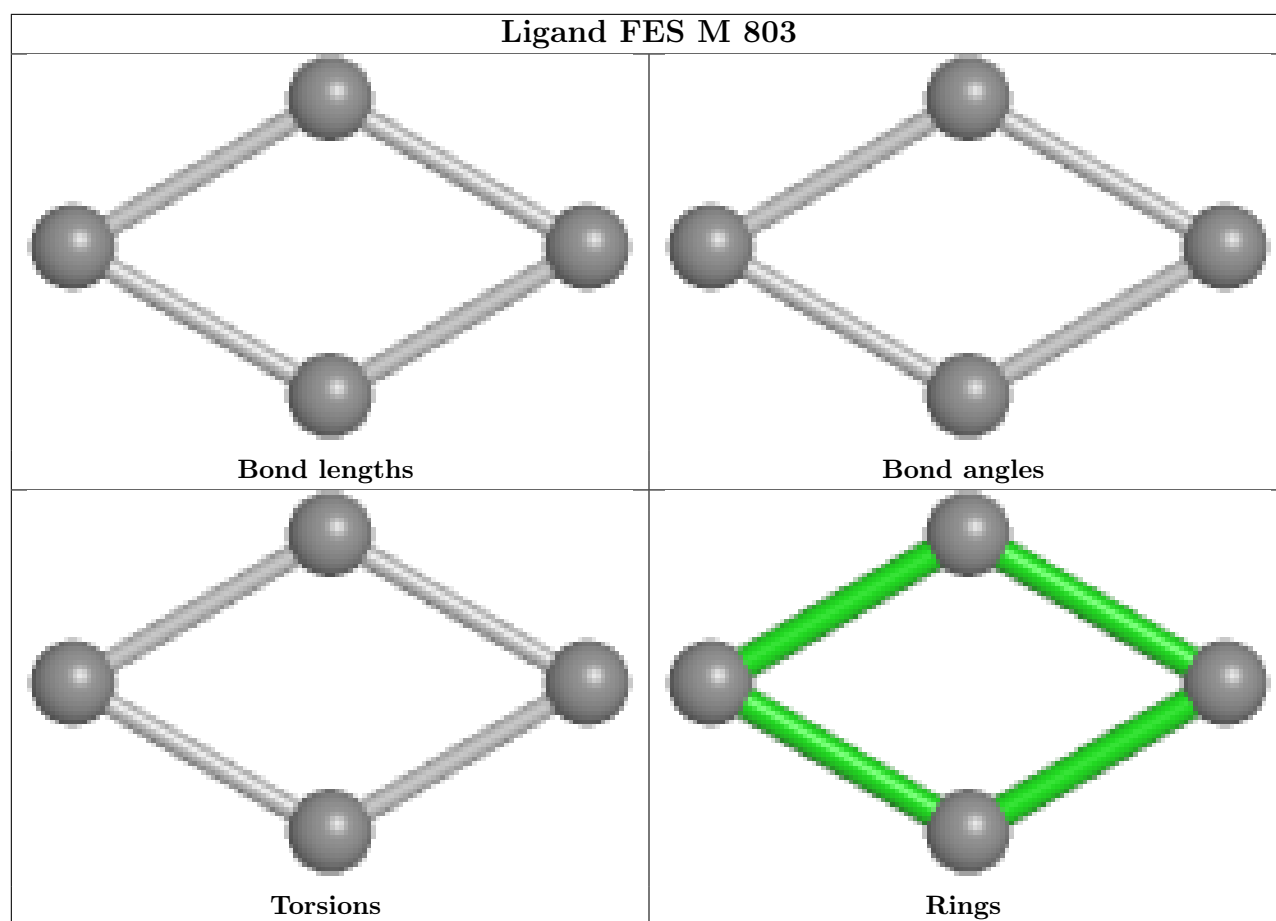


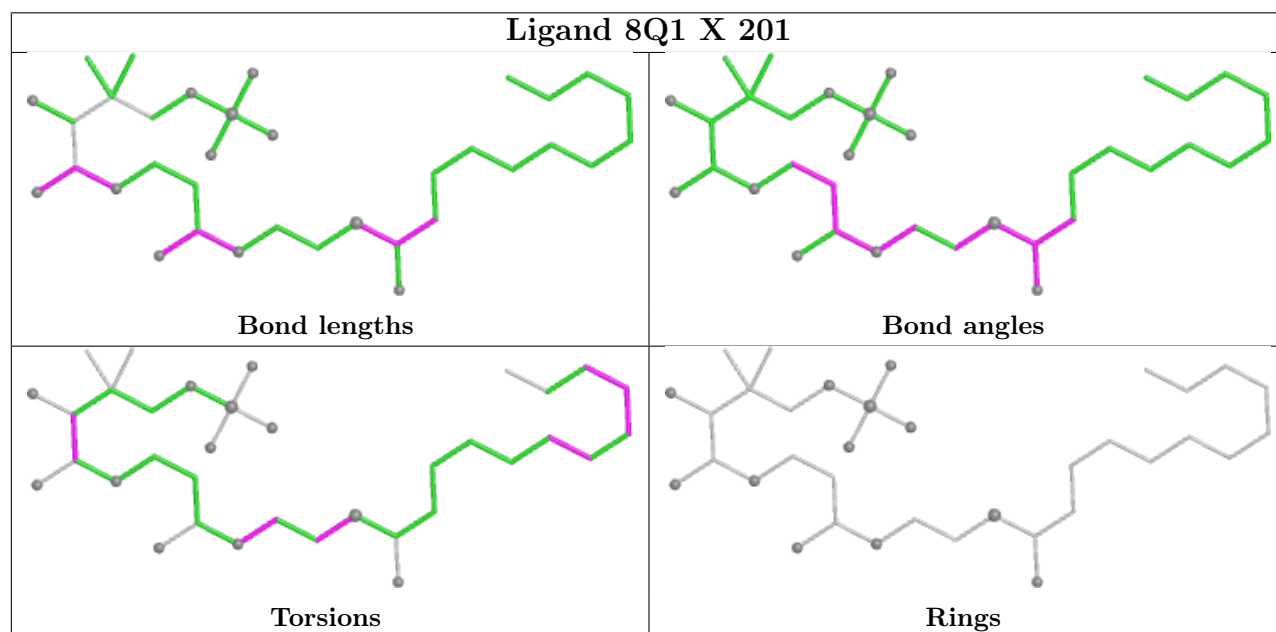
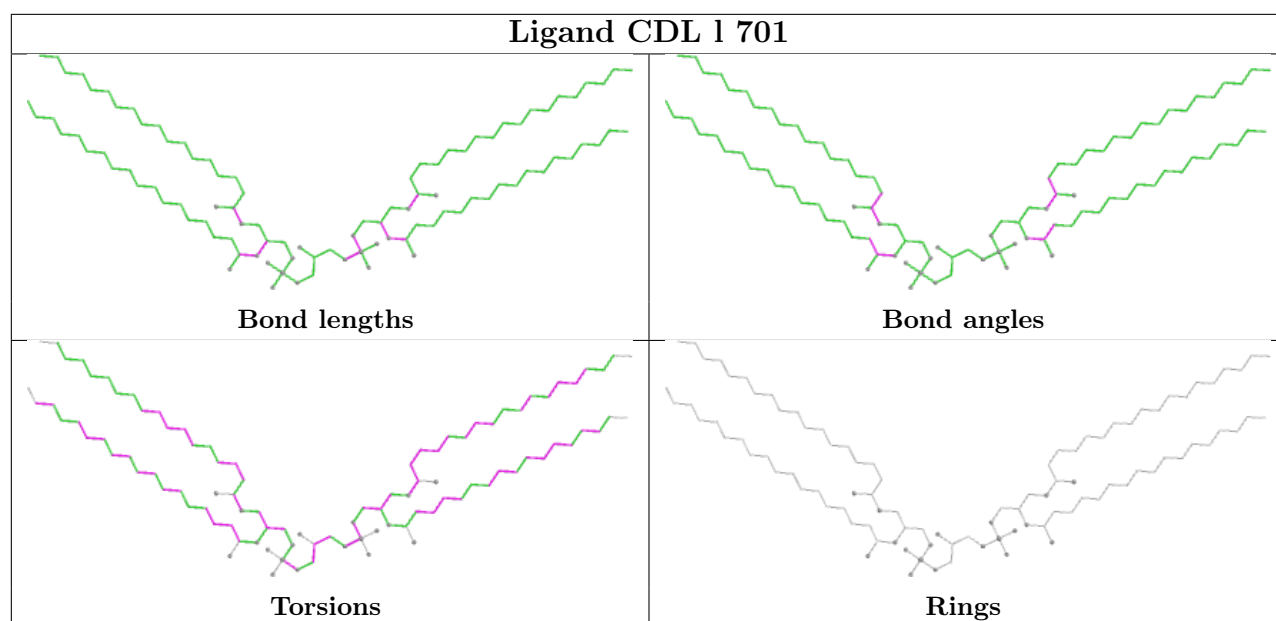


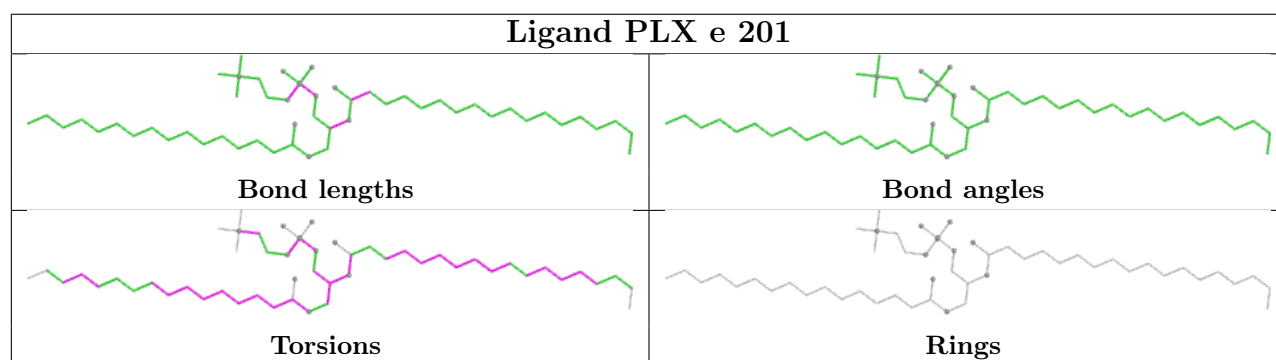
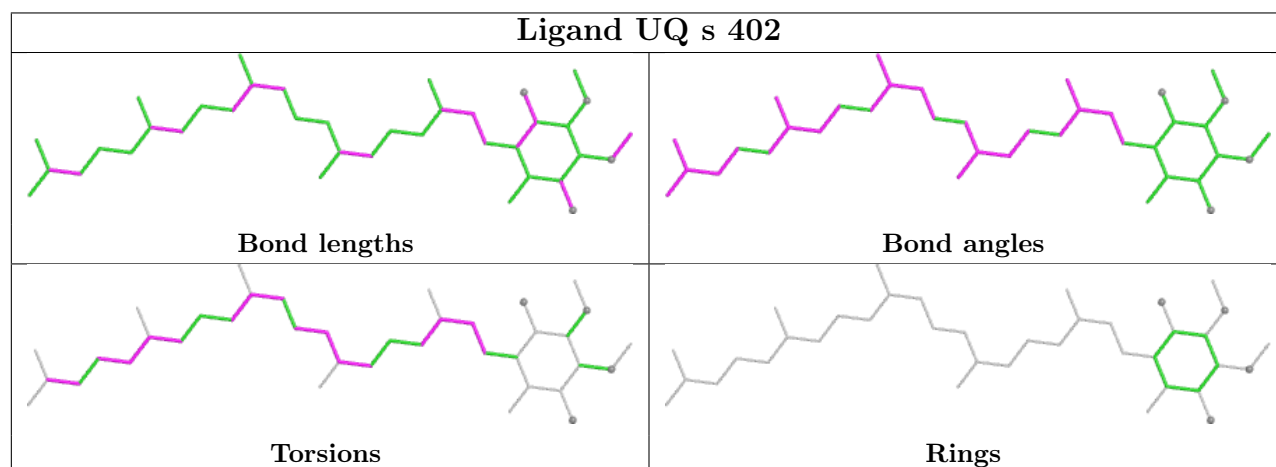
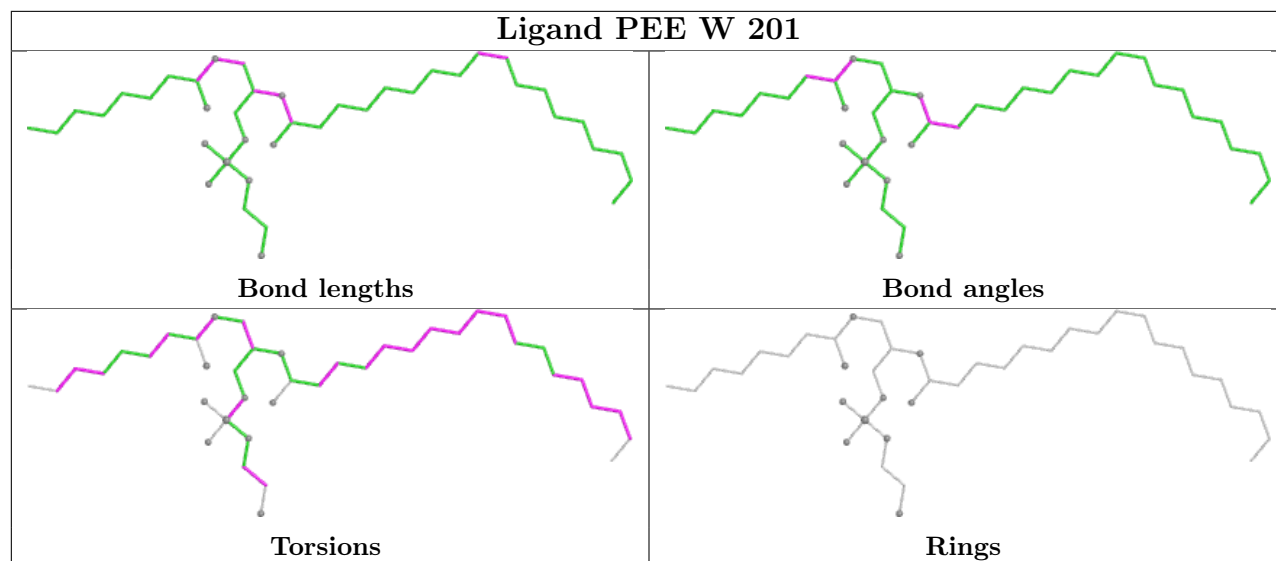


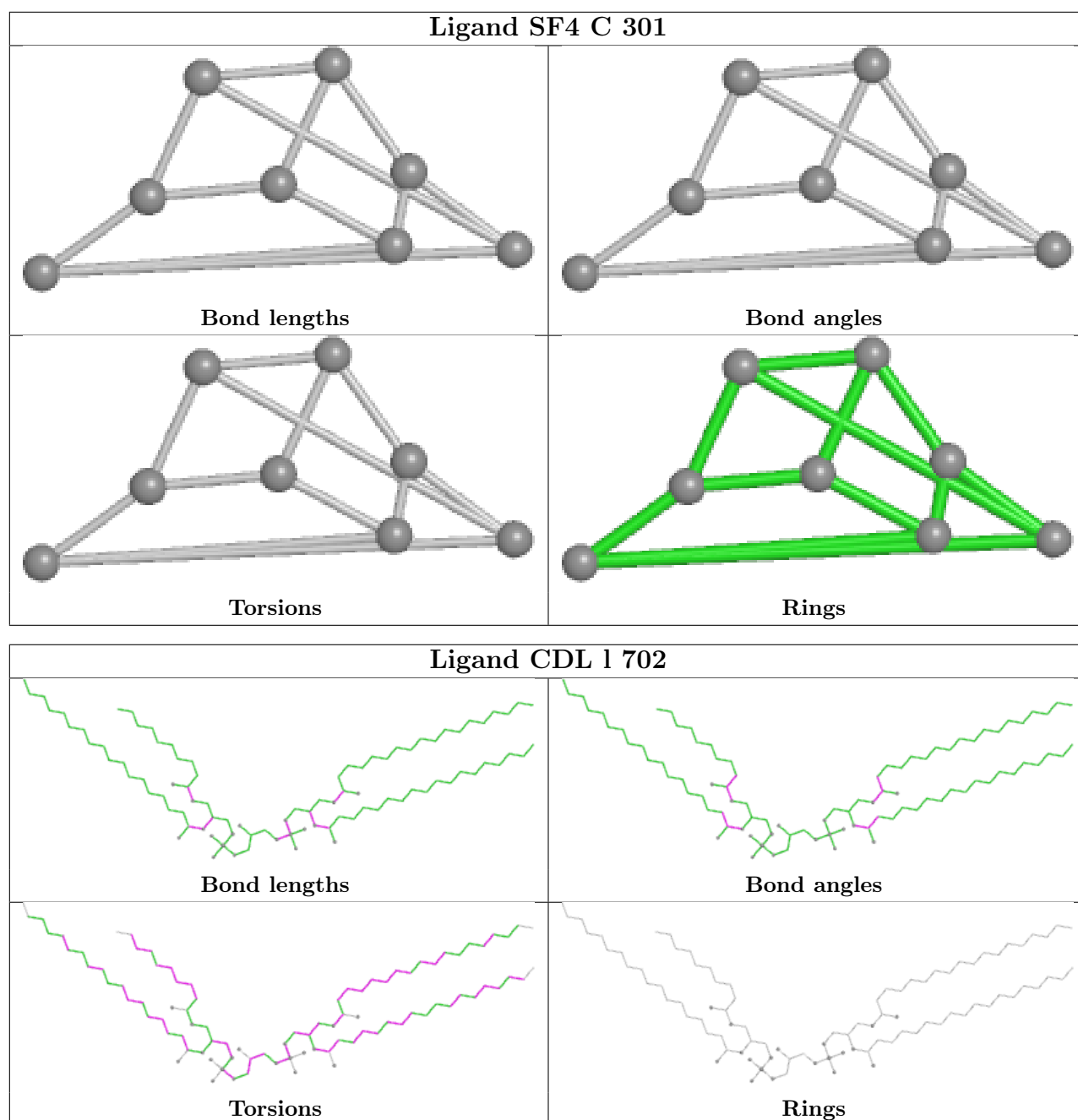












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

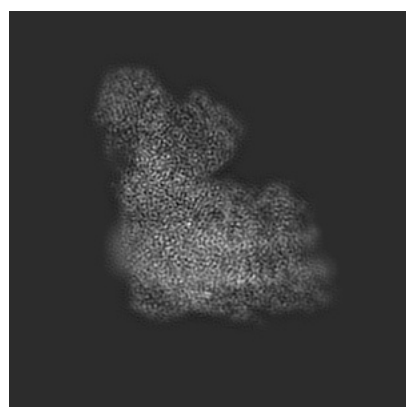
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32267. These allow visual inspection of the internal detail of the map and identification of artifacts.

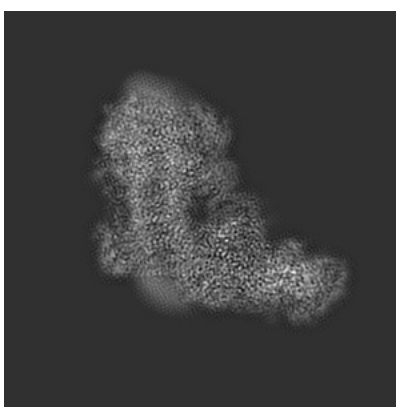
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

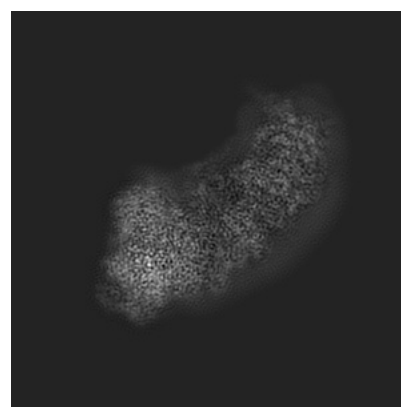
#### 6.1.1 Primary map



X



Y

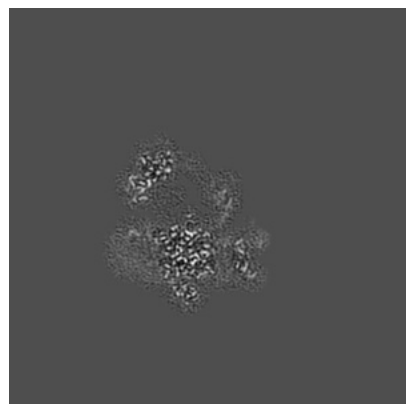


Z

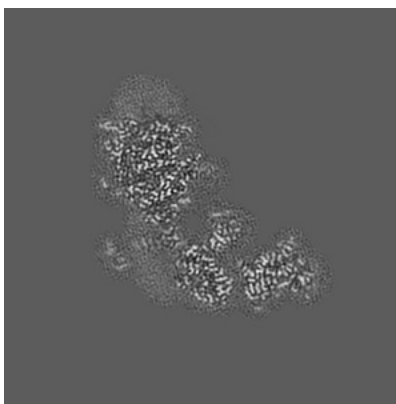
The images above show the map projected in three orthogonal directions.

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

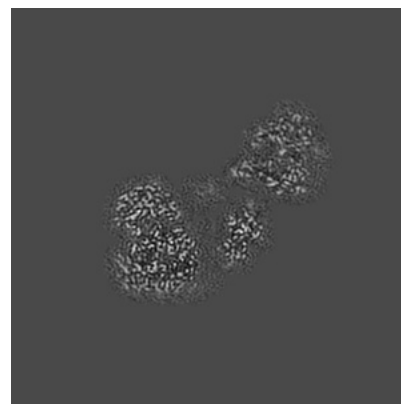
#### 6.2.1 Primary map



X Index: 155



Y Index: 155

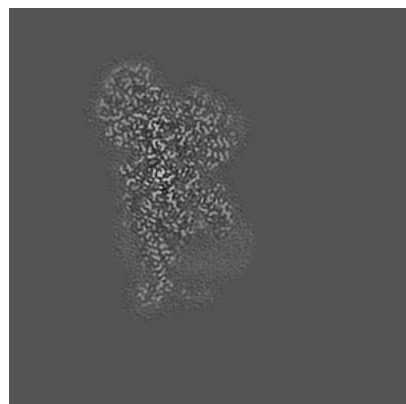


Z Index: 155

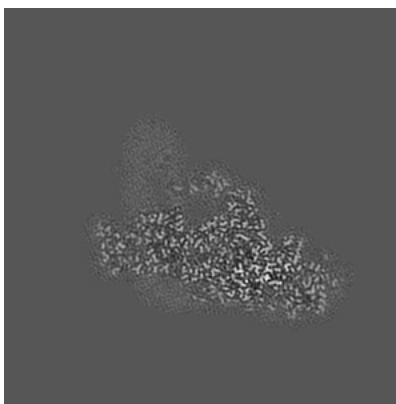
The images above show central slices of the map in three orthogonal directions.

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

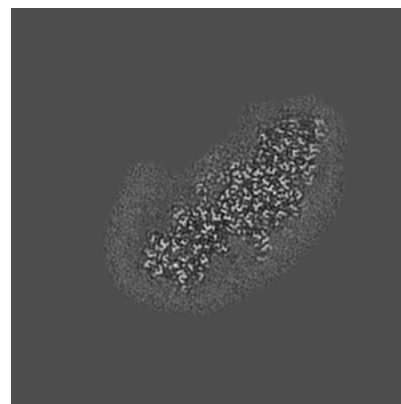
### 6.3.1 Primary map



X Index: 106



Y Index: 112

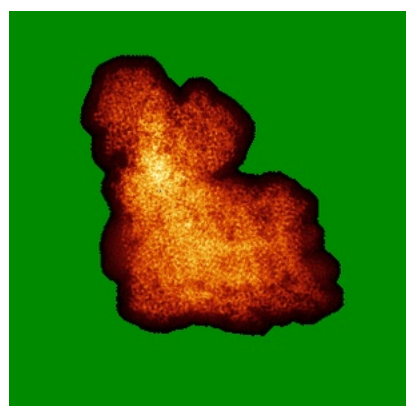


Z Index: 126

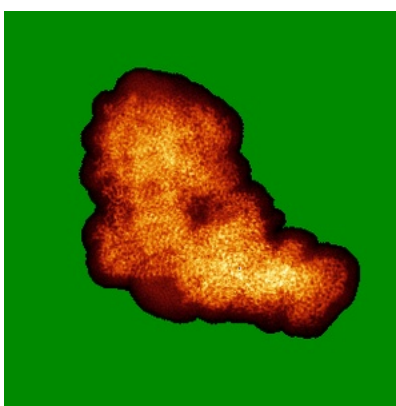
The images above show the largest variance slices of the map in three orthogonal directions.

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

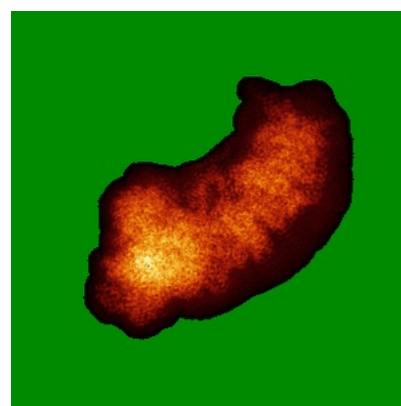
### 6.4.1 Primary map



X



Y

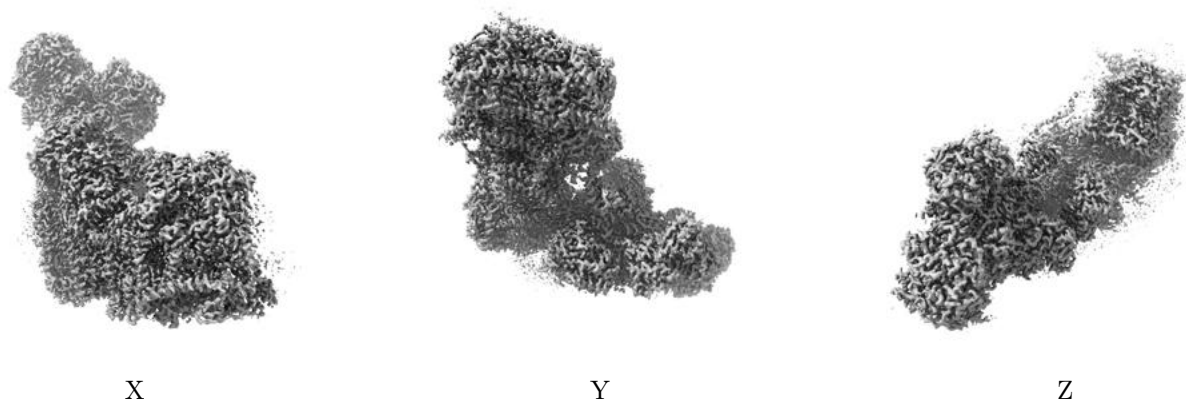


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

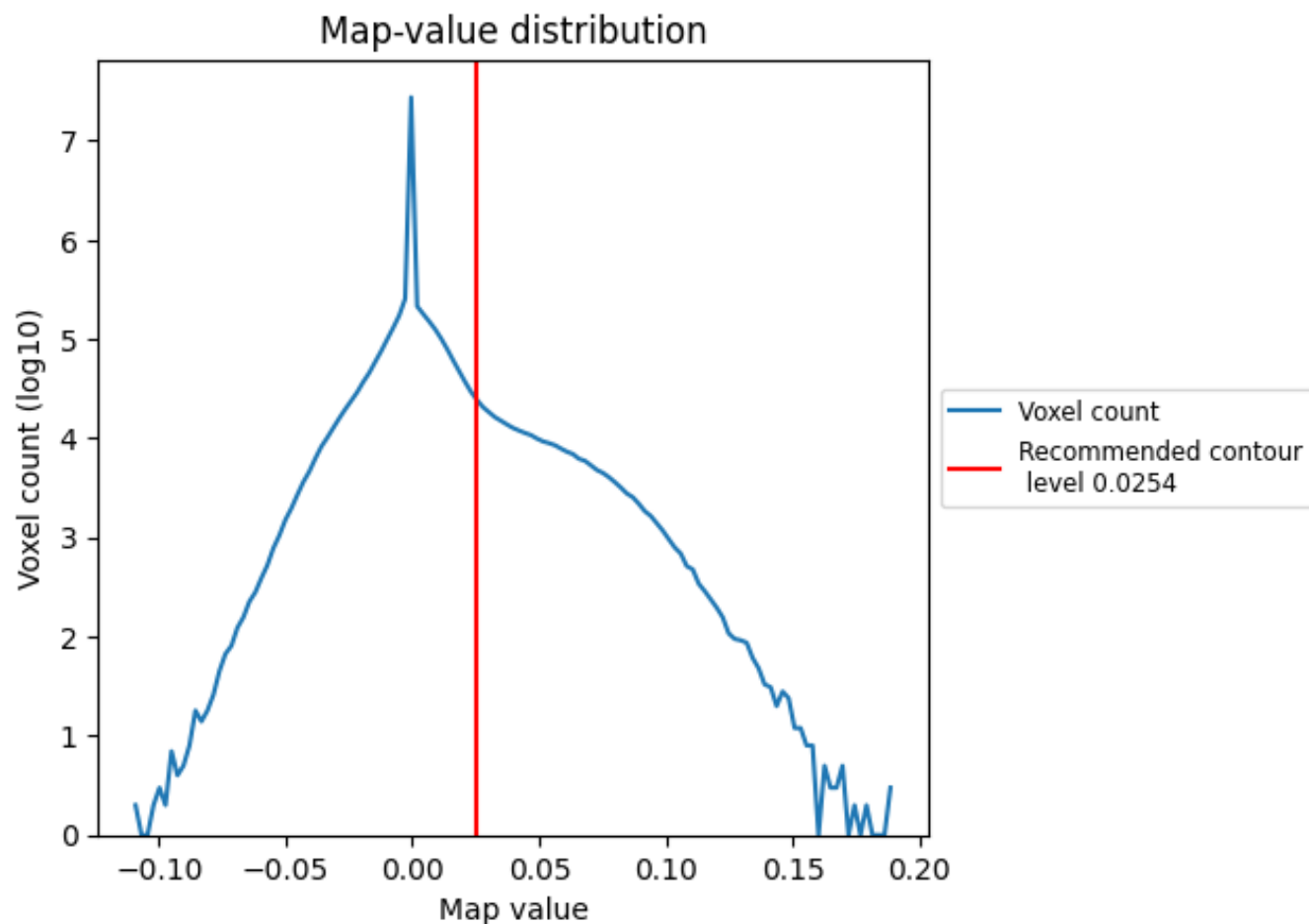
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

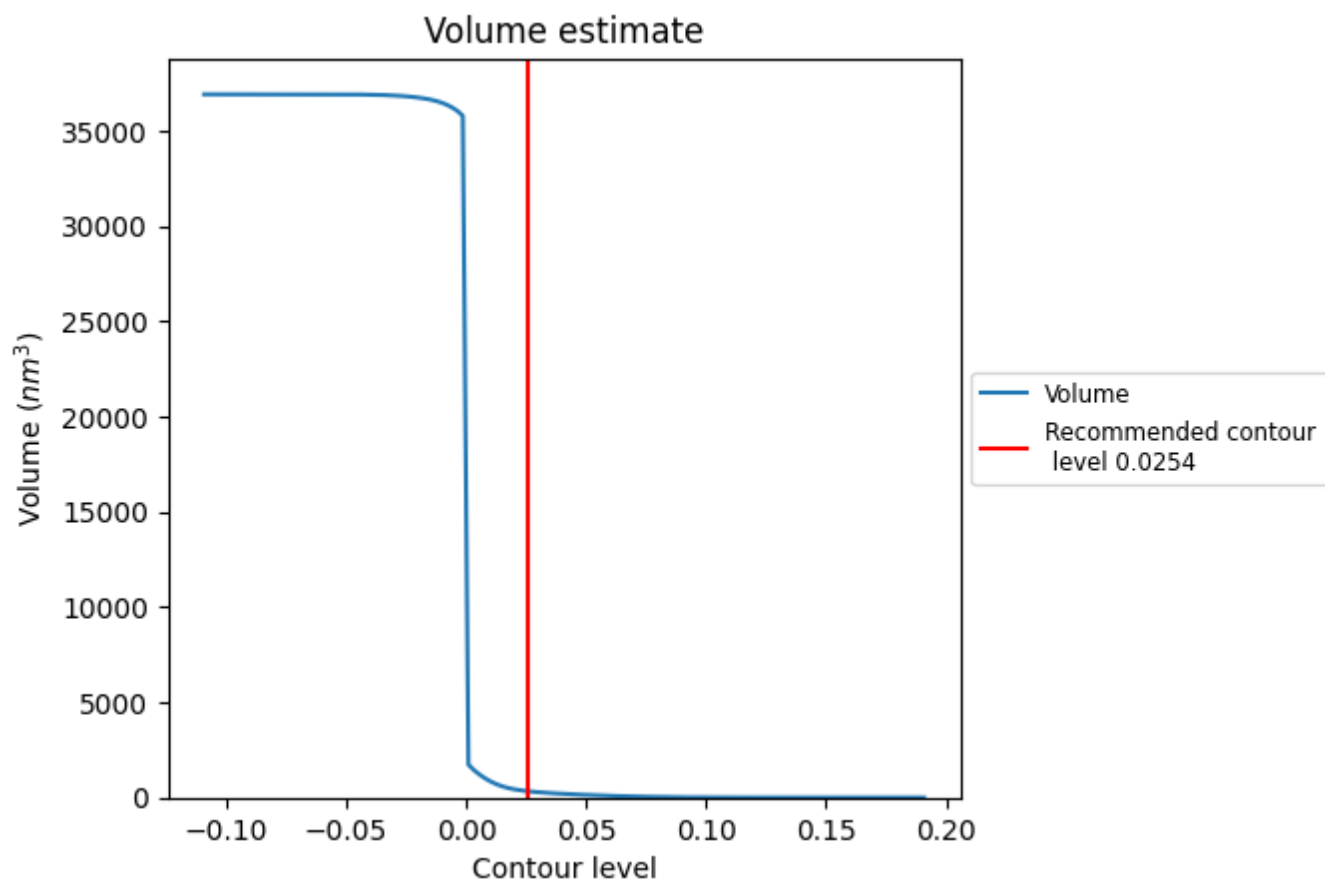
This section contains the results of statistical analysis of the map.

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



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

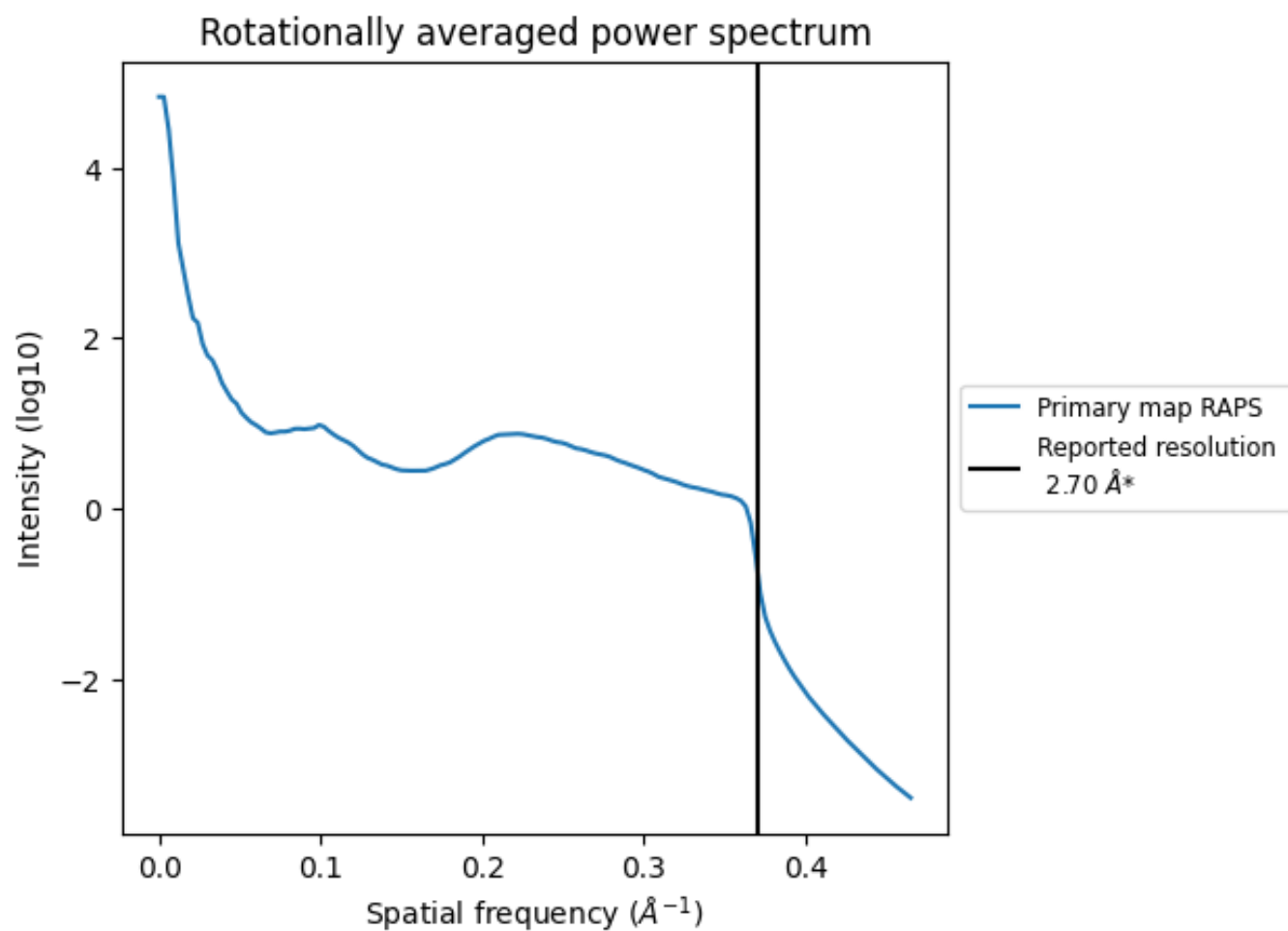
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm<sup>3</sup>; this corresponds to an approximate mass of 305 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 0.370 Å<sup>-1</sup>

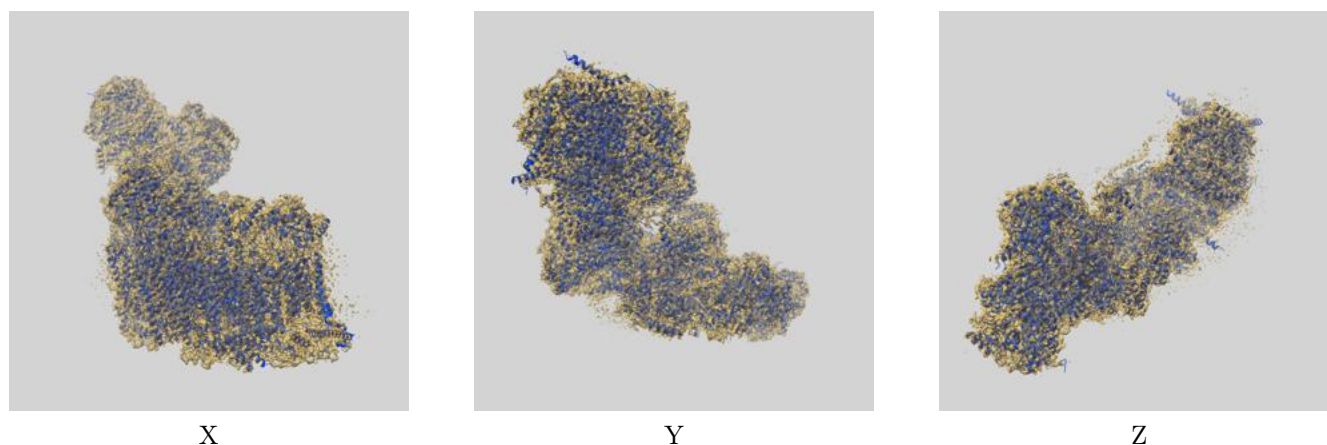
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

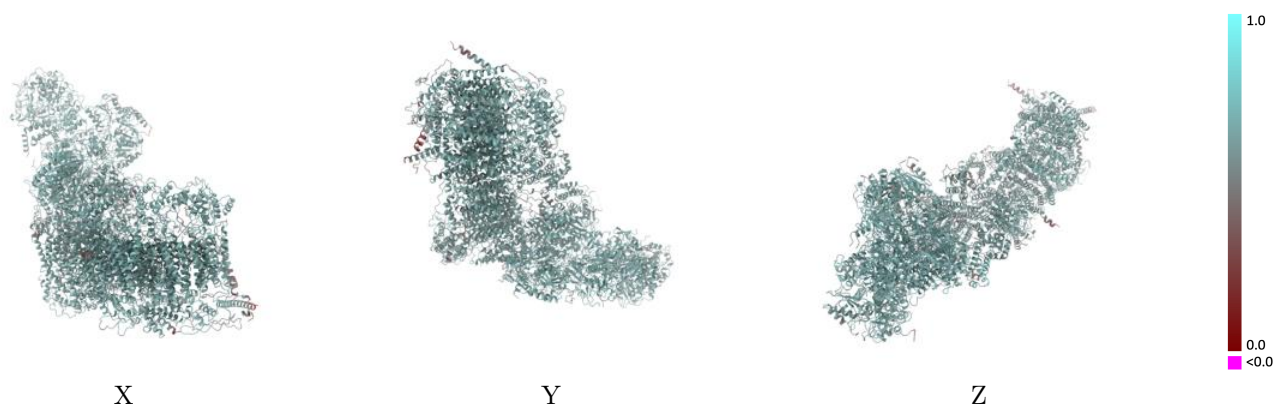
This section contains information regarding the fit between EMDB map EMD-32267 and PDB model 7W2Y. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



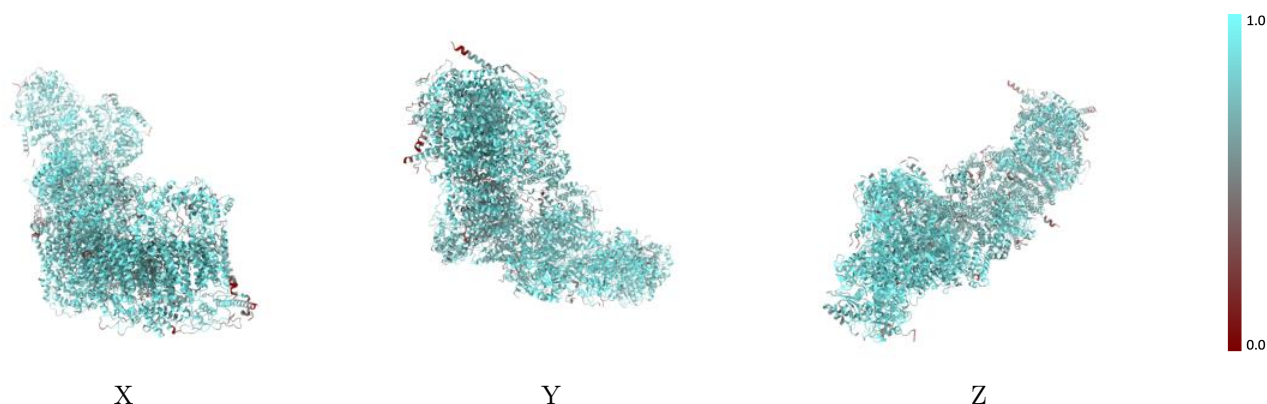
The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



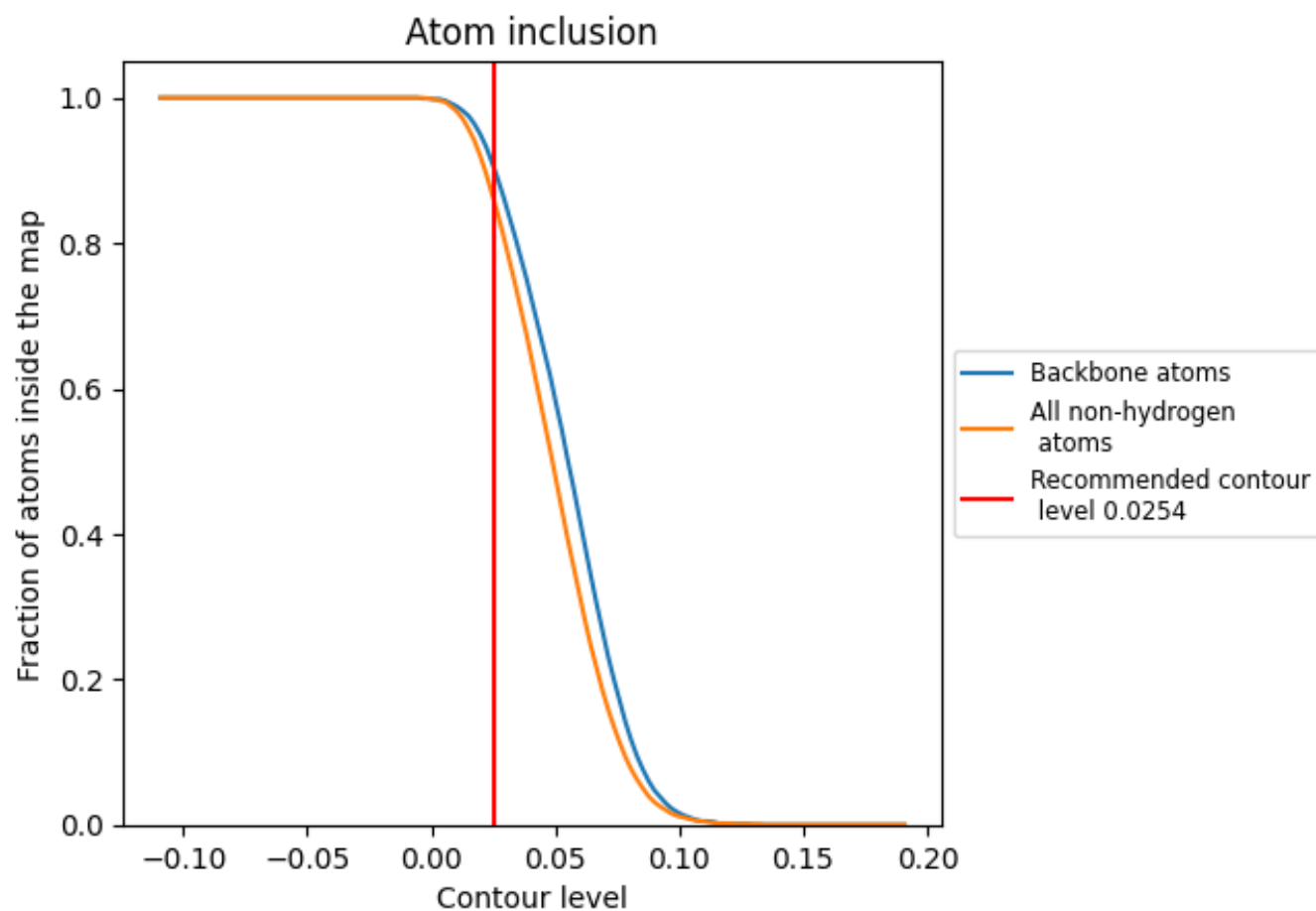
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0254).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (0.0254) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8580   |  0.6260   |
| A     |  0.8670   |  0.6190   |
| B     |  0.9370   |  0.6610   |
| C     |  0.9270   |  0.6570   |
| E     |  0.8800   |  0.6400   |
| F     |  0.7930   |  0.5900   |
| G     |  0.6270   |  0.5350   |
| H     |  0.8740   |  0.6320   |
| I     |  0.7340   |  0.5900   |
| J     |  0.8890   |  0.6350   |
| K     |  0.7800   |  0.5930   |
| L     |  0.8880   |  0.6480   |
| M     |  0.9090   |  0.6420   |
| N     |  0.7340   |  0.6060   |
| O     |  0.8300  |  0.6090  |
| P     |  0.9550 |  0.6680 |
| Q     |  0.9510 |  0.6610 |
| S     |  0.9020 |  0.6380 |
| T     |  0.8090 |  0.6220 |
| U     |  0.8280 |  0.6060 |
| V     |  0.6860 |  0.5850 |
| W     |  0.8310 |  0.6140 |
| X     |  0.7850 |  0.6040 |
| Y     |  0.7190 |  0.5620 |
| Z     |  0.6460 |  0.5530 |
| a     |  0.8400 |  0.6290 |
| b     |  0.7830 |  0.5940 |
| c     |  0.8370 |  0.6170 |
| d     |  0.7840 |  0.6000 |
| e     |  0.7780 |  0.5960 |
| f     |  0.6570 |  0.5620 |
| g     |  0.8640 |  0.6260 |
| h     |  0.8560 |  0.6130 |
| i     |  0.9280 |  0.6510 |
| j     |  0.8500 |  0.6340 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| k     |  0.9300 |  0.6460 |
| l     |  0.8630 |  0.6290 |
| m     |  0.8110 |  0.6060 |
| n     |  0.6920 |  0.5690 |
| o     |  0.8380 |  0.6270 |
| p     |  0.8500 |  0.6220 |
| r     |  0.9110 |  0.6410 |
| s     |  0.9180 |  0.6480 |
| u     |  0.8520 |  0.6170 |
| v     |  0.7270 |  0.5640 |
| w     |  0.8580 |  0.6220 |