



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:48 AM UTC

PDB ID : 7V2R / pdb\_00007v2r  
EMDB ID : EMD-31647  
Title : Active state complex I from Q1-NADH dataset  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-08-09  
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

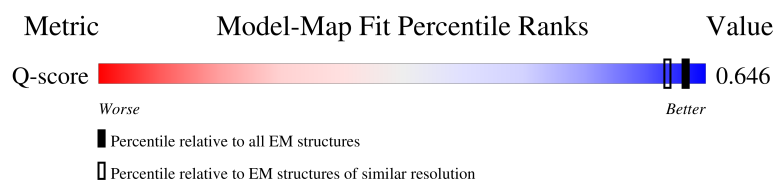
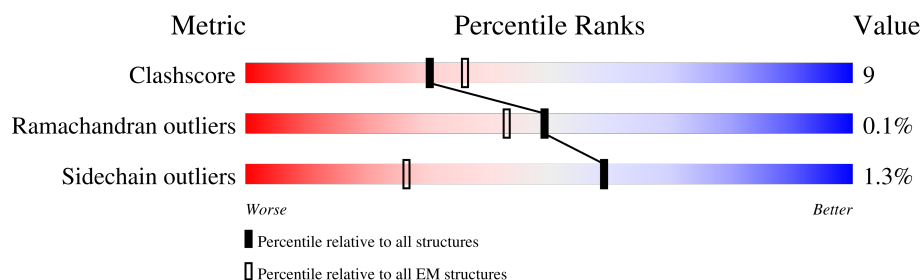
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8728 ( 2.10 - 3.10 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 433    | <br>76% 23% .    |
| 2   | B     | 176    | <br>86% 13% .    |
| 3   | C     | 156    | <br>87% 13% .    |
| 4   | E     | 115    | <br>82% 17% .    |

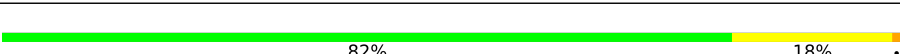
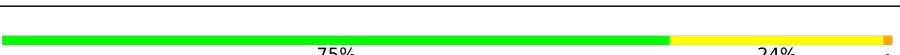
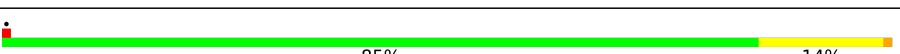
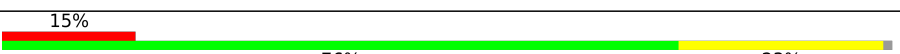
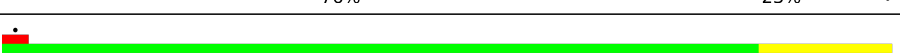
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | F     | 86     |                  |
| 6   | G     | 88     |                  |
| 6   | X     | 88     |                  |
| 7   | H     | 112    |                  |
| 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    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 45  | SF4  | A     | 501 | -         | -        | X       | -                |
| 45  | SF4  | M     | 802 | -         | -        | X       | -                |
| 54  | FES  | O     | 301 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68260 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, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | G     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 693   | 447 | 102 | 139 | 5 |         |       |
| 6   | X     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 703   | 453 | 104 | 141 | 5 |         |       |

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

| 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     |
|     |       |          | 2751  | 1783 | 481 | 478 | 9 |         |       |

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 752 | 200 | 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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| 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     |
|     |       |          | 4816  | 3193 | 746 | 826 | 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     |
|     |       |          | 1292  | 863 | 188 | 228 | 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 |         |       |

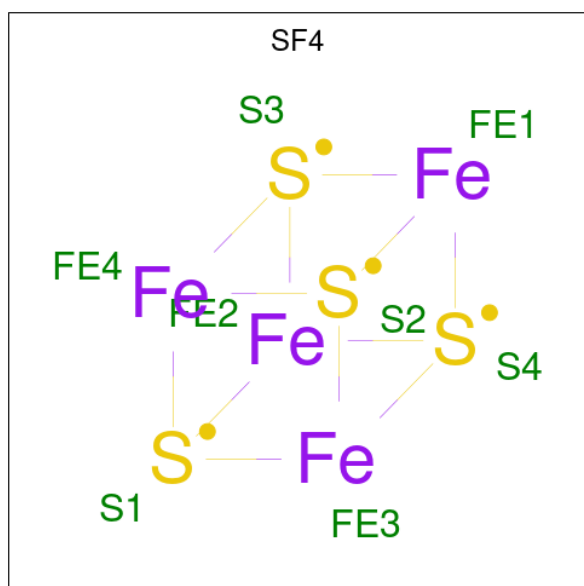
There is a discrepancy between the modelled and reference sequences:

| 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.

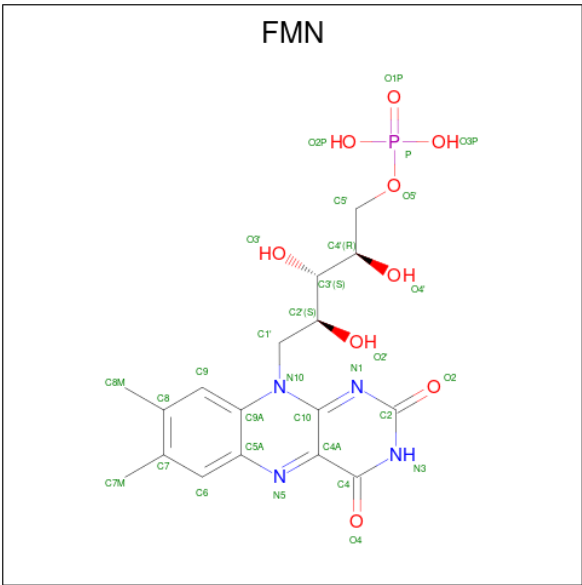
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | w     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2582  | 1643 | 438 | 491 | 10 |         | 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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



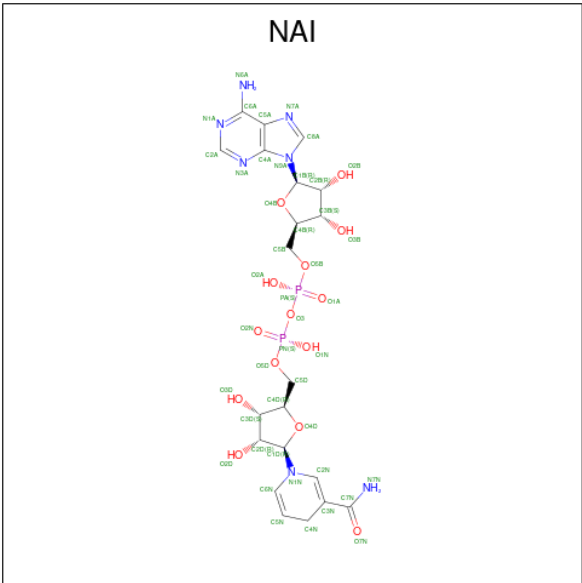
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 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:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



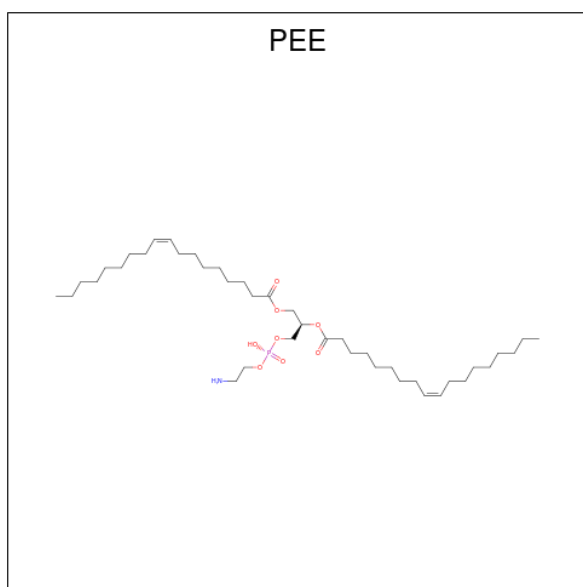
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- 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).



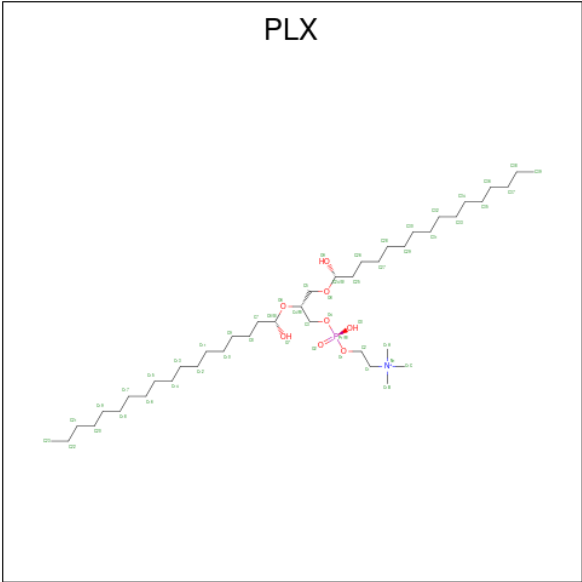
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 47  | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |

- 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).



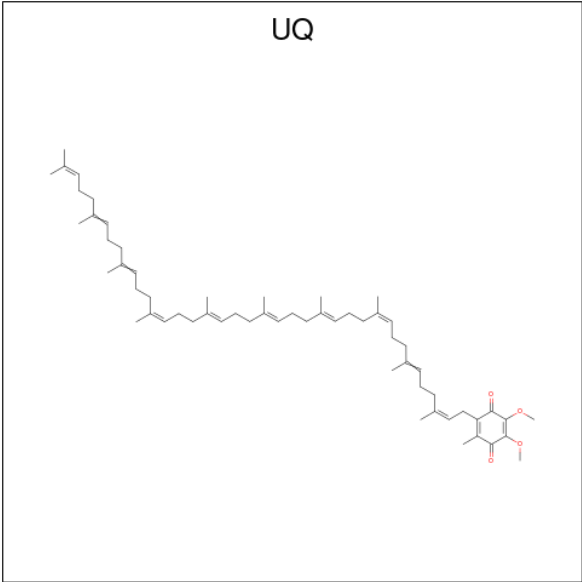
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | Q     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | V     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 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  | s     | 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).



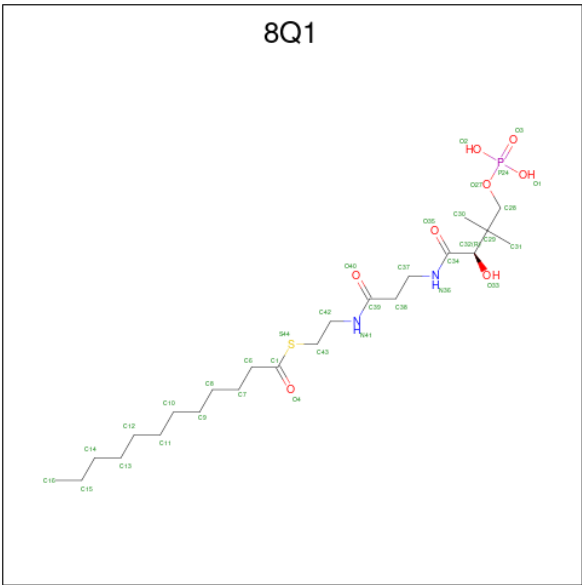
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 49  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | J     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 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 Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 50  | C     | 1        | Total | C  | O | 0       |
|     |       |          | 38    | 34 | 4 |         |
| 50  | J     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 29 | 4 |         |

- Molecule 51 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}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 |         |

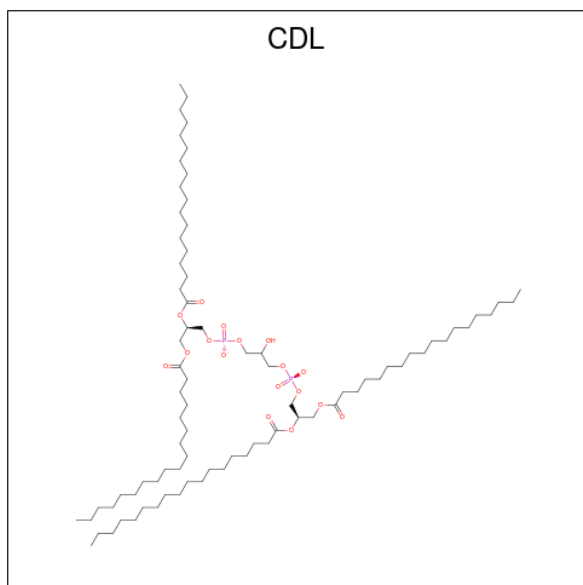
Continued on next page...



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

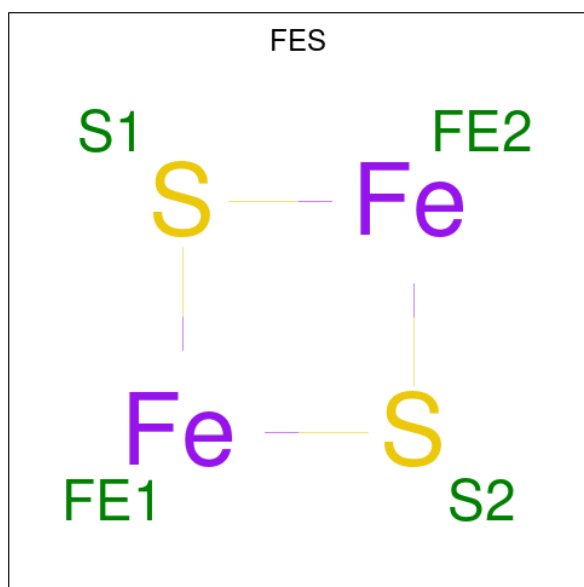
- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 52  | I     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 32 | 17 | 2 |         |
| 52  | J     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 89    | 70 | 17 | 2 |         |
| 52  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 94    | 75 | 17 | 2 |         |
| 52  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 52  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 52  | k     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 94    | 75 | 17 | 2 |         |
| 52  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 99    | 80 | 17 | 2 |         |
| 52  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 52  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 52  | u     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 55    | 36 | 17 | 2 |         |

- # NDP

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

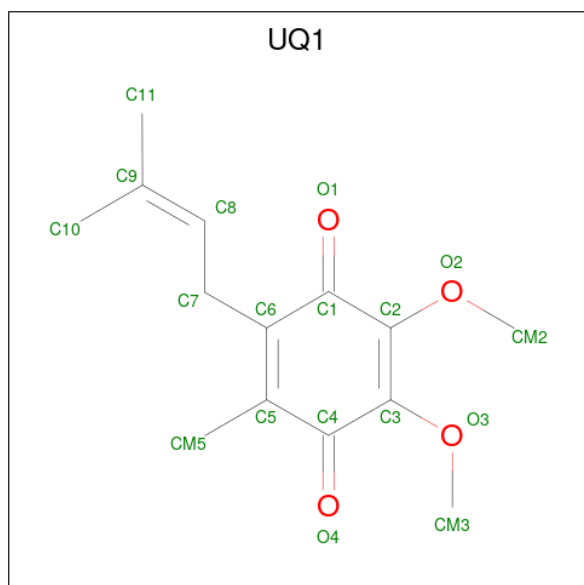


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 54  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 54  | O     | 1        | Total | Fe | S | 0       |
|     |       |          | 4  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

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

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

- Molecule 56 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C<sub>14</sub>H<sub>18</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).

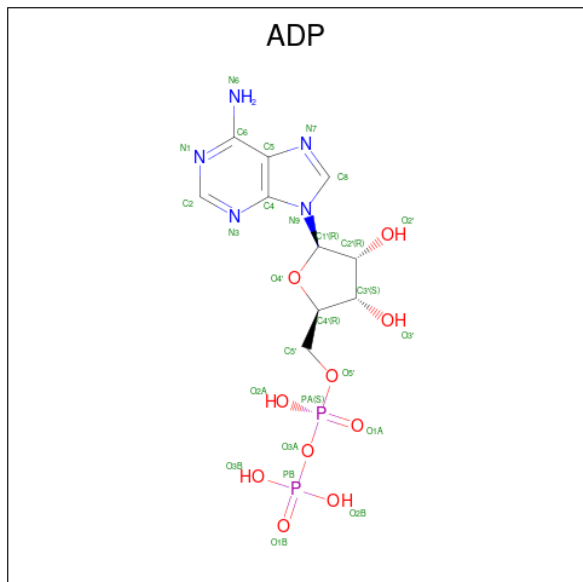


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 56  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 14 | 4 |         |
| 56  | Q     | 1        | Total | C  | O | 0       |
|     |       |          | 18    | 14 | 4 |         |

- 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).

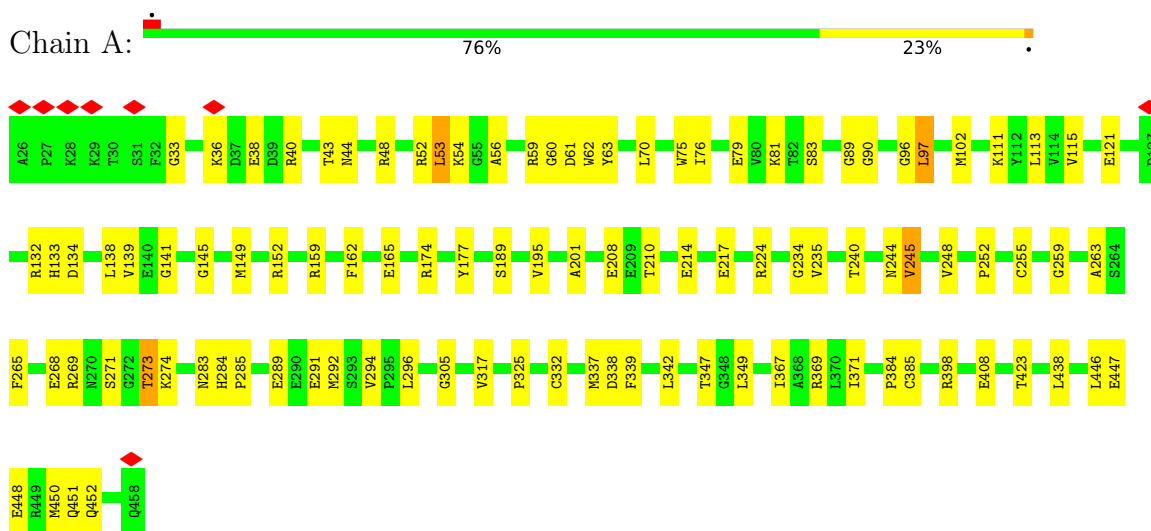


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
|     |       |          | Total | C  | N | O  | P |         |
| 58  | w     | 1        | 27    | 10 | 5 | 10 | 2 | 0       |

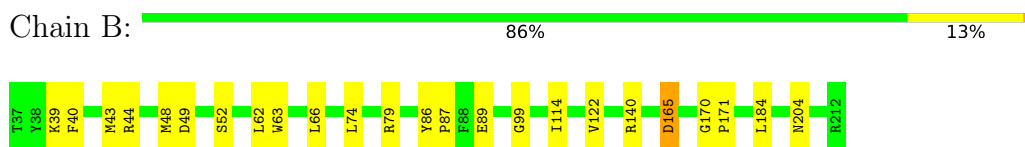
### 3 Residue-property plots

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.

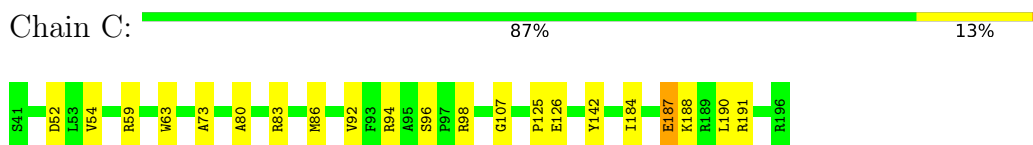
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



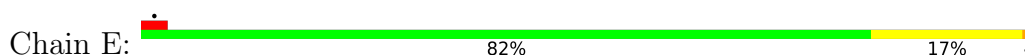
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

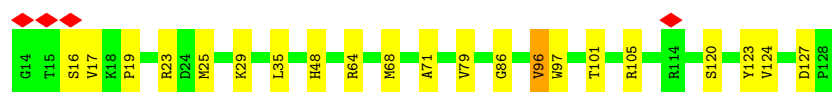


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

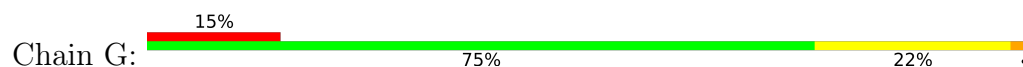




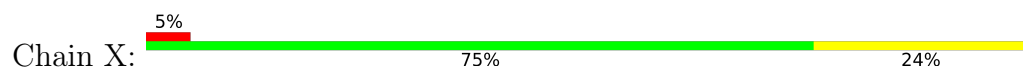
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



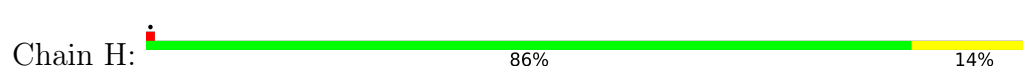
- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 6: Acyl carrier protein, mitochondrial



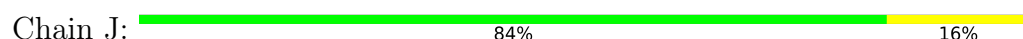
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

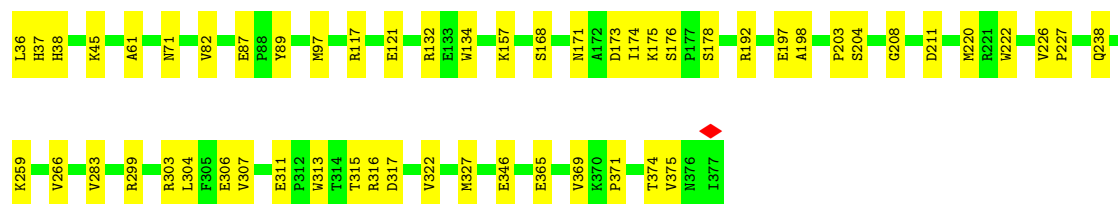


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

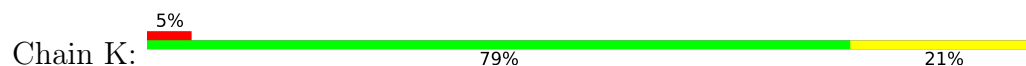


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

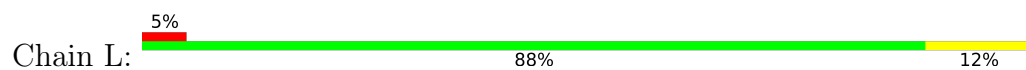




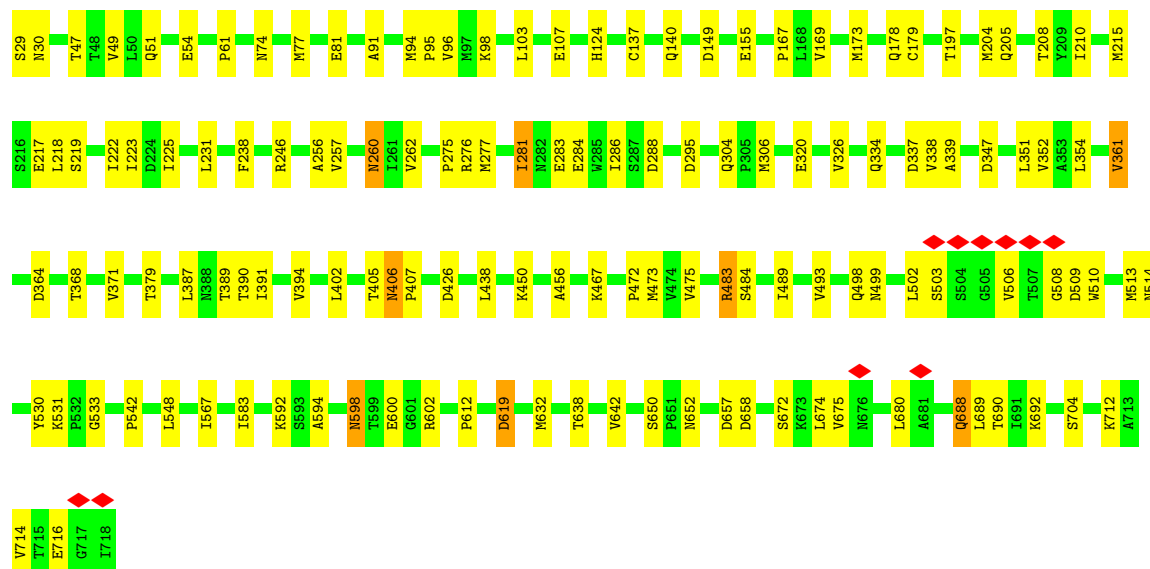
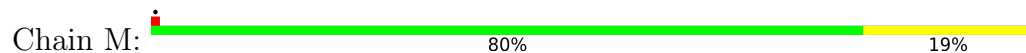
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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



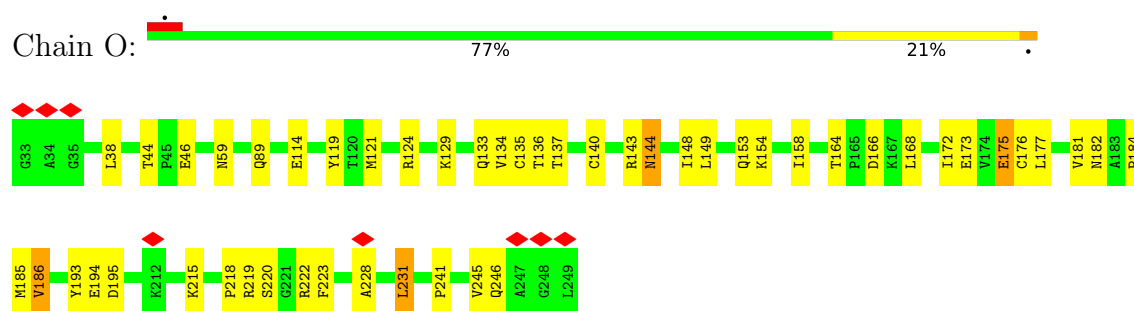
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



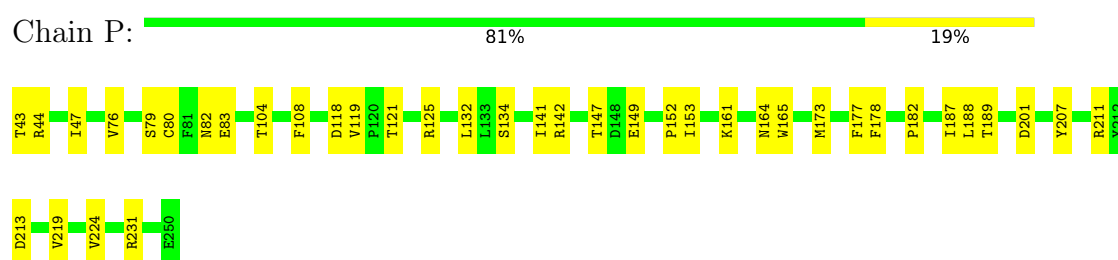
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



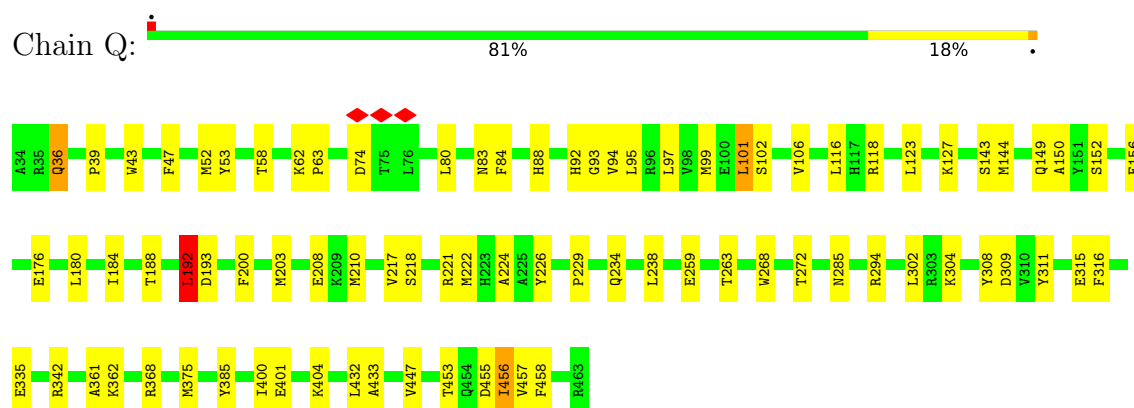
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



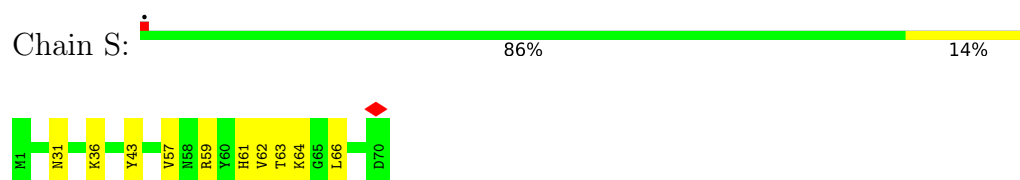
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



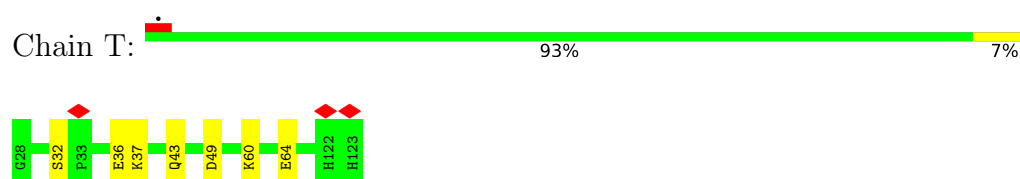
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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



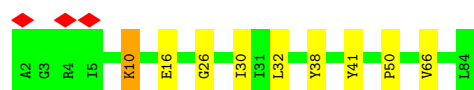
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial





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

Chain U:  89% 10%



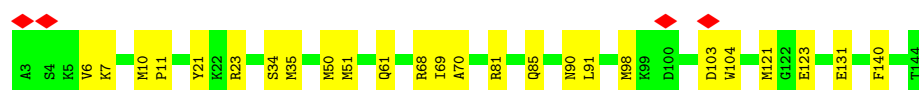
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  83% 17%



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W:  82% 18%



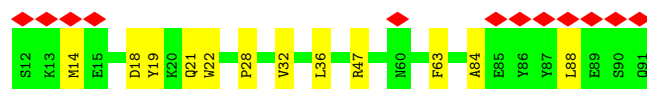
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:  12% 73% 27%



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

Chain Z:  15% 85% 15%



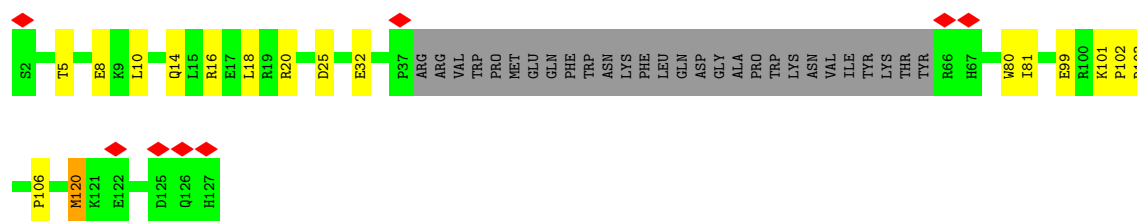
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:  87% 13%

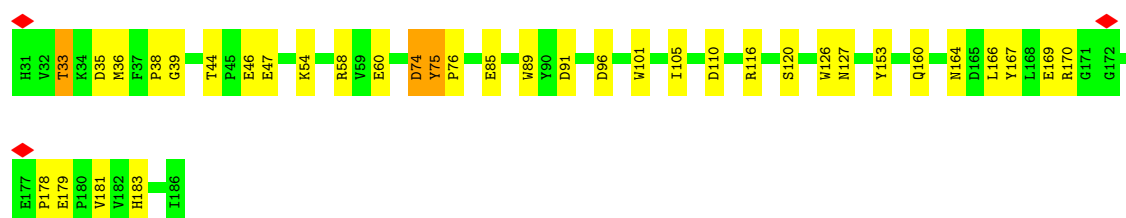
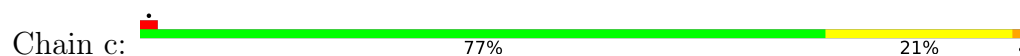


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

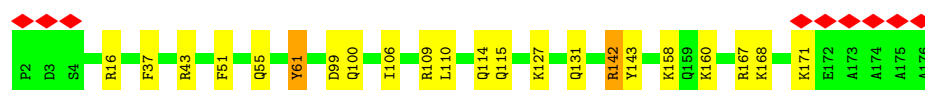
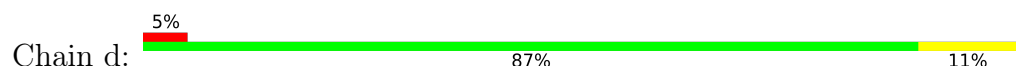
Chain b:  6% 64% 13% 22%



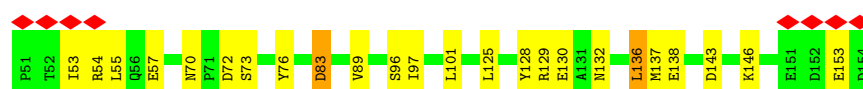
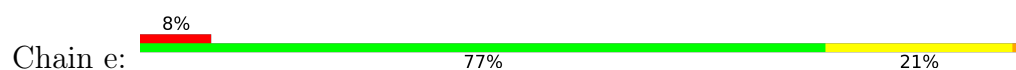
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



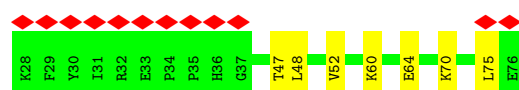
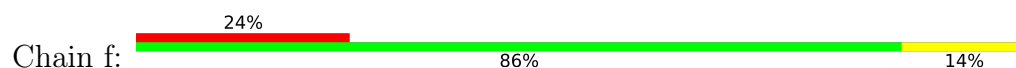
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



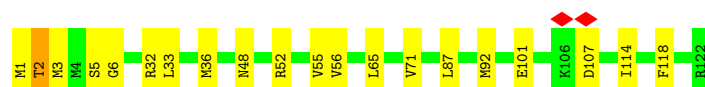
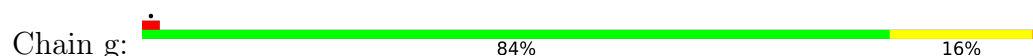
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



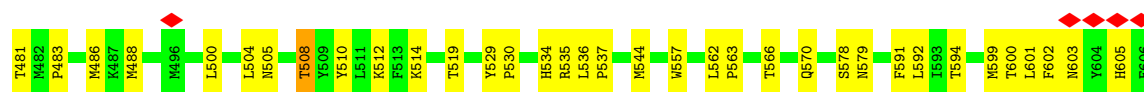
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



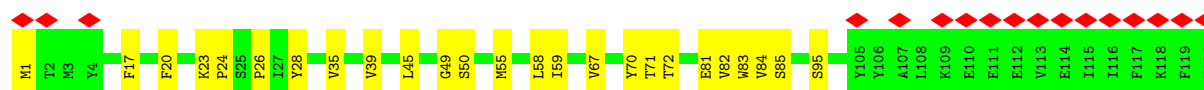
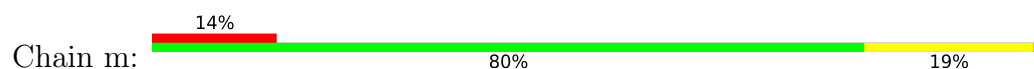
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



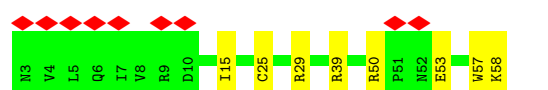
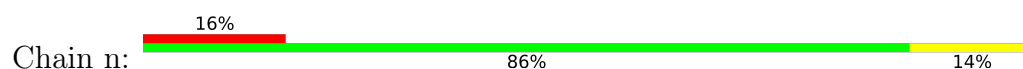




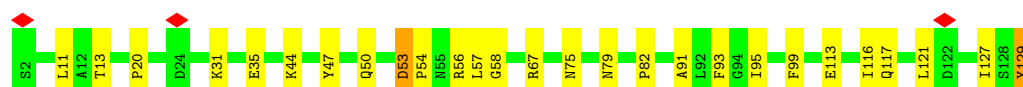
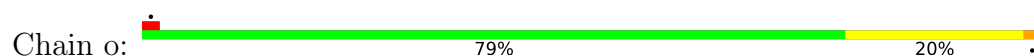
- Molecule 36: NADH-ubiquinone oxidoreductase chain 6



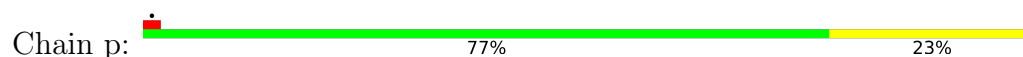
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



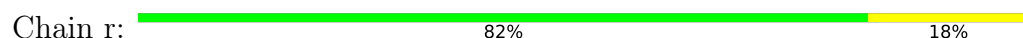
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

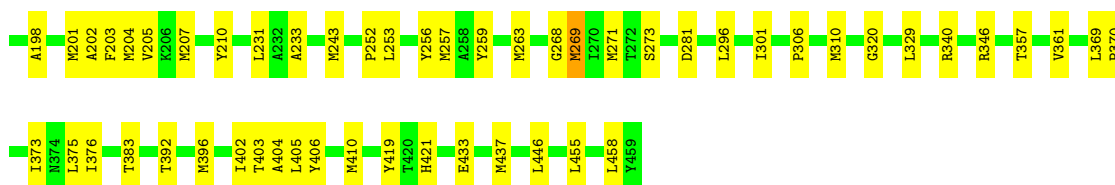


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4





- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 75% 24% .



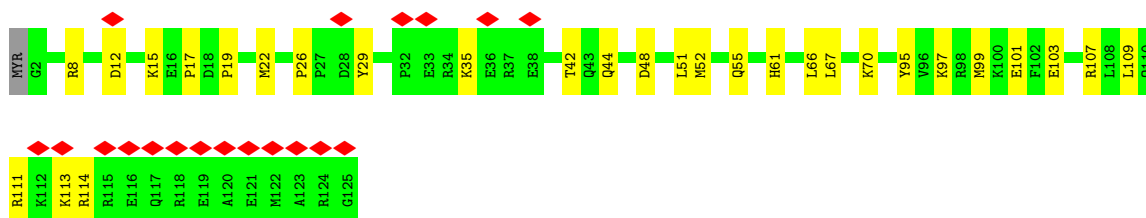
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 85% 14% .



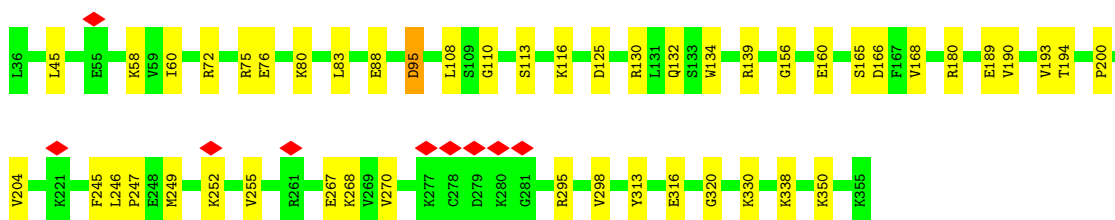
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 15% 76% 23% .



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

Chain w: 85% 15% .



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 302353                                  | 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                    | 0.268                                   | Depositor |
| Minimum map value                    | -0.140                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.007                                   | Depositor |
| Recommended contour level            | 0.027                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 333.7616, 333.7616, 333.7616            | wwPDB     |
| Map dimensions                       | 304, 304, 304                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0979, 1.0979, 1.0979                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, UQ, NAI, UQ1, 8Q1, FMN, FES, PLX, ADP, 2MR, SF4, ZN, PEE, CDL, NDP

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     | 0.17         | 0/3406        | 0.38        | 0/4603        |
| 2   | B     | 0.18         | 0/1443        | 0.34        | 0/1952        |
| 3   | C     | 0.17         | 0/1279        | 0.36        | 0/1730        |
| 4   | E     | 0.18         | 0/995         | 0.40        | 1/1340 (0.1%) |
| 5   | F     | 0.17         | 0/698         | 0.41        | 0/940         |
| 6   | G     | 0.21         | 0/705         | 0.55        | 0/956         |
| 6   | X     | 0.20         | 0/715         | 0.48        | 1/967 (0.1%)  |
| 7   | H     | 0.17         | 0/929         | 0.41        | 0/1258        |
| 8   | I     | 0.30         | 0/798         | 0.97        | 5/1079 (0.5%) |
| 9   | J     | 0.19         | 0/2828        | 0.41        | 0/3834        |
| 10  | K     | 0.20         | 0/377         | 0.58        | 1/509 (0.2%)  |
| 11  | L     | 0.19         | 0/1039        | 0.43        | 0/1403        |
| 12  | M     | 0.26         | 0/5384        | 0.59        | 6/7295 (0.1%) |
| 13  | N     | 0.14         | 0/1245        | 0.32        | 0/1694        |
| 14  | O     | 0.20         | 0/1711        | 0.47        | 1/2328 (0.0%) |
| 15  | P     | 0.29         | 0/1789        | 0.62        | 1/2436 (0.0%) |
| 16  | Q     | 0.36         | 2/3538 (0.1%) | 0.52        | 7/4796 (0.1%) |
| 17  | S     | 0.25         | 0/581         | 0.58        | 0/781         |
| 18  | T     | 0.20         | 0/755         | 0.42        | 0/1018        |
| 19  | U     | 0.13         | 0/664         | 0.31        | 0/912         |
| 20  | V     | 0.16         | 0/1042        | 0.35        | 0/1411        |
| 21  | W     | 0.21         | 0/1198        | 0.44        | 0/1617        |
| 22  | Y     | 0.13         | 0/610         | 0.38        | 0/836         |
| 23  | Z     | 0.12         | 0/660         | 0.34        | 0/892         |
| 24  | a     | 0.18         | 0/1184        | 0.38        | 0/1603        |
| 25  | b     | 0.19         | 0/844         | 0.46        | 0/1149        |
| 26  | c     | 0.20         | 0/1371        | 0.54        | 3/1875 (0.2%) |
| 27  | d     | 0.18         | 0/1494        | 0.42        | 2/2015 (0.1%) |
| 28  | e     | 0.17         | 0/891         | 0.39        | 0/1210        |
| 29  | f     | 0.15         | 0/386         | 0.38        | 0/523         |
| 30  | g     | 0.18         | 0/1036        | 0.42        | 1/1401 (0.1%) |
| 31  | h     | 0.19         | 0/889         | 0.45        | 0/1190        |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 32  | i     | 0.23         | 0/2773         | 0.54        | 3/3768 (0.1%)   |
| 33  | j     | 0.19         | 0/938          | 0.38        | 0/1281          |
| 34  | k     | 0.27         | 0/759          | 0.54        | 1/1029 (0.1%)   |
| 35  | l     | 0.20         | 0/4947         | 0.48        | 5/6728 (0.1%)   |
| 36  | m     | 0.20         | 0/1325         | 0.45        | 0/1800          |
| 37  | n     | 0.12         | 0/491          | 0.29        | 0/663           |
| 38  | o     | 0.19         | 0/1092         | 0.51        | 3/1481 (0.2%)   |
| 39  | p     | 0.13         | 0/1590         | 0.30        | 0/2155          |
| 40  | r     | 0.21         | 0/3723         | 0.43        | 1/5078 (0.0%)   |
| 41  | s     | 0.26         | 0/2581         | 0.60        | 8/3529 (0.2%)   |
| 42  | u     | 0.17         | 0/1436         | 0.43        | 1/1938 (0.1%)   |
| 43  | v     | 0.18         | 0/1052         | 0.40        | 0/1411          |
| 44  | w     | 0.13         | 0/2642         | 0.34        | 0/3580          |
| All | All   | 0.21         | 2/67833 (0.0%) | 0.47        | 51/91994 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 16  | Q     | 193 | ASP  | C-N   | 11.44 | 1.46        | 1.34     |
| 16  | Q     | 92  | HIS  | C-N   | 9.73  | 1.47        | 1.33     |

All (51) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | I     | 28  | TYR  | N-CA-C | 11.00 | 123.35      | 111.36   |
| 8   | I     | 44  | GLY  | CA-C-N | 10.39 | 130.58      | 119.05   |
| 8   | I     | 44  | GLY  | C-N-CA | 10.39 | 130.58      | 119.05   |
| 8   | I     | 43  | VAL  | N-CA-C | 9.93  | 120.75      | 110.72   |
| 12  | M     | 74  | ASN  | N-CA-C | 9.66  | 121.89      | 111.36   |
| 26  | c     | 75  | TYR  | CA-C-N | 9.25  | 129.01      | 119.76   |
| 26  | c     | 75  | TYR  | C-N-CA | 9.25  | 129.01      | 119.76   |
| 41  | s     | 206 | GLU  | N-CA-C | 8.24  | 120.35      | 111.36   |
| 35  | l     | 26  | ILE  | N-CA-C | -8.01 | 106.10      | 113.71   |
| 15  | P     | 82  | ASN  | N-CA-C | 7.80  | 122.27      | 111.74   |
| 12  | M     | 406 | ASN  | CA-C-N | 7.64  | 127.68      | 119.28   |
| 12  | M     | 406 | ASN  | C-N-CA | 7.64  | 127.68      | 119.28   |
| 6   | X     | 137 | LYS  | N-CA-C | 7.18  | 119.11      | 111.28   |
| 38  | o     | 53  | ASP  | CA-C-N | 6.98  | 126.80      | 119.05   |
| 38  | o     | 53  | ASP  | C-N-CA | 6.98  | 126.80      | 119.05   |
| 16  | Q     | 456 | ILE  | N-CA-C | 6.97  | 118.33      | 108.36   |
| 16  | Q     | 102 | SER  | N-CA-C | -6.68 | 97.63       | 108.52   |
| 14  | O     | 144 | ASN  | N-CA-C | 6.60  | 120.51      | 111.54   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 16  | Q     | 193 | ASP  | O-C-N   | 6.46  | 128.97      | 122.12   |
| 41  | s     | 217 | ALA  | N-CA-C  | 6.35  | 118.82      | 108.08   |
| 41  | s     | 67  | SER  | N-CA-C  | -6.29 | 99.75       | 109.76   |
| 38  | o     | 127 | ILE  | N-CA-C  | 6.28  | 117.06      | 110.72   |
| 35  | l     | 198 | LEU  | N-CA-C  | 6.22  | 118.06      | 111.28   |
| 41  | s     | 204 | GLU  | N-CA-C  | 6.19  | 117.70      | 111.07   |
| 27  | d     | 142 | ARG  | N-CA-C  | 6.18  | 117.82      | 111.14   |
| 12  | M     | 173 | MET  | N-CA-C  | 6.12  | 119.84      | 112.38   |
| 34  | k     | 54  | THR  | N-CA-C  | 6.11  | 117.94      | 111.28   |
| 35  | l     | 600 | THR  | N-CA-C  | 6.10  | 117.73      | 111.14   |
| 35  | l     | 68  | TRP  | N-CA-C  | 6.03  | 117.65      | 111.14   |
| 41  | s     | 200 | LEU  | N-CA-C  | 5.94  | 117.84      | 111.36   |
| 42  | u     | 169 | PHE  | N-CA-C  | 5.87  | 118.63      | 111.82   |
| 16  | Q     | 192 | LEU  | CA-C-N  | 5.86  | 128.13      | 120.28   |
| 16  | Q     | 192 | LEU  | C-N-CA  | 5.86  | 128.13      | 120.28   |
| 41  | s     | 66  | SER  | N-CA-C  | 5.77  | 118.63      | 110.50   |
| 10  | K     | 72  | THR  | N-CA-C  | 5.75  | 117.95      | 110.53   |
| 41  | s     | 217 | ALA  | CB-CA-C | -5.51 | 110.23      | 116.63   |
| 12  | M     | 612 | PRO  | CA-C-N  | 5.46  | 125.37      | 119.85   |
| 12  | M     | 612 | PRO  | C-N-CA  | 5.46  | 125.37      | 119.85   |
| 16  | Q     | 101 | LEU  | N-CA-C  | 5.43  | 118.31      | 109.24   |
| 26  | c     | 74  | ASP  | N-CA-C  | 5.30  | 117.06      | 111.28   |
| 4   | E     | 97  | TRP  | N-CA-C  | -5.28 | 105.52      | 111.28   |
| 8   | I     | 41  | LEU  | N-CA-C  | 5.17  | 121.25      | 109.81   |
| 32  | i     | 109 | SER  | CA-C-N  | 5.17  | 139.40      | 127.00   |
| 32  | i     | 109 | SER  | C-N-CA  | 5.17  | 139.40      | 127.00   |
| 30  | g     | 3   | MET  | N-CA-C  | 5.16  | 116.98      | 111.36   |
| 40  | r     | 421 | HIS  | N-CA-C  | 5.13  | 116.87      | 111.28   |
| 16  | Q     | 192 | LEU  | O-C-N   | -5.10 | 116.71      | 122.12   |
| 27  | d     | 143 | TYR  | N-CA-C  | 5.09  | 120.88      | 114.31   |
| 32  | i     | 109 | SER  | C-N-CD  | -5.09 | 109.40      | 120.60   |
| 41  | s     | 207 | LEU  | N-CA-C  | 5.03  | 118.94      | 112.41   |
| 35  | l     | 389 | PHE  | N-CA-C  | 5.02  | 116.75      | 111.28   |

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     | 86      | 0            |
| 2   | B     | 1412  | 0        | 1363     | 19      | 0            |
| 3   | C     | 1248  | 0        | 1254     | 22      | 0            |
| 4   | E     | 971   | 0        | 975      | 20      | 0            |
| 5   | F     | 687   | 0        | 700      | 18      | 0            |
| 6   | G     | 693   | 0        | 671      | 26      | 0            |
| 6   | X     | 703   | 0        | 693      | 25      | 0            |
| 7   | H     | 910   | 0        | 950      | 9       | 0            |
| 8   | I     | 780   | 0        | 808      | 29      | 0            |
| 9   | J     | 2751  | 0        | 2773     | 43      | 0            |
| 10  | K     | 366   | 0        | 338      | 9       | 0            |
| 11  | L     | 1016  | 0        | 1016     | 14      | 0            |
| 12  | M     | 5296  | 0        | 5327     | 100     | 0            |
| 13  | N     | 1204  | 0        | 1162     | 14      | 0            |
| 14  | O     | 1671  | 0        | 1675     | 55      | 0            |
| 15  | P     | 1738  | 0        | 1693     | 30      | 0            |
| 16  | Q     | 3459  | 0        | 3395     | 61      | 0            |
| 17  | S     | 566   | 0        | 561      | 8       | 0            |
| 18  | T     | 741   | 0        | 702      | 10      | 0            |
| 19  | U     | 643   | 0        | 642      | 14      | 0            |
| 20  | V     | 1021  | 0        | 1025     | 23      | 0            |
| 21  | W     | 1167  | 0        | 1155     | 25      | 0            |
| 22  | Y     | 584   | 0        | 529      | 14      | 0            |
| 23  | Z     | 641   | 0        | 620      | 11      | 0            |
| 24  | a     | 1151  | 0        | 1164     | 21      | 0            |
| 25  | b     | 819   | 0        | 835      | 17      | 0            |
| 26  | c     | 1315  | 0        | 1208     | 28      | 0            |
| 27  | d     | 1461  | 0        | 1429     | 29      | 0            |
| 28  | e     | 867   | 0        | 817      | 30      | 0            |
| 29  | f     | 378   | 0        | 356      | 5       | 0            |
| 30  | g     | 1005  | 0        | 999      | 21      | 0            |
| 31  | h     | 867   | 0        | 873      | 10      | 0            |
| 32  | i     | 2710  | 0        | 2874     | 72      | 0            |
| 33  | j     | 914   | 0        | 951      | 23      | 0            |
| 34  | k     | 748   | 0        | 799      | 27      | 0            |
| 35  | l     | 4816  | 0        | 4955     | 120     | 0            |
| 36  | m     | 1292  | 0        | 1261     | 33      | 0            |
| 37  | n     | 479   | 0        | 486      | 6       | 0            |
| 38  | o     | 1062  | 0        | 1072     | 22      | 0            |
| 39  | p     | 1534  | 0        | 1470     | 32      | 0            |
| 40  | r     | 3631  | 0        | 3839     | 60      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | s     | 2508  | 0        | 2607     | 65      | 0            |
| 42  | u     | 1398  | 0        | 1374     | 20      | 0            |
| 43  | v     | 1028  | 0        | 982      | 30      | 0            |
| 44  | w     | 2582  | 0        | 2531     | 34      | 0            |
| 45  | A     | 8     | 0        | 0        | 2       | 0            |
| 45  | B     | 16    | 0        | 0        | 0       | 0            |
| 45  | C     | 8     | 0        | 0        | 1       | 0            |
| 45  | M     | 16    | 0        | 0        | 3       | 0            |
| 46  | A     | 31    | 0        | 19       | 4       | 0            |
| 47  | A     | 44    | 0        | 27       | 4       | 0            |
| 48  | C     | 47    | 0        | 71       | 6       | 0            |
| 48  | Q     | 47    | 0        | 71       | 11      | 0            |
| 48  | V     | 91    | 0        | 136      | 11      | 0            |
| 48  | W     | 41    | 0        | 59       | 8       | 0            |
| 48  | j     | 92    | 0        | 141      | 20      | 0            |
| 48  | l     | 97    | 0        | 151      | 16      | 0            |
| 48  | s     | 51    | 0        | 82       | 4       | 0            |
| 49  | C     | 52    | 0        | 88       | 7       | 0            |
| 49  | J     | 52    | 0        | 88       | 6       | 0            |
| 49  | a     | 52    | 0        | 88       | 0       | 0            |
| 49  | e     | 52    | 0        | 88       | 7       | 0            |
| 49  | g     | 52    | 0        | 88       | 3       | 0            |
| 49  | j     | 52    | 0        | 88       | 3       | 0            |
| 49  | r     | 52    | 0        | 88       | 3       | 0            |
| 50  | C     | 38    | 0        | 47       | 7       | 0            |
| 50  | J     | 33    | 0        | 39       | 11      | 0            |
| 51  | G     | 35    | 0        | 0        | 4       | 0            |
| 51  | X     | 35    | 0        | 0        | 3       | 0            |
| 52  | I     | 51    | 0        | 46       | 2       | 0            |
| 52  | J     | 89    | 0        | 125      | 8       | 0            |
| 52  | V     | 194   | 0        | 294      | 10      | 0            |
| 52  | a     | 100   | 0        | 156      | 4       | 0            |
| 52  | k     | 94    | 0        | 141      | 7       | 0            |
| 52  | l     | 199   | 0        | 307      | 33      | 0            |
| 52  | r     | 100   | 0        | 156      | 7       | 0            |
| 52  | u     | 55    | 0        | 54       | 3       | 0            |
| 53  | J     | 48    | 0        | 26       | 1       | 0            |
| 54  | M     | 4     | 0        | 0        | 0       | 0            |
| 54  | O     | 4     | 0        | 0        | 3       | 0            |
| 55  | M     | 1     | 0        | 0        | 0       | 0            |
| 56  | Q     | 36    | 0        | 36       | 7       | 0            |
| 57  | T     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 58  | w     | 27    | 0        | 11       | 3       | 0            |
| All | All   | 68260 | 0        | 69012    | 1229    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1229) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:68:MET:HE1    | 51:G:201:8Q1:C30  | 1.34                     | 1.54              |
| 4:E:68:MET:CE     | 51:G:201:8Q1:C30  | 2.09                     | 1.30              |
| 48:Q:503:PEE:H42  | 48:Q:503:PEE:H34  | 1.26                     | 1.16              |
| 16:Q:208:GLU:OE2  | 16:Q:221:ARG:NH2  | 1.83                     | 1.11              |
| 1:A:285:PRO:HG3   | 14:O:143:ARG:NH1  | 1.67                     | 1.10              |
| 27:d:99:ASP:CG    | 28:e:137:MET:HE3  | 1.77                     | 1.10              |
| 20:V:141:VAL:O    | 24:a:169:TYR:OH   | 1.70                     | 1.09              |
| 6:G:133:ILE:O     | 6:G:134:ASP:HB2   | 1.46                     | 1.09              |
| 35:l:599:MET:O    | 35:l:603:ASN:HB3  | 1.54                     | 1.07              |
| 14:O:135:CYS:SG   | 14:O:175:GLU:O    | 2.11                     | 1.07              |
| 35:l:331:MET:SD   | 35:l:387:THR:HG23 | 1.95                     | 1.07              |
| 52:l:702:CDL:H371 | 52:l:702:CDL:H601 | 1.34                     | 1.05              |
| 14:O:134:VAL:HG12 | 14:O:186:VAL:HG22 | 1.37                     | 1.03              |
| 14:O:140:CYS:SG   | 54:O:301:FES:FE1  | 1.49                     | 1.03              |
| 6:G:105:MET:HE2   | 6:G:139:MET:HE1   | 1.41                     | 1.01              |
| 49:e:201:PLX:H21  | 48:l:704:PEE:H2   | 1.42                     | 1.01              |
| 52:l:702:CDL:H642 | 52:l:702:CDL:H431 | 1.41                     | 1.00              |
| 8:I:40:LYS:HB3    | 21:W:7:LYS:H      | 1.22                     | 1.00              |
| 14:O:134:VAL:HG12 | 14:O:186:VAL:CG2  | 1.93                     | 0.99              |
| 4:E:64:ARG:NH2    | 6:G:114:ASP:OD1   | 1.95                     | 0.99              |
| 6:X:105:MET:HE3   | 6:X:139:MET:HE1   | 1.46                     | 0.97              |
| 1:A:48:ARG:NH1    | 10:K:70:ASN:O     | 1.97                     | 0.97              |
| 43:v:15:LYS:HA    | 43:v:109:LEU:HD22 | 1.46                     | 0.97              |
| 12:M:391:ILE:N    | 12:M:600:GLU:OE2  | 1.98                     | 0.96              |
| 21:W:140:PHE:O    | 48:W:201:PEE:H11  | 1.65                     | 0.95              |
| 48:Q:503:PEE:H37  | 48:Q:503:PEE:C37  | 1.96                     | 0.95              |
| 52:l:702:CDL:H642 | 52:l:702:CDL:C43  | 1.98                     | 0.93              |
| 35:l:119:LYS:NZ   | 52:l:701:CDL:OA3  | 2.01                     | 0.93              |
| 12:M:179:CYS:SG   | 45:M:802:SF4:FE1  | 1.61                     | 0.93              |
| 44:w:139:ARG:HH12 | 58:w:401:ADP:HN61 | 1.16                     | 0.92              |
| 48:Q:503:PEE:H37  | 48:Q:503:PEE:H60  | 1.50                     | 0.91              |
| 24:a:170:GLN:HB2  | 30:g:6:GLY:O      | 1.69                     | 0.91              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:95:MET:HE3   | 32:i:149:ILE:HD12 | 1.51                     | 0.90              |
| 16:Q:156:GLU:OE2  | 16:Q:229:PRO:O    | 1.90                     | 0.89              |
| 44:w:139:ARG:HH12 | 58:w:401:ADP:N6   | 1.71                     | 0.89              |
| 6:G:105:MET:HE2   | 6:G:139:MET:CE    | 2.02                     | 0.89              |
| 6:G:133:ILE:O     | 6:G:134:ASP:CB    | 2.19                     | 0.88              |
| 27:d:99:ASP:OD2   | 28:e:137:MET:HE3  | 1.72                     | 0.88              |
| 35:l:294:THR:HG22 | 52:l:702:CDL:HB62 | 1.53                     | 0.88              |
| 27:d:99:ASP:CG    | 28:e:137:MET:CE   | 2.47                     | 0.88              |
| 12:M:483:ARG:NH1  | 12:M:489:ILE:HD11 | 1.89                     | 0.87              |
| 43:v:15:LYS:HA    | 43:v:109:LEU:CD2  | 2.03                     | 0.87              |
| 24:a:161:ARG:NH2  | 30:g:1:MET:CB     | 2.38                     | 0.87              |
| 9:J:313:TRP:CG    | 50:J:402:UQ:H8    | 2.12                     | 0.85              |
| 27:d:99:ASP:HB3   | 28:e:137:MET:HE1  | 1.59                     | 0.84              |
| 35:l:294:THR:CG2  | 52:l:702:CDL:HB62 | 2.08                     | 0.83              |
| 12:M:295:ASP:OD1  | 12:M:704:SER:OG   | 1.95                     | 0.83              |
| 12:M:179:CYS:HG   | 45:M:802:SF4:FE1  | 0.96                     | 0.82              |
| 9:J:313:TRP:CD1   | 50:J:402:UQ:H8    | 2.14                     | 0.82              |
| 6:G:130:ILE:CG2   | 6:G:135:ALA:HB2   | 2.09                     | 0.81              |
| 48:Q:503:PEE:H34  | 48:Q:503:PEE:C25  | 2.09                     | 0.81              |
| 51:X:201:8Q1:O40  | 39:p:12:HIS:HE1   | 1.64                     | 0.81              |
| 40:r:253:LEU:HD12 | 40:r:256:TYR:CE1  | 2.16                     | 0.81              |
| 9:J:304:LEU:HD11  | 49:J:403:PLX:H312 | 1.63                     | 0.80              |
| 35:l:419:THR:HA   | 35:l:422:TYR:CE2  | 2.16                     | 0.80              |
| 3:C:126:GLU:OE1   | 33:j:33:LYS:NZ    | 2.14                     | 0.79              |
| 48:C:302:PEE:H81  | 41:s:56:PHE:CE2   | 2.18                     | 0.79              |
| 15:P:83:GLU:OE1   | 15:P:142:ARG:NH2  | 2.16                     | 0.79              |
| 35:l:360:GLY:HA3  | 35:l:435:PRO:HA   | 1.65                     | 0.78              |
| 6:X:139:MET:HA    | 6:X:139:MET:CE    | 2.14                     | 0.78              |
| 15:P:125:ARG:NH2  | 15:P:201:ASP:OD1  | 2.16                     | 0.78              |
| 37:n:50:ARG:HB2   | 37:n:53:GLU:HG2   | 1.65                     | 0.78              |
| 32:i:7:THR:HG22   | 32:i:11:MET:HE2   | 1.66                     | 0.78              |
| 11:L:109:ASN:ND2  | 11:L:111:LEU:O    | 2.17                     | 0.77              |
| 26:c:54:LYS:NZ    | 26:c:74:ASP:OD2   | 2.17                     | 0.77              |
| 48:W:201:PEE:H42  | 48:W:201:PEE:H33  | 1.64                     | 0.77              |
| 43:v:51:LEU:O     | 43:v:52:MET:HG2   | 1.85                     | 0.76              |
| 14:O:136:THR:HG21 | 14:O:173:GLU:OE1  | 1.86                     | 0.76              |
| 3:C:73:ALA:HB1    | 56:Q:501:UQ1:H112 | 1.66                     | 0.76              |
| 1:A:285:PRO:CG    | 14:O:143:ARG:NH1  | 2.48                     | 0.76              |
| 6:G:139:MET:HE2   | 6:G:139:MET:HA    | 1.68                     | 0.76              |
| 9:J:306:GLU:HG2   | 9:J:315:THR:HG22  | 1.68                     | 0.76              |
| 6:G:105:MET:CE    | 6:G:139:MET:HE1   | 2.14                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:Q:503:PEE:H37  | 48:Q:503:PEE:H61  | 1.67                     | 0.75              |
| 28:e:129:ARG:NH1  | 28:e:136:LEU:O    | 2.19                     | 0.75              |
| 9:J:220:MET:CE    | 9:J:227:PRO:HD2   | 2.17                     | 0.75              |
| 24:a:94:GLY:O     | 27:d:61:TYR:OH    | 2.02                     | 0.75              |
| 35:l:66:TRP:CD1   | 48:l:704:PEE:H16  | 2.22                     | 0.75              |
| 32:i:258:SER:OG   | 32:i:333:SER:O    | 2.05                     | 0.74              |
| 41:s:288:LEU:HD11 | 48:s:401:PEE:H7   | 1.67                     | 0.74              |
| 2:B:48:MET:O      | 19:U:10:LYS:NZ    | 2.20                     | 0.74              |
| 12:M:338:VAL:HG21 | 12:M:361:VAL:HG11 | 1.70                     | 0.74              |
| 41:s:288:LEU:CD1  | 48:s:401:PEE:H7   | 2.17                     | 0.74              |
| 15:P:231:ARG:HG3  | 15:P:231:ARG:HH11 | 1.54                     | 0.73              |
| 6:X:139:MET:HA    | 6:X:139:MET:HE3   | 1.68                     | 0.73              |
| 30:g:36:MET:HE1   | 49:g:201:PLX:H393 | 1.70                     | 0.73              |
| 21:W:121:MET:HG3  | 36:m:130:THR:HB   | 1.71                     | 0.73              |
| 36:m:26:PRO:HB2   | 36:m:71:THR:CG2   | 2.18                     | 0.73              |
| 20:V:3:LYS:H      | 35:l:605:HIS:HE1  | 1.37                     | 0.72              |
| 27:d:167:ARG:HH21 | 28:e:153:GLU:HG3  | 1.54                     | 0.72              |
| 12:M:483:ARG:HH11 | 12:M:489:ILE:HD11 | 1.52                     | 0.72              |
| 36:m:72:THR:HG21  | 41:s:133:LEU:HD21 | 1.70                     | 0.72              |
| 48:j:202:PEE:O1P  | 41:s:62:ARG:NH2   | 2.22                     | 0.72              |
| 22:Y:43:ARG:O     | 22:Y:46:GLN:NE2   | 2.22                     | 0.72              |
| 14:O:177:LEU:HD12 | 14:O:185:MET:SD   | 2.30                     | 0.71              |
| 41:s:209:SER:HB3  | 41:s:213:VAL:HA   | 1.72                     | 0.71              |
| 24:a:106:VAL:HB   | 37:n:50:ARG:HH21  | 1.55                     | 0.71              |
| 14:O:140:CYS:HG   | 54:O:301:FES:FE1  | 0.42                     | 0.71              |
| 6:G:139:MET:CE    | 6:G:139:MET:HA    | 2.21                     | 0.71              |
| 12:M:149:ASP:HB2  | 16:Q:361:ALA:HB3  | 1.73                     | 0.71              |
| 1:A:121:GLU:HB2   | 47:A:503:NAI:H42N | 1.72                     | 0.71              |
| 12:M:179:CYS:SG   | 45:M:802:SF4:S4   | 2.89                     | 0.71              |
| 48:Q:503:PEE:H28  | 48:Q:503:PEE:H36  | 1.72                     | 0.71              |
| 35:l:2:ASN:OD1    | 35:l:59:GLN:NE2   | 2.21                     | 0.70              |
| 52:l:702:CDL:H432 | 52:l:702:CDL:H662 | 1.73                     | 0.70              |
| 42:u:88:CYS:SG    | 42:u:103:GLN:NE2  | 2.64                     | 0.70              |
| 12:M:493:VAL:HG12 | 12:M:513:MET:HE1  | 1.72                     | 0.70              |
| 12:M:256:ALA:O    | 12:M:598:ASN:ND2  | 2.24                     | 0.70              |
| 16:Q:62:LYS:HE2   | 16:Q:63:PRO:HD2   | 1.73                     | 0.70              |
| 26:c:58:ARG:NH2   | 26:c:60:GLU:OE1   | 2.24                     | 0.70              |
| 48:W:201:PEE:H33  | 48:W:201:PEE:C25  | 2.21                     | 0.70              |
| 32:i:97:MET:HA    | 32:i:100:MET:HE2  | 1.72                     | 0.70              |
| 32:i:258:SER:HB2  | 32:i:336:VAL:HG12 | 1.74                     | 0.70              |
| 5:F:20:ARG:HB2    | 5:F:66:TRP:HB2    | 1.73                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:J:402:UQ:C24   | 50:J:402:UQ:H201  | 2.22                     | 0.70              |
| 32:i:95:MET:CE    | 32:i:149:ILE:HD12 | 2.22                     | 0.70              |
| 48:V:202:PEE:H78  | 40:r:201:MET:HE2  | 1.71                     | 0.69              |
| 8:I:92:LYS:HA     | 8:I:92:LYS:HE2    | 1.74                     | 0.69              |
| 8:I:46:SER:O      | 8:I:52:ASN:ND2    | 2.24                     | 0.69              |
| 50:J:402:UQ:H103  | 50:J:402:UQ:O1    | 1.93                     | 0.69              |
| 52:l:701:CDL:H1O1 | 40:r:357:THR:HG1  | 1.39                     | 0.69              |
| 12:M:337:ASP:O    | 12:M:542:PRO:HB2  | 1.93                     | 0.69              |
| 32:i:68:MET:HE2   | 32:i:68:MET:HA    | 1.74                     | 0.68              |
| 34:k:44:SER:HB2   | 34:k:59:MET:HE1   | 1.74                     | 0.68              |
| 33:j:6:THR:HG21   | 41:s:87:VAL:HG11  | 1.74                     | 0.68              |
| 43:v:109:LEU:O    | 43:v:109:LEU:HD23 | 1.93                     | 0.68              |
| 2:B:44:ARG:HH11   | 2:B:44:ARG:HG2    | 1.59                     | 0.68              |
| 6:G:130:ILE:HG22  | 6:G:135:ALA:HB2   | 1.74                     | 0.68              |
| 32:i:88:LYS:HG2   | 32:i:148:SER:HB3  | 1.75                     | 0.68              |
| 2:B:165:ASP:OD1   | 16:Q:368:ARG:NH2  | 2.27                     | 0.68              |
| 9:J:37:HIS:CE1    | 18:T:49:ASP:HA    | 2.28                     | 0.68              |
| 35:l:331:MET:SD   | 35:l:387:THR:CG2  | 2.78                     | 0.68              |
| 28:e:54:ARG:NH2   | 44:w:313:TYR:O    | 2.26                     | 0.68              |
| 16:Q:156:GLU:CG   | 16:Q:229:PRO:O    | 2.42                     | 0.68              |
| 1:A:132:ARG:HB3   | 1:A:165:GLU:HG3   | 1.75                     | 0.67              |
| 48:W:201:PEE:H42  | 48:W:201:PEE:C21  | 2.24                     | 0.67              |
| 36:m:26:PRO:HB2   | 36:m:71:THR:HG21  | 1.77                     | 0.67              |
| 34:k:23:ARG:HG3   | 36:m:23:LYS:HE2   | 1.75                     | 0.67              |
| 1:A:285:PRO:HG3   | 14:O:143:ARG:HH11 | 1.56                     | 0.67              |
| 9:J:192:ARG:NH1   | 9:J:198:ALA:O     | 2.28                     | 0.67              |
| 32:i:236:LYS:HG3  | 32:i:237:MET:HG3  | 1.76                     | 0.67              |
| 49:J:403:PLX:H141 | 33:j:19:LEU:HD23  | 1.76                     | 0.66              |
| 10:K:78:HIS:CE1   | 10:K:79:HIS:CE1   | 2.83                     | 0.66              |
| 35:l:69:MET:HE3   | 35:l:76:LEU:HD12  | 1.76                     | 0.66              |
| 24:a:154:LEU:HD21 | 32:i:272:LYS:HG2  | 1.77                     | 0.66              |
| 31:h:18:MET:HE3   | 34:k:56:ALA:HA    | 1.76                     | 0.66              |
| 39:p:105:ASP:OD1  | 39:p:122:ARG:NH1  | 2.26                     | 0.66              |
| 9:J:304:LEU:O     | 9:J:307:VAL:HG22  | 1.94                     | 0.66              |
| 16:Q:302:LEU:HB2  | 16:Q:401:GLU:HB2  | 1.77                     | 0.66              |
| 16:Q:88:HIS:HE1   | 41:s:205:SER:O    | 1.79                     | 0.66              |
| 8:I:40:LYS:HB3    | 21:W:7:LYS:N      | 2.05                     | 0.66              |
| 48:Q:503:PEE:H60  | 48:Q:503:PEE:C23  | 2.24                     | 0.66              |
| 16:Q:83:ASN:HB2   | 33:j:38:GLU:HG2   | 1.77                     | 0.65              |
| 44:w:125:ASP:O    | 44:w:130:ARG:NH2  | 2.30                     | 0.65              |
| 32:i:190:MET:HE2  | 32:i:205:LEU:HA   | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:k:80:MET:HE3   | 36:m:172:THR:HA   | 1.79                     | 0.65              |
| 16:Q:259:GLU:OE2  | 21:W:23:ARG:NH1   | 2.26                     | 0.65              |
| 2:B:63:TRP:HB3    | 2:B:66:LEU:HD12   | 1.77                     | 0.65              |
| 5:F:71:PHE:HE1    | 12:M:334:GLN:NE2  | 1.94                     | 0.65              |
| 41:s:277:TYR:CE2  | 48:s:401:PEE:H59  | 2.32                     | 0.65              |
| 43:v:52:MET:HB2   | 43:v:55:GLN:HG3   | 1.76                     | 0.65              |
| 43:v:111:ARG:HG2  | 43:v:114:ARG:HH21 | 1.61                     | 0.65              |
| 29:f:70:LYS:HA    | 29:f:75:LEU:HD23  | 1.79                     | 0.65              |
| 39:p:47:ARG:NH2   | 39:p:70:GLU:OE1   | 2.29                     | 0.65              |
| 1:A:174:ARG:HA    | 10:K:93:LEU:HD21  | 1.78                     | 0.65              |
| 17:S:63:THR:HG23  | 42:u:21:SER:HB2   | 1.78                     | 0.65              |
| 52:V:201:CDL:H731 | 52:V:201:CDL:H601 | 1.79                     | 0.65              |
| 35:l:228:GLY:HA3  | 48:l:703:PEE:H38  | 1.79                     | 0.65              |
| 40:r:253:LEU:HD12 | 40:r:256:TYR:HE1  | 1.62                     | 0.64              |
| 43:v:35:LYS:HE2   | 43:v:35:LYS:H     | 1.62                     | 0.64              |
| 49:J:403:PLX:H131 | 48:j:202:PEE:C37  | 2.27                     | 0.64              |
| 19:U:16:GLU:HG3   | 48:j:201:PEE:H49  | 1.79                     | 0.64              |
| 32:i:108:LEU:HD11 | 32:i:191:THR:HG21 | 1.77                     | 0.64              |
| 14:O:215:LYS:O    | 14:O:219:ARG:NH2  | 2.31                     | 0.64              |
| 40:r:97:THR:HG21  | 52:r:502:CDL:H241 | 1.80                     | 0.64              |
| 52:u:201:CDL:H581 | 52:u:201:CDL:H541 | 1.78                     | 0.64              |
| 14:O:182:ASN:HD22 | 14:O:194:GLU:CD   | 2.05                     | 0.64              |
| 30:g:56:VAL:HG21  | 40:r:17:MET:HE1   | 1.79                     | 0.64              |
| 49:e:201:PLX:C2   | 48:l:704:PEE:H2   | 2.24                     | 0.64              |
| 34:k:27:MET:HE1   | 36:m:70:TYR:HB3   | 1.79                     | 0.64              |
| 1:A:89:GLY:O      | 47:A:503:NAI:H2N  | 1.97                     | 0.64              |
| 39:p:35:ASP:OD1   | 39:p:36:LYS:N     | 2.30                     | 0.64              |
| 32:i:258:SER:CB   | 32:i:336:VAL:HG12 | 2.27                     | 0.64              |
| 40:r:74:PRO:O     | 40:r:78:MET:HG3   | 1.98                     | 0.64              |
| 16:Q:36:GLN:HG2   | 40:r:138:ASN:HA   | 1.80                     | 0.64              |
| 32:i:42:PRO:HG2   | 36:m:167:VAL:HG22 | 1.80                     | 0.64              |
| 35:l:294:THR:HG22 | 52:l:702:CDL:CB6  | 2.28                     | 0.64              |
| 1:A:385:CYS:HB3   | 45:A:501:SF4:S2   | 2.37                     | 0.63              |
| 44:w:139:ARG:NH1  | 44:w:166:ASP:OD2  | 2.31                     | 0.63              |
| 44:w:139:ARG:NH1  | 58:w:401:ADP:HN61 | 1.90                     | 0.63              |
| 5:F:71:PHE:CE1    | 12:M:334:GLN:NE2  | 2.66                     | 0.63              |
| 1:A:56:ALA:HB1    | 1:A:61:ASP:HB2    | 1.81                     | 0.63              |
| 34:k:65:VAL:HG11  | 36:m:157:THR:HG23 | 1.79                     | 0.63              |
| 14:O:166:ASP:HB3  | 14:O:168:LEU:HD22 | 1.79                     | 0.63              |
| 27:d:99:ASP:OD2   | 28:e:137:MET:CE   | 2.43                     | 0.63              |
| 35:l:500:LEU:CD1  | 52:l:702:CDL:H352 | 2.29                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:U:26:GLY:HA3   | 48:j:201:PEE:C23  | 2.29                     | 0.63              |
| 1:A:244:ASN:ND2   | 46:A:502:FMN:O2   | 2.27                     | 0.63              |
| 34:k:20:LEU:HD12  | 35:l:592:LEU:HD13 | 1.80                     | 0.63              |
| 44:w:132:GLN:NE2  | 44:w:166:ASP:OD1  | 2.32                     | 0.63              |
| 16:Q:192:LEU:HD21 | 56:Q:502:UQ1:HM22 | 1.81                     | 0.62              |
| 44:w:113:SER:HB3  | 44:w:116:LYS:HG2  | 1.80                     | 0.62              |
| 1:A:285:PRO:HG3   | 14:O:143:ARG:HH12 | 1.63                     | 0.62              |
| 7:H:83:GLN:HG3    | 15:P:104:THR:HG22 | 1.80                     | 0.62              |
| 3:C:92:VAL:HG11   | 50:C:304:UQ:H103  | 1.81                     | 0.62              |
| 4:E:64:ARG:NH1    | 6:G:117:GLU:OE1   | 2.32                     | 0.62              |
| 1:A:337:MET:HE2   | 1:A:342:LEU:HD11  | 1.80                     | 0.62              |
| 26:c:36:MET:HE2   | 38:o:67:ARG:HH21  | 1.64                     | 0.62              |
| 15:P:211:ARG:NH2  | 15:P:213:ASP:OD2  | 2.33                     | 0.62              |
| 12:M:257:VAL:C    | 12:M:598:ASN:HD21 | 2.08                     | 0.62              |
| 12:M:275:PRO:HG3  | 12:M:286:ILE:HG12 | 1.81                     | 0.62              |
| 1:A:113:LEU:HD13  | 1:A:149:MET:HE1   | 1.82                     | 0.62              |
| 11:L:123:ASN:OD1  | 12:M:246:ARG:NH2  | 2.33                     | 0.61              |
| 43:v:103:GLU:HA   | 43:v:103:GLU:OE1  | 2.00                     | 0.61              |
| 14:O:177:LEU:HD12 | 14:O:185:MET:HE1  | 1.81                     | 0.61              |
| 28:e:143:ASP:HB3  | 28:e:146:LYS:HD3  | 1.82                     | 0.61              |
| 14:O:181:VAL:CG1  | 14:O:222:ARG:HH22 | 2.14                     | 0.61              |
| 33:j:18:VAL:HG12  | 48:j:202:PEE:H16  | 1.81                     | 0.61              |
| 33:j:57:LEU:HD21  | 36:m:169:MET:HE3  | 1.81                     | 0.61              |
| 48:j:201:PEE:H40  | 41:s:302:MET:HE1  | 1.81                     | 0.61              |
| 21:W:61:GLN:HE22  | 41:s:317:GLN:H    | 1.46                     | 0.61              |
| 32:i:54:GLU:HG3   | 34:k:93:LEU:HB3   | 1.82                     | 0.61              |
| 32:i:111:PHE:HA   | 35:l:591:PHE:CE1  | 2.35                     | 0.61              |
| 41:s:66:SER:HB2   | 41:s:122:ALA:O    | 2.00                     | 0.61              |
| 49:J:403:PLX:C13  | 48:j:202:PEE:C37  | 2.79                     | 0.61              |
| 12:M:47:THR:O     | 12:M:96:VAL:HG22  | 2.01                     | 0.61              |
| 26:c:179:GLU:H    | 26:c:179:GLU:CD   | 2.08                     | 0.61              |
| 33:j:97:LEU:HD21  | 49:j:203:PLX:H391 | 1.83                     | 0.61              |
| 40:r:281:ASP:OD2  | 40:r:340:ARG:NH1  | 2.34                     | 0.61              |
| 16:Q:99:MET:HE3   | 16:Q:101:LEU:HD21 | 1.83                     | 0.61              |
| 3:C:125:PRO:HG2   | 41:s:58:LYS:HE3   | 1.81                     | 0.60              |
| 13:N:106:ARG:HB2  | 13:N:109:ILE:HG13 | 1.83                     | 0.60              |
| 19:U:30:ILE:HD11  | 33:j:96:ILE:HD11  | 1.83                     | 0.60              |
| 35:l:505:ASN:O    | 35:l:508:THR:OG1  | 2.19                     | 0.60              |
| 1:A:159:ARG:NH2   | 14:O:176:CYS:O    | 2.34                     | 0.60              |
| 16:Q:149:GLN:NE2  | 16:Q:309:ASP:OD2  | 2.33                     | 0.60              |
| 32:i:110:PRO:CG   | 35:l:594:THR:HG21 | 2.31                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:285:PRO:CG    | 14:O:143:ARG:HH12 | 2.15                     | 0.60              |
| 12:M:222:ILE:HA   | 12:M:225:ILE:HG12 | 1.84                     | 0.60              |
| 12:M:506:VAL:HG12 | 12:M:508:GLY:H    | 1.66                     | 0.60              |
| 23:Z:84:ALA:O     | 23:Z:88:LEU:HB2   | 2.01                     | 0.60              |
| 27:d:114:GLN:HG3  | 35:l:203:MET:HG2  | 1.82                     | 0.60              |
| 30:g:52:ARG:NH1   | 32:i:318:GLU:OE1  | 2.35                     | 0.60              |
| 35:l:562:LEU:HB3  | 35:l:563:PRO:HD3  | 1.83                     | 0.60              |
| 1:A:268:GLU:OE1   | 1:A:269:ARG:NH1   | 2.35                     | 0.60              |
| 52:V:203:CDL:H622 | 52:V:203:CDL:H762 | 1.83                     | 0.60              |
| 1:A:48:ARG:NH2    | 14:O:231:LEU:HD11 | 2.17                     | 0.60              |
| 43:v:15:LYS:CA    | 43:v:109:LEU:HD22 | 2.27                     | 0.60              |
| 1:A:195:VAL:O     | 10:K:97:ARG:NH1   | 2.33                     | 0.60              |
| 32:i:265:MET:HE2  | 32:i:343:LEU:HD21 | 1.83                     | 0.60              |
| 9:J:283:VAL:HG22  | 9:J:369:VAL:HG21  | 1.83                     | 0.60              |
| 14:O:38:LEU:O     | 14:O:124:ARG:NH2  | 2.35                     | 0.59              |
| 48:Q:503:PEE:H36  | 48:Q:503:PEE:C18  | 2.31                     | 0.59              |
| 52:l:702:CDL:H642 | 52:l:702:CDL:H432 | 1.82                     | 0.59              |
| 4:E:96:VAL:HG12   | 4:E:96:VAL:O      | 2.00                     | 0.59              |
| 12:M:472:PRO:O    | 12:M:510:TRP:NE1  | 2.29                     | 0.59              |
| 12:M:483:ARG:HH11 | 12:M:489:ILE:CD1  | 2.15                     | 0.59              |
| 27:d:99:ASP:CB    | 28:e:137:MET:HE1  | 2.29                     | 0.59              |
| 40:r:253:LEU:CD1  | 40:r:256:TYR:CE1  | 2.85                     | 0.59              |
| 14:O:59:ASN:ND2   | 14:O:89:GLN:OE1   | 2.32                     | 0.59              |
| 5:F:24:CYS:N      | 5:F:58:CYS:SG     | 2.75                     | 0.59              |
| 13:N:8:ARG:O      | 13:N:12:GLN:HG2   | 2.03                     | 0.59              |
| 14:O:44:THR:HG22  | 14:O:46:GLU:H     | 1.68                     | 0.59              |
| 48:Q:503:PEE:H42  | 48:Q:503:PEE:C21  | 2.10                     | 0.59              |
| 9:J:313:TRP:CD2   | 50:J:402:UQ:C8    | 2.85                     | 0.59              |
| 12:M:456:ALA:O    | 12:M:499:ASN:ND2  | 2.35                     | 0.59              |
| 4:E:71:ALA:HB1    | 51:G:201:8Q1:O33  | 2.01                     | 0.59              |
| 48:j:202:PEE:O1P  | 41:s:62:ARG:NH1   | 2.36                     | 0.59              |
| 35:l:504:LEU:HD12 | 52:l:702:CDL:H511 | 1.83                     | 0.59              |
| 1:A:214:GLU:OE1   | 11:L:175:LYS:NZ   | 2.32                     | 0.59              |
| 16:Q:39:PRO:HB3   | 16:Q:43:TRP:CD1   | 2.37                     | 0.59              |
| 20:V:61:PHE:HD2   | 20:V:104:ARG:HH21 | 1.51                     | 0.59              |
| 32:i:207:ILE:HD13 | 32:i:262:PRO:HD3  | 1.85                     | 0.59              |
| 19:U:26:GLY:HA3   | 48:j:201:PEE:H37  | 1.84                     | 0.59              |
| 35:l:227:PHE:O    | 35:l:230:HIS:ND1  | 2.36                     | 0.59              |
| 39:p:136:GLU:OE2  | 39:p:167:TRP:NE1  | 2.36                     | 0.59              |
| 41:s:205:SER:OG   | 41:s:279:ARG:NH2  | 2.35                     | 0.58              |
| 5:F:68:ARG:NH2    | 12:M:364:ASP:OD1  | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:368:THR:O    | 12:M:533:GLY:O    | 2.21                     | 0.58              |
| 12:M:674:LEU:HD12 | 12:M:675:VAL:HG23 | 1.85                     | 0.58              |
| 15:P:231:ARG:HG3  | 15:P:231:ARG:NH1  | 2.14                     | 0.58              |
| 27:d:160:LYS:NZ   | 30:g:114:ILE:O    | 2.36                     | 0.58              |
| 35:l:599:MET:C    | 35:l:603:ASN:HB3  | 2.25                     | 0.58              |
| 6:G:115:GLN:HG3   | 6:G:139:MET:HE1   | 1.85                     | 0.58              |
| 15:P:173:MET:HE1  | 15:P:189:THR:HG23 | 1.85                     | 0.58              |
| 16:Q:226:TYR:OH   | 16:Q:234:GLN:O    | 2.14                     | 0.58              |
| 1:A:52:ARG:O      | 1:A:54:LYS:N      | 2.37                     | 0.58              |
| 12:M:498:GLN:O    | 12:M:498:GLN:NE2  | 2.35                     | 0.58              |
| 20:V:49:PHE:HA    | 52:k:101:CDL:HA61 | 1.85                     | 0.58              |
| 32:i:88:LYS:O     | 32:i:148:SER:CB   | 2.51                     | 0.58              |
| 8:I:8:ILE:HG13    | 52:l:201:CDL:OA4  | 2.03                     | 0.58              |
| 49:e:201:PLX:H141 | 52:l:701:CDL:H802 | 1.85                     | 0.58              |
| 35:l:346:ILE:HA   | 35:l:366:MET:HE1  | 1.84                     | 0.58              |
| 11:L:78:ARG:NH1   | 11:L:148:GLU:OE2  | 2.36                     | 0.58              |
| 21:W:61:GLN:NE2   | 41:s:317:GLN:OE1  | 2.36                     | 0.58              |
| 32:i:110:PRO:HG2  | 35:l:594:THR:HG21 | 1.84                     | 0.58              |
| 40:r:346:ARG:O    | 40:r:419:TYR:HA   | 2.03                     | 0.58              |
| 1:A:217:GLU:CD    | 11:L:171:ARG:HH22 | 2.12                     | 0.58              |
| 3:C:54:VAL:HG21   | 48:C:302:PEE:H55  | 1.84                     | 0.58              |
| 12:M:493:VAL:CG1  | 12:M:513:MET:HE1  | 2.34                     | 0.58              |
| 20:V:110:ILE:HD11 | 48:V:204:PEE:H8   | 1.85                     | 0.58              |
| 21:W:90:ASN:ND2   | 21:W:123:GLU:O    | 2.37                     | 0.58              |
| 35:l:103:PHE:HB2  | 35:l:341:MET:HE3  | 1.86                     | 0.58              |
| 5:F:71:PHE:HE1    | 12:M:334:GLN:HE21 | 1.51                     | 0.58              |
| 9:J:313:TRP:CD2   | 50:J:402:UQ:H8    | 2.38                     | 0.58              |
| 14:O:134:VAL:HG21 | 14:O:149:LEU:HD13 | 1.84                     | 0.58              |
| 10:K:78:HIS:HE1   | 10:K:79:HIS:CE1   | 2.21                     | 0.58              |
| 20:V:38:ALA:HA    | 52:k:101:CDL:H212 | 1.86                     | 0.57              |
| 31:h:43:CYS:HG    | 31:h:56:CYS:HG    | 0.60                     | 0.57              |
| 16:Q:144:MET:HG2  | 16:Q:222:MET:O    | 2.03                     | 0.57              |
| 16:Q:156:GLU:CD   | 16:Q:229:PRO:O    | 2.47                     | 0.57              |
| 26:c:85:GLU:OE2   | 38:o:13:THR:OG1   | 2.22                     | 0.57              |
| 34:k:19:LEU:HD23  | 34:k:36:MET:HE1   | 1.86                     | 0.57              |
| 16:Q:152:SER:HB3  | 16:Q:229:PRO:HA   | 1.86                     | 0.57              |
| 9:J:173:ASP:HB3   | 9:J:176:SER:HB2   | 1.87                     | 0.57              |
| 40:r:269:MET:HE1  | 40:r:296:LEU:HD13 | 1.87                     | 0.57              |
| 14:O:148:ILE:HG13 | 14:O:184:PRO:HG2  | 1.87                     | 0.57              |
| 41:s:18:ALA:O     | 41:s:21:THR:OG1   | 2.21                     | 0.57              |
| 50:C:304:UQ:HM31  | 56:Q:502:UQ1:HM31 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:104:PHE:HD1   | 6:G:108:LEU:HD12  | 1.70                     | 0.57              |
| 12:M:178:GLN:HG2  | 12:M:204:MET:HE3  | 1.87                     | 0.57              |
| 48:W:201:PEE:H50  | 36:m:45:LEU:HD21  | 1.85                     | 0.57              |
| 1:A:56:ALA:HB1    | 1:A:61:ASP:CB     | 2.35                     | 0.57              |
| 1:A:60:GLY:HA2    | 14:O:241:PRO:HA   | 1.87                     | 0.56              |
| 41:s:101:GLY:O    | 41:s:105:MET:HG2  | 2.05                     | 0.56              |
| 8:I:7:VAL:HA      | 8:I:10:LEU:HD12   | 1.87                     | 0.56              |
| 12:M:98:LYS:HD3   | 12:M:98:LYS:C     | 2.30                     | 0.56              |
| 27:d:142:ARG:NE   | 28:e:138:GLU:O    | 2.35                     | 0.56              |
| 52:l:701:CDL:H242 | 48:l:704:PEE:H34  | 1.86                     | 0.56              |
| 39:p:22:ARG:NH2   | 39:p:68:GLU:OE1   | 2.38                     | 0.56              |
| 1:A:56:ALA:O      | 1:A:61:ASP:HB2    | 2.05                     | 0.56              |
| 1:A:325:PRO:O     | 1:A:347:THR:OG1   | 2.19                     | 0.56              |
| 52:l:701:CDL:H352 | 40:r:361:VAL:HG13 | 1.85                     | 0.56              |
| 40:r:306:PRO:HB3  | 40:r:458:LEU:HD12 | 1.87                     | 0.56              |
| 41:s:62:ARG:HD2   | 41:s:68:ILE:CD1   | 2.35                     | 0.56              |
| 43:v:109:LEU:HD23 | 43:v:109:LEU:C    | 2.30                     | 0.56              |
| 50:J:402:UQ:O1    | 50:J:402:UQ:HM23  | 2.04                     | 0.56              |
| 48:V:202:PEE:C46  | 40:r:201:MET:HE2  | 2.33                     | 0.56              |
| 34:k:20:LEU:HD13  | 35:l:592:LEU:HB2  | 1.87                     | 0.56              |
| 11:L:112:MET:SD   | 13:N:126:PRO:HB2  | 2.46                     | 0.56              |
| 12:M:509:ASP:N    | 12:M:509:ASP:OD1  | 2.39                     | 0.56              |
| 41:s:40:VAL:O     | 41:s:40:VAL:HG22  | 2.04                     | 0.56              |
| 16:Q:304:LYS:NZ   | 16:Q:316:PHE:O    | 2.35                     | 0.56              |
| 20:V:3:LYS:H      | 35:l:605:HIS:CE1  | 2.21                     | 0.56              |
| 6:X:105:MET:CE    | 6:X:139:MET:HE1   | 2.28                     | 0.56              |
| 52:l:702:CDL:H321 | 52:l:702:CDL:H112 | 1.88                     | 0.56              |
| 1:A:398:ARG:NH1   | 12:M:155:GLU:OE2  | 2.38                     | 0.56              |
| 52:J:404:CDL:H561 | 48:W:201:PEE:H45  | 1.88                     | 0.56              |
| 21:W:98:MET:HE2   | 21:W:104:TRP:CD2  | 2.41                     | 0.56              |
| 18:T:43:GLN:NE2   | 18:T:60:LYS:NZ    | 2.54                     | 0.56              |
| 38:o:91:ALA:O     | 38:o:95:ILE:HB    | 2.06                     | 0.56              |
| 2:B:89:GLU:OE2    | 13:N:34:ARG:NH2   | 2.38                     | 0.56              |
| 5:F:65:LEU:HB2    | 5:F:79:LEU:HD11   | 1.87                     | 0.56              |
| 1:A:265:PHE:HB3   | 1:A:291:GLU:HG3   | 1.88                     | 0.55              |
| 52:J:404:CDL:H222 | 48:j:202:PEE:H31  | 1.88                     | 0.55              |
| 52:u:201:CDL:H581 | 52:u:201:CDL:C54  | 2.36                     | 0.55              |
| 9:J:346:GLU:HG2   | 9:J:371:PRO:HB3   | 1.87                     | 0.55              |
| 12:M:371:VAL:HG22 | 12:M:533:GLY:HA2  | 1.87                     | 0.55              |
| 32:i:221:HIS:HB2  | 32:i:323:MET:HE1  | 1.88                     | 0.55              |
| 43:v:12:ASP:OD2   | 43:v:15:LYS:NZ    | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:83:LEU:HD22  | 44:w:156:GLY:HA3  | 1.89                     | 0.55              |
| 35:l:72:GLN:CD    | 35:l:72:GLN:H     | 2.13                     | 0.55              |
| 52:l:702:CDL:H112 | 52:l:702:CDL:C32  | 2.36                     | 0.55              |
| 12:M:337:ASP:O    | 12:M:542:PRO:CB   | 2.54                     | 0.55              |
| 27:d:109:ARG:NH1  | 28:e:130:GLU:OE2  | 2.29                     | 0.55              |
| 32:i:171:ASN:ND2  | 35:l:578:SER:OG   | 2.36                     | 0.55              |
| 35:l:271:LYS:N    | 35:l:271:LYS:HE2  | 2.21                     | 0.55              |
| 3:C:188:LYS:HG2   | 3:C:191:ARG:HH11  | 1.71                     | 0.55              |
| 12:M:390:THR:HB   | 12:M:600:GLU:OE2  | 2.06                     | 0.55              |
| 21:W:10:MET:HE3   | 21:W:11:PRO:HD2   | 1.89                     | 0.55              |
| 52:a:201:CDL:H191 | 52:a:201:CDL:H752 | 1.88                     | 0.55              |
| 48:C:302:PEE:H31  | 49:C:303:PLX:H392 | 1.88                     | 0.55              |
| 7:H:9:THR:O       | 7:H:76:GLN:NE2    | 2.39                     | 0.55              |
| 14:O:135:CYS:SG   | 14:O:176:CYS:HA   | 2.47                     | 0.55              |
| 16:Q:156:GLU:HG3  | 16:Q:229:PRO:O    | 2.06                     | 0.55              |
| 1:A:201:ALA:HA    | 14:O:121:MET:HE2  | 1.89                     | 0.55              |
| 14:O:148:ILE:HG13 | 14:O:184:PRO:CG   | 2.37                     | 0.55              |
| 1:A:56:ALA:C      | 1:A:61:ASP:HB2    | 2.31                     | 0.55              |
| 1:A:384:PRO:HB2   | 1:A:423:THR:HG22  | 1.87                     | 0.55              |
| 14:O:129:LYS:H    | 14:O:168:LEU:HA   | 1.72                     | 0.55              |
| 16:Q:52:MET:HE2   | 32:i:173:THR:HG22 | 1.88                     | 0.55              |
| 32:i:117:GLU:OE2  | 34:k:98:CYS:SG    | 2.63                     | 0.55              |
| 35:l:293:ILE:HG13 | 35:l:294:THR:HG23 | 1.89                     | 0.55              |
| 15:P:201:ASP:OD1  | 15:P:201:ASP:N    | 2.40                     | 0.55              |
| 24:a:134:GLU:OE1  | 37:n:57:TRP:NE1   | 2.26                     | 0.55              |
| 32:i:243:LEU:HD23 | 52:r:502:CDL:H361 | 1.88                     | 0.55              |
| 41:s:24:GLU:OE1   | 41:s:228:TYR:OH   | 2.16                     | 0.55              |
| 48:C:302:PEE:O5   | 48:C:302:PEE:H52  | 2.07                     | 0.55              |
| 31:h:69:ARG:O     | 31:h:73:MET:HG3   | 2.06                     | 0.55              |
| 32:i:128:LEU:HD12 | 32:i:216:PHE:HB3  | 1.89                     | 0.55              |
| 35:l:483:PRO:HD2  | 35:l:486:MET:HE2  | 1.89                     | 0.55              |
| 35:l:534:HIS:CD2  | 48:l:703:PEE:H13  | 2.42                     | 0.55              |
| 12:M:387:LEU:HD12 | 12:M:514:ASN:HB3  | 1.88                     | 0.54              |
| 26:c:75:TYR:CG    | 26:c:76:PRO:HD2   | 2.41                     | 0.54              |
| 39:p:54:GLU:HG2   | 39:p:59:LYS:HD3   | 1.89                     | 0.54              |
| 49:e:201:PLX:H382 | 40:r:67:VAL:HG12  | 1.89                     | 0.54              |
| 32:i:172:GLN:HB2  | 32:i:178:ILE:HG13 | 1.89                     | 0.54              |
| 6:G:92:LYS:HE2    | 6:G:114:ASP:OD2   | 2.07                     | 0.54              |
| 14:O:164:THR:HG22 | 14:O:166:ASP:H    | 1.71                     | 0.54              |
| 35:l:407:TRP:O    | 35:l:411:MET:HG2  | 2.08                     | 0.54              |
| 4:E:25:MET:HE1    | 4:E:79:VAL:HG21   | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:299:ARG:HG3   | 9:J:316:ARG:HG2   | 1.88                     | 0.54              |
| 12:M:394:VAL:HA   | 12:M:473:MET:HE1  | 1.88                     | 0.54              |
| 32:i:88:LYS:O     | 32:i:148:SER:HB3  | 2.05                     | 0.54              |
| 35:l:375:ILE:HD12 | 35:l:458:LEU:HD11 | 1.88                     | 0.54              |
| 1:A:285:PRO:O     | 14:O:222:ARG:NH2  | 2.40                     | 0.54              |
| 26:c:39:GLY:O     | 26:c:74:ASP:HB2   | 2.08                     | 0.54              |
| 44:w:180:ARG:NH1  | 44:w:316:GLU:OE2  | 2.40                     | 0.54              |
| 44:w:204:VAL:HG21 | 44:w:249:MET:HG2  | 1.88                     | 0.54              |
| 2:B:62:LEU:HD12   | 21:W:35:MET:HE3   | 1.89                     | 0.54              |
| 9:J:204:SER:OG    | 9:J:238:GLN:O     | 2.25                     | 0.54              |
| 16:Q:53:TYR:OH    | 32:i:295:ARG:NH2  | 2.40                     | 0.54              |
| 40:r:370:PRO:HG3  | 40:r:375:LEU:HD13 | 1.90                     | 0.54              |
| 16:Q:404:LYS:HE2  | 16:Q:457:VAL:HG23 | 1.89                     | 0.54              |
| 22:Y:99:ILE:HG21  | 43:v:107:ARG:HG3  | 1.88                     | 0.54              |
| 26:c:116:ARG:HG2  | 48:l:703:PEE:H49  | 1.89                     | 0.54              |
| 1:A:210:THR:HB    | 1:A:224:ARG:HG2   | 1.90                     | 0.54              |
| 2:B:171:PRO:HB3   | 13:N:93:MET:HE1   | 1.90                     | 0.54              |
| 9:J:178:SER:OG    | 9:J:317:ASP:OD1   | 2.23                     | 0.54              |
| 26:c:38:PRO:HD3   | 38:o:67:ARG:HG2   | 1.89                     | 0.54              |
| 5:F:61:VAL:HG23   | 5:F:62:GLN:H      | 1.73                     | 0.54              |
| 36:m:82:VAL:HG22  | 36:m:85:SER:HB3   | 1.90                     | 0.54              |
| 9:J:117:ARG:O     | 9:J:121:GLU:HG3   | 2.08                     | 0.54              |
| 9:J:313:TRP:CG    | 50:J:402:UQ:C8    | 2.89                     | 0.54              |
| 15:P:187:ILE:HG23 | 15:P:188:LEU:HG   | 1.90                     | 0.54              |
| 12:M:217:GLU:HG2  | 12:M:218:LEU:HG   | 1.90                     | 0.53              |
| 25:b:106:PRO:HG2  | 25:b:120:MET:SD   | 2.47                     | 0.53              |
| 44:w:108:LEU:HD21 | 44:w:330:LYS:HD3  | 1.90                     | 0.53              |
| 4:E:68:MET:HE2    | 51:G:201:8Q1:C30  | 2.26                     | 0.53              |
| 6:G:93:ILE:HD11   | 6:G:110:LEU:HD11  | 1.88                     | 0.53              |
| 35:l:166:THR:CG2  | 48:l:703:PEE:H2   | 2.39                     | 0.53              |
| 40:r:403:THR:HA   | 40:r:406:TYR:CE2  | 2.43                     | 0.53              |
| 14:O:140:CYS:SG   | 54:O:301:FES:S2   | 3.06                     | 0.53              |
| 24:a:161:ARG:CZ   | 30:g:1:MET:CB     | 2.86                     | 0.53              |
| 12:M:51:GLN:HA    | 12:M:54:GLU:HG2   | 1.89                     | 0.53              |
| 41:s:67:SER:O     | 41:s:71:PHE:HB2   | 2.08                     | 0.53              |
| 2:B:49:ASP:OD1    | 2:B:52:SER:OG     | 2.25                     | 0.53              |
| 52:V:203:CDL:H742 | 52:V:203:CDL:H601 | 1.90                     | 0.53              |
| 6:X:126:PHE:CE2   | 6:X:148:ILE:HD13  | 2.44                     | 0.53              |
| 32:i:93:VAL:HG13  | 35:l:599:MET:HE1  | 1.91                     | 0.53              |
| 32:i:147:GLN:CD   | 32:i:147:GLN:H    | 2.17                     | 0.53              |
| 52:r:502:CDL:H201 | 52:r:502:CDL:H351 | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:246:LEU:HD22 | 44:w:255:VAL:HG11 | 1.90                     | 0.53              |
| 8:I:12:ARG:HB3    | 8:I:20:LEU:HD12   | 1.90                     | 0.53              |
| 9:J:168:SER:O     | 9:J:203:PRO:HD2   | 2.09                     | 0.53              |
| 14:O:177:LEU:HD12 | 14:O:185:MET:CE   | 2.38                     | 0.53              |
| 15:P:43:THR:HA    | 15:P:47:ILE:HD12  | 1.89                     | 0.53              |
| 52:a:201:CDL:H362 | 25:b:80:TRP:HB3   | 1.91                     | 0.53              |
| 21:W:103:ASP:OD1  | 21:W:103:ASP:N    | 2.40                     | 0.53              |
| 35:l:536:LEU:HB3  | 35:l:537:PRO:HD3  | 1.90                     | 0.53              |
| 33:j:95:LEU:HD13  | 41:s:302:MET:HG3  | 1.91                     | 0.53              |
| 12:M:390:THR:HA   | 12:M:600:GLU:HG2  | 1.91                     | 0.53              |
| 1:A:263:ALA:HA    | 1:A:271:SER:HB3   | 1.91                     | 0.52              |
| 1:A:448:GLU:O     | 1:A:452:GLN:HG2   | 2.10                     | 0.52              |
| 20:V:106:ARG:HA   | 20:V:106:ARG:NE   | 2.24                     | 0.52              |
| 26:c:153:TYR:OH   | 43:v:8:ARG:NH1    | 2.37                     | 0.52              |
| 4:E:120:SER:O     | 4:E:124:VAL:HG22  | 2.08                     | 0.52              |
| 21:W:70:ALA:HB2   | 42:u:125:LEU:HD13 | 1.91                     | 0.52              |
| 25:b:5:THR:OG1    | 25:b:8:GLU:HG3    | 2.09                     | 0.52              |
| 32:i:30:TRP:O     | 32:i:34:GLU:HG2   | 2.09                     | 0.52              |
| 32:i:246:VAL:HG11 | 52:r:502:CDL:H392 | 1.91                     | 0.52              |
| 35:l:51:LEU:O     | 35:l:55:MET:HG3   | 2.09                     | 0.52              |
| 41:s:63:PRO:HB2   | 41:s:66:SER:HB3   | 1.92                     | 0.52              |
| 41:s:85:MET:HE1   | 41:s:109:SER:HB3  | 1.90                     | 0.52              |
| 6:X:123:GLU:OE1   | 39:p:25:ARG:NH2   | 2.36                     | 0.52              |
| 28:e:97:ILE:O     | 28:e:101:LEU:HB2  | 2.09                     | 0.52              |
| 35:l:68:TRP:CZ3   | 35:l:69:MET:HE2   | 2.44                     | 0.52              |
| 1:A:369:ARG:NH2   | 14:O:136:THR:OG1  | 2.41                     | 0.52              |
| 12:M:391:ILE:HG13 | 12:M:600:GLU:CD   | 2.34                     | 0.52              |
| 25:b:25:ASP:OD2   | 39:p:125:TRP:NE1  | 2.36                     | 0.52              |
| 3:C:126:GLU:HG2   | 9:J:89:TYR:OH     | 2.09                     | 0.52              |
| 34:k:79:VAL:HG12  | 34:k:80:MET:HE2   | 1.90                     | 0.52              |
| 22:Y:69:ILE:HD13  | 35:l:383:MET:HE2  | 1.92                     | 0.52              |
| 28:e:89:VAL:HG21  | 40:r:25:ILE:HG23  | 1.92                     | 0.52              |
| 41:s:62:ARG:HD2   | 41:s:68:ILE:HD11  | 1.91                     | 0.52              |
| 1:A:235:VAL:H     | 1:A:240:THR:HG21  | 1.74                     | 0.52              |
| 8:I:30:GLU:CD     | 8:I:30:GLU:H      | 2.17                     | 0.52              |
| 16:Q:95:LEU:HB2   | 16:Q:458:PHE:CZ   | 2.45                     | 0.52              |
| 32:i:72:MET:HE2   | 32:i:76:ILE:HG13  | 1.92                     | 0.52              |
| 51:X:201:8Q1:O40  | 39:p:12:HIS:CE1   | 2.54                     | 0.52              |
| 27:d:16:ARG:NH2   | 43:v:48:ASP:OD2   | 2.42                     | 0.52              |
| 29:f:60:LYS:O     | 29:f:64:GLU:HG3   | 2.10                     | 0.52              |
| 35:l:601:LEU:HD23 | 35:l:602:PHE:CE1  | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:351:LEU:O    | 12:M:530:TYR:OH   | 2.28                     | 0.52              |
| 15:P:44:ARG:HB2   | 15:P:44:ARG:CZ    | 2.39                     | 0.52              |
| 35:l:356:ILE:HA   | 35:l:359:MET:SD   | 2.50                     | 0.52              |
| 40:r:273:SER:HB3  | 40:r:402:ILE:CG2  | 2.39                     | 0.52              |
| 1:A:296:LEU:HD22  | 1:A:332:CYS:HB3   | 1.91                     | 0.52              |
| 4:E:48:HIS:NE2    | 9:J:365:GLU:OE1   | 2.37                     | 0.52              |
| 5:F:86:GLN:O      | 5:F:90:THR:HG22   | 2.11                     | 0.52              |
| 16:Q:53:TYR:OH    | 48:Q:503:PEE:O2P  | 2.12                     | 0.52              |
| 51:X:201:8Q1:O4   | 39:p:48:PHE:HA    | 2.10                     | 0.52              |
| 48:j:202:PEE:O1P  | 41:s:62:ARG:CZ    | 2.58                     | 0.52              |
| 14:O:177:LEU:CD1  | 14:O:185:MET:HE1  | 2.39                     | 0.51              |
| 46:A:502:FMN:N5   | 47:A:503:NAI:H4N  | 2.25                     | 0.51              |
| 6:X:85:TYR:OH     | 23:Z:22:TRP:NE1   | 2.30                     | 0.51              |
| 9:J:222:TRP:HZ3   | 52:J:404:CDL:HA4  | 1.74                     | 0.51              |
| 32:i:270:MET:O    | 32:i:275:SER:HB3  | 2.10                     | 0.51              |
| 48:l:703:PEE:H7   | 48:l:703:PEE:H14  | 1.93                     | 0.51              |
| 38:o:20:PRO:HB3   | 39:p:65:ARG:HH12  | 1.74                     | 0.51              |
| 1:A:217:GLU:OE1   | 11:L:171:ARG:NH2  | 2.43                     | 0.51              |
| 6:G:107:ASP:OD1   | 6:G:107:ASP:N     | 2.44                     | 0.51              |
| 20:V:110:ILE:HD11 | 48:V:204:PEE:C3   | 2.41                     | 0.51              |
| 25:b:32:GLU:OE1   | 39:p:115:TYR:HA   | 2.10                     | 0.51              |
| 32:i:62:THR:HG21  | 32:i:114:TRP:CD1  | 2.44                     | 0.51              |
| 39:p:101:GLU:O    | 39:p:122:ARG:NH2  | 2.44                     | 0.51              |
| 1:A:83:SER:HB2    | 1:A:259:GLY:HA2   | 1.92                     | 0.51              |
| 6:G:116:VAL:HG12  | 6:G:120:MET:HE2   | 1.90                     | 0.51              |
| 17:S:63:THR:HG23  | 42:u:21:SER:CB    | 2.40                     | 0.51              |
| 30:g:52:ARG:NH2   | 44:w:338:LYS:O    | 2.43                     | 0.51              |
| 36:m:35:VAL:O     | 36:m:39:VAL:HG22  | 2.11                     | 0.51              |
| 41:s:24:GLU:HG3   | 41:s:271:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:115:VAL:HG22  | 1:A:248:VAL:HG21  | 1.93                     | 0.51              |
| 1:A:398:ARG:NH2   | 1:A:408:GLU:OE1   | 2.38                     | 0.51              |
| 20:V:46:PRO:HB2   | 20:V:51:GLU:HG2   | 1.93                     | 0.51              |
| 22:Y:100:LEU:HD13 | 22:Y:104:GLU:HB2  | 1.92                     | 0.51              |
| 25:b:10:LEU:O     | 25:b:14:GLN:HG3   | 2.11                     | 0.51              |
| 46:A:502:FMN:N1   | 46:A:502:FMN:O3'  | 2.39                     | 0.51              |
| 5:F:42:VAL:O      | 5:F:46:LYS:HG2    | 2.10                     | 0.51              |
| 8:I:54:TYR:CZ     | 16:Q:362:LYS:HD2  | 2.46                     | 0.51              |
| 12:M:306:MET:HB2  | 12:M:583:ILE:HB   | 1.93                     | 0.51              |
| 15:P:161:LYS:HG2  | 16:Q:285:ASN:HD22 | 1.76                     | 0.51              |
| 6:X:91:ASP:OD1    | 23:Z:47:ARG:NH2   | 2.31                     | 0.51              |
| 27:d:99:ASP:CB    | 28:e:137:MET:CE   | 2.88                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:l:599:MET:O    | 35:l:603:ASN:CB   | 2.43                     | 0.51              |
| 4:E:123:TYR:CZ    | 12:M:320:GLU:HG3  | 2.46                     | 0.51              |
| 6:G:130:ILE:HG21  | 6:G:135:ALA:HB2   | 1.92                     | 0.51              |
| 43:v:42:THR:HG22  | 43:v:44:GLN:H     | 1.76                     | 0.51              |
| 9:J:220:MET:HE2   | 9:J:227:PRO:HD2   | 1.92                     | 0.50              |
| 12:M:379:THR:O    | 12:M:379:THR:HG22 | 2.10                     | 0.50              |
| 24:a:153:GLU:HG3  | 30:g:92:MET:HE2   | 1.92                     | 0.50              |
| 33:j:90:MET:HE1   | 49:j:203:PLX:H281 | 1.92                     | 0.50              |
| 43:v:97:LYS:O     | 43:v:101:GLU:HG2  | 2.11                     | 0.50              |
| 31:h:29:ILE:HG21  | 36:m:138:GLU:HG3  | 1.92                     | 0.50              |
| 3:C:80:ALA:HA     | 3:C:86:MET:HG2    | 1.94                     | 0.50              |
| 16:Q:47:PHE:HD1   | 16:Q:52:MET:HE1   | 1.76                     | 0.50              |
| 19:U:26:GLY:HA3   | 48:j:201:PEE:H38  | 1.94                     | 0.50              |
| 20:V:136:PHE:HD1  | 32:i:155:LEU:HD13 | 1.77                     | 0.50              |
| 23:Z:32:VAL:O     | 23:Z:36:LEU:HG    | 2.12                     | 0.50              |
| 32:i:128:LEU:O    | 32:i:132:THR:OG1  | 2.24                     | 0.50              |
| 1:A:234:GLY:HA3   | 1:A:240:THR:HG22  | 1.93                     | 0.50              |
| 32:i:122:ILE:O    | 32:i:176:ARG:NH1  | 2.41                     | 0.50              |
| 1:A:367:ILE:HG13  | 1:A:438:LEU:HD13  | 1.94                     | 0.50              |
| 13:N:7:LEU:O      | 13:N:11:LEU:HG    | 2.11                     | 0.50              |
| 34:k:31:LEU:HD21  | 36:m:67:VAL:HG11  | 1.93                     | 0.50              |
| 35:l:190:LEU:HD22 | 40:r:383:THR:HG21 | 1.93                     | 0.50              |
| 1:A:214:GLU:OE2   | 1:A:224:ARG:NH2   | 2.40                     | 0.50              |
| 16:Q:218:SER:OG   | 16:Q:224:ALA:HB1  | 2.12                     | 0.50              |
| 36:m:45:LEU:HD12  | 36:m:50:SER:HA    | 1.92                     | 0.50              |
| 41:s:170:GLU:OE1  | 42:u:98:ARG:NH1   | 2.44                     | 0.50              |
| 9:J:87:GLU:HG3    | 9:J:89:TYR:H      | 1.77                     | 0.50              |
| 35:l:102:GLU:OE1  | 35:l:456:ARG:NH2  | 2.34                     | 0.50              |
| 39:p:132:SER:OG   | 39:p:136:GLU:OE2  | 2.27                     | 0.50              |
| 42:u:83:THR:HA    | 42:u:86:TRP:CD1   | 2.47                     | 0.50              |
| 43:v:109:LEU:CD2  | 43:v:109:LEU:C    | 2.85                     | 0.50              |
| 7:H:38:ILE:O      | 7:H:45:ARG:NH1    | 2.36                     | 0.50              |
| 16:Q:218:SER:CB   | 16:Q:224:ALA:HB1  | 2.42                     | 0.50              |
| 22:Y:65:MET:SD    | 35:l:375:ILE:HG12 | 2.52                     | 0.50              |
| 38:o:75:ASN:O     | 38:o:79:ASN:ND2   | 2.45                     | 0.50              |
| 42:u:34:ALA:HB2   | 42:u:120:PRO:HG3  | 1.93                     | 0.50              |
| 2:B:86:TYR:CD1    | 2:B:87:PRO:HA     | 2.47                     | 0.49              |
| 32:i:222:SER:O    | 32:i:224:ALA:N    | 2.45                     | 0.49              |
| 33:j:83:ASN:HD21  | 36:m:148:SER:HB2  | 1.77                     | 0.49              |
| 52:J:404:CDL:HB61 | 52:J:404:CDL:H322 | 1.94                     | 0.49              |
| 25:b:99:GLU:CD    | 35:l:61:MET:HE2   | 2.37                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:c:75:TYR:OH    | 26:c:105:ILE:O    | 2.17                     | 0.49              |
| 27:d:106:ILE:HD11 | 28:e:136:LEU:HD21 | 1.93                     | 0.49              |
| 41:s:145:THR:HG21 | 41:s:289:LEU:HD12 | 1.93                     | 0.49              |
| 44:w:58:LYS:O     | 44:w:60:ILE:HG13  | 2.12                     | 0.49              |
| 6:X:89:LEU:HD21   | 23:Z:19:TYR:HB2   | 1.93                     | 0.49              |
| 40:r:373:ILE:HA   | 40:r:376:ILE:HD12 | 1.93                     | 0.49              |
| 8:I:66:PRO:HB3    | 15:P:79:SER:HA    | 1.94                     | 0.49              |
| 8:I:69:VAL:O      | 15:P:76:VAL:HB    | 2.11                     | 0.49              |
| 18:T:43:GLN:HE21  | 18:T:60:LYS:HZ1   | 1.59                     | 0.49              |
| 34:k:21:MET:HE1   | 52:k:101:CDL:H591 | 1.95                     | 0.49              |
| 35:l:519:THR:HG22 | 52:l:702:CDL:H711 | 1.95                     | 0.49              |
| 40:r:133:ILE:HD11 | 40:r:231:LEU:HD11 | 1.94                     | 0.49              |
| 6:G:84:LEU:O      | 6:G:88:LYS:HG2    | 2.13                     | 0.49              |
| 12:M:531:LYS:HB2  | 12:M:531:LYS:NZ   | 2.27                     | 0.49              |
| 35:l:394:LEU:HA   | 35:l:397:GLU:HG2  | 1.94                     | 0.49              |
| 52:l:701:CDL:H371 | 40:r:369:LEU:HD23 | 1.94                     | 0.49              |
| 1:A:255:CYS:O     | 14:O:246:GLN:OE1  | 2.30                     | 0.49              |
| 1:A:283:ASN:ND2   | 1:A:305:GLY:O     | 2.46                     | 0.49              |
| 19:U:38:TYR:HB2   | 41:s:310:MET:O    | 2.12                     | 0.49              |
| 6:X:82:ARG:HH12   | 35:l:440:LEU:HD22 | 1.78                     | 0.49              |
| 15:P:147:THR:HB   | 15:P:153:ILE:HD11 | 1.94                     | 0.49              |
| 49:e:201:PLX:H102 | 52:l:701:CDL:H641 | 1.93                     | 0.49              |
| 32:i:68:MET:HE1   | 34:k:37:MET:SD    | 2.53                     | 0.49              |
| 38:o:95:ILE:HG23  | 38:o:99:PHE:HE2   | 1.77                     | 0.49              |
| 39:p:55:LYS:HD3   | 39:p:55:LYS:N     | 2.26                     | 0.49              |
| 8:I:26:LEU:HD13   | 13:N:55:PHE:CD2   | 2.48                     | 0.49              |
| 9:J:238:GLN:HG2   | 9:J:266:VAL:HB    | 1.94                     | 0.49              |
| 24:a:66:ARG:HH12  | 28:e:72:ASP:HB2   | 1.76                     | 0.49              |
| 52:l:702:CDL:H601 | 52:l:702:CDL:C37  | 2.25                     | 0.49              |
| 44:w:95:ASP:OD1   | 44:w:95:ASP:N     | 2.46                     | 0.49              |
| 1:A:134:ASP:N     | 1:A:134:ASP:OD1   | 2.45                     | 0.48              |
| 50:J:402:UQ:H201  | 50:J:402:UQ:C23   | 2.43                     | 0.48              |
| 25:b:81:ILE:HG23  | 48:l:704:PEE:H58  | 1.94                     | 0.48              |
| 20:V:69:ILE:O     | 20:V:73:THR:HG23  | 2.12                     | 0.48              |
| 30:g:2:THR:HG21   | 30:g:5:SER:HB2    | 1.94                     | 0.48              |
| 32:i:81:SER:O     | 32:i:83:GLN:N     | 2.43                     | 0.48              |
| 34:k:19:LEU:CD2   | 34:k:36:MET:HE1   | 2.42                     | 0.48              |
| 36:m:26:PRO:HB2   | 36:m:71:THR:HG23  | 1.94                     | 0.48              |
| 49:J:403:PLX:H132 | 48:j:202:PEE:C37  | 2.44                     | 0.48              |
| 12:M:29:SER:OG    | 12:M:30:ASN:N     | 2.45                     | 0.48              |
| 14:O:175:GLU:OE1  | 14:O:175:GLU:HA   | 2.11                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:X:139:MET:HA    | 6:X:139:MET:HE2   | 1.92                     | 0.48              |
| 28:e:125:LEU:O    | 28:e:129:ARG:HG3  | 2.13                     | 0.48              |
| 38:o:57:LEU:C     | 38:o:57:LEU:HD13  | 2.38                     | 0.48              |
| 40:r:392:THR:O    | 40:r:396:MET:HG2  | 2.12                     | 0.48              |
| 1:A:44:ASN:ND2    | 1:A:133:HIS:O     | 2.47                     | 0.48              |
| 1:A:273:THR:OG1   | 1:A:274:LYS:N     | 2.47                     | 0.48              |
| 1:A:385:CYS:HB2   | 45:A:501:SF4:S4   | 2.53                     | 0.48              |
| 4:E:101:THR:OG1   | 15:P:219:VAL:O    | 2.21                     | 0.48              |
| 34:k:4:VAL:O      | 34:k:8:ILE:HG12   | 2.12                     | 0.48              |
| 3:C:59:ARG:NH1    | 49:C:303:PLX:O2   | 2.45                     | 0.48              |
| 16:Q:94:VAL:HG21  | 16:Q:116:LEU:HB2  | 1.95                     | 0.48              |
| 48:V:202:PEE:H22  | 40:r:198:ALA:HB2  | 1.95                     | 0.48              |
| 33:j:106:TRP:CD2  | 48:j:201:PEE:H15  | 2.48                     | 0.48              |
| 35:l:173:LEU:HD12 | 40:r:405:LEU:HD21 | 1.96                     | 0.48              |
| 38:o:129:TYR:CD1  | 38:o:129:TYR:N    | 2.81                     | 0.48              |
| 9:J:174:ILE:HG23  | 9:J:175:LYS:HG2   | 1.95                     | 0.48              |
| 18:T:64:GLU:OE2   | 18:T:64:GLU:HA    | 2.14                     | 0.48              |
| 26:c:166:LEU:O    | 26:c:170:ARG:HG3  | 2.13                     | 0.48              |
| 32:i:119:THR:HG22 | 32:i:176:ARG:HB3  | 1.95                     | 0.48              |
| 34:k:37:MET:HE3   | 34:k:67:ALA:HB2   | 1.95                     | 0.48              |
| 3:C:52:ASP:HB3    | 49:C:303:PLX:H251 | 1.96                     | 0.48              |
| 5:F:91:LEU:O      | 5:F:95:LEU:HD12   | 2.12                     | 0.48              |
| 27:d:110:LEU:HD11 | 35:l:203:MET:HE2  | 1.96                     | 0.48              |
| 33:j:67:LEU:HD22  | 36:m:59:ILE:HD12  | 1.96                     | 0.48              |
| 37:n:39:ARG:HG3   | 37:n:57:TRP:CE2   | 2.49                     | 0.48              |
| 43:v:15:LYS:HA    | 43:v:109:LEU:HD21 | 1.91                     | 0.48              |
| 12:M:619:ASP:OD1  | 12:M:619:ASP:N    | 2.46                     | 0.48              |
| 20:V:40:SER:HA    | 52:V:201:CDL:HB61 | 1.95                     | 0.48              |
| 48:V:204:PEE:O2P  | 48:V:204:PEE:H7   | 2.14                     | 0.48              |
| 22:Y:103:ASP:OD1  | 22:Y:103:ASP:N    | 2.47                     | 0.48              |
| 10:K:98:MET:HE3   | 10:K:98:MET:HB3   | 1.77                     | 0.48              |
| 12:M:638:THR:O    | 12:M:642:VAL:HG23 | 2.13                     | 0.48              |
| 38:o:95:ILE:HG23  | 38:o:99:PHE:CE2   | 2.48                     | 0.48              |
| 2:B:44:ARG:HG2    | 2:B:44:ARG:NH1    | 2.22                     | 0.48              |
| 8:I:2:ALA:HB3     | 8:I:21:GLN:HE22   | 1.78                     | 0.48              |
| 17:S:66:LEU:HD11  | 42:u:74:ILE:HG22  | 1.95                     | 0.48              |
| 12:M:222:ILE:HD12 | 12:M:231:LEU:HD13 | 1.96                     | 0.47              |
| 12:M:347:ASP:HB3  | 12:M:594:ALA:HB1  | 1.96                     | 0.47              |
| 26:c:164:ASN:HA   | 26:c:181:VAL:HB   | 1.95                     | 0.47              |
| 31:h:84:ASP:HA    | 31:h:87:ILE:HG12  | 1.96                     | 0.47              |
| 32:i:267:ILE:HG12 | 32:i:279:PRO:HB3  | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:283:ALA:HB1  | 40:r:158:LEU:HD13 | 1.94                     | 0.47              |
| 39:p:28:GLU:OE2   | 39:p:34:ARG:NH1   | 2.46                     | 0.47              |
| 44:w:75:ARG:HG3   | 44:w:75:ARG:HH11  | 1.78                     | 0.47              |
| 6:G:93:ILE:HD13   | 6:G:108:LEU:HD13  | 1.95                     | 0.47              |
| 15:P:165:TRP:CD2  | 16:Q:433:ALA:HB2  | 2.48                     | 0.47              |
| 17:S:43:TYR:CZ    | 21:W:68:ARG:HG3   | 2.49                     | 0.47              |
| 20:V:34:LEU:HD11  | 52:k:101:CDL:H441 | 1.96                     | 0.47              |
| 21:W:61:GLN:NE2   | 41:s:317:GLN:H    | 2.11                     | 0.47              |
| 35:l:14:ILE:HD11  | 35:l:43:ALA:HA    | 1.95                     | 0.47              |
| 35:l:599:MET:HA   | 35:l:603:ASN:HB3  | 1.96                     | 0.47              |
| 1:A:208:GLU:OE1   | 1:A:210:THR:OG1   | 2.29                     | 0.47              |
| 20:V:141:VAL:C    | 24:a:161:ARG:HH11 | 2.22                     | 0.47              |
| 52:V:203:CDL:H782 | 35:l:557:TRP:CD2  | 2.49                     | 0.47              |
| 28:e:128:TYR:CZ   | 28:e:132:ASN:ND2  | 2.83                     | 0.47              |
| 48:j:201:PEE:H26  | 41:s:295:PRO:HB3  | 1.95                     | 0.47              |
| 34:k:3:LEU:HD23   | 36:m:121:GLY:HA2  | 1.96                     | 0.47              |
| 46:A:502:FMN:H9   | 46:A:502:FMN:H1'1 | 1.70                     | 0.47              |
| 49:C:303:PLX:H102 | 49:C:303:PLX:H261 | 1.97                     | 0.47              |
| 12:M:169:VAL:HG22 | 12:M:223:ILE:HD11 | 1.95                     | 0.47              |
| 12:M:262:VAL:HG23 | 12:M:276:ARG:HB2  | 1.96                     | 0.47              |
| 12:M:483:ARG:HH12 | 12:M:489:ILE:HD11 | 1.78                     | 0.47              |
| 12:M:690:THR:CG2  | 12:M:692:LYS:HG2  | 2.45                     | 0.47              |
| 25:b:18:LEU:HD11  | 39:p:163:LEU:HD22 | 1.97                     | 0.47              |
| 26:c:166:LEU:HB3  | 26:c:169:GLU:HB2  | 1.96                     | 0.47              |
| 40:r:271:MET:HE2  | 40:r:271:MET:HA   | 1.97                     | 0.47              |
| 23:Z:28:PRO:O     | 23:Z:32:VAL:HG23  | 2.15                     | 0.47              |
| 26:c:33:THR:OG1   | 26:c:35:ASP:OD1   | 2.19                     | 0.47              |
| 30:g:32:ARG:HB3   | 32:i:339:MET:HE1  | 1.97                     | 0.47              |
| 30:g:101:GLU:H    | 30:g:101:GLU:CD   | 2.22                     | 0.47              |
| 39:p:100:PRO:HD3  | 40:r:419:TYR:CZ   | 2.50                     | 0.47              |
| 40:r:253:LEU:CD1  | 40:r:256:TYR:HE1  | 2.27                     | 0.47              |
| 1:A:36:LYS:HG3    | 1:A:38:GLU:HG2    | 1.96                     | 0.47              |
| 1:A:40:ARG:NH2    | 1:A:289:GLU:O     | 2.43                     | 0.47              |
| 48:C:302:PEE:H31  | 49:C:303:PLX:C39  | 2.45                     | 0.47              |
| 9:J:71:ASN:HB2    | 9:J:97:MET:HE2    | 1.95                     | 0.47              |
| 12:M:347:ASP:OD1  | 12:M:347:ASP:N    | 2.39                     | 0.47              |
| 16:Q:84:PHE:HB3   | 16:Q:97:LEU:HB3   | 1.97                     | 0.47              |
| 16:Q:88:HIS:CE1   | 41:s:205:SER:O    | 2.65                     | 0.47              |
| 35:l:358:LYS:HG3  | 39:p:80:TYR:CE1   | 2.50                     | 0.47              |
| 35:l:359:MET:O    | 35:l:436:ARG:NH2  | 2.48                     | 0.47              |
| 36:m:17:PHE:HA    | 36:m:20:PHE:CE2   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:X:129:GLU:OE2   | 26:c:89:TRP:HZ2   | 1.98                     | 0.47              |
| 33:j:83:ASN:OD1   | 33:j:83:ASN:N     | 2.45                     | 0.47              |
| 35:l:534:HIS:CG   | 48:l:703:PEE:H13  | 2.49                     | 0.47              |
| 44:w:88:GLU:N     | 44:w:160:GLU:HG3  | 2.30                     | 0.47              |
| 1:A:90:GLY:HA3    | 47:A:503:NAI:H1D  | 1.97                     | 0.47              |
| 12:M:406:ASN:ND2  | 12:M:688:GLN:O    | 2.47                     | 0.47              |
| 6:X:123:GLU:HG2   | 6:X:129:GLU:HA    | 1.97                     | 0.47              |
| 26:c:39:GLY:C     | 26:c:74:ASP:HB2   | 2.40                     | 0.47              |
| 35:l:246:LEU:O    | 35:l:251:THR:OG1  | 2.32                     | 0.47              |
| 48:s:401:PEE:H61  | 48:s:401:PEE:H55  | 1.58                     | 0.47              |
| 4:E:23:ARG:NH2    | 11:L:52:LEU:O     | 2.48                     | 0.47              |
| 8:I:40:LYS:CG     | 21:W:6:VAL:HA     | 2.44                     | 0.47              |
| 35:l:510:TYR:HB3  | 35:l:512:LYS:HE3  | 1.97                     | 0.47              |
| 9:J:71:ASN:HA     | 9:J:97:MET:HG2    | 1.97                     | 0.46              |
| 16:Q:176:GLU:OE2  | 16:Q:311:TYR:OH   | 2.24                     | 0.46              |
| 16:Q:208:GLU:CD   | 16:Q:221:ARG:HH22 | 2.21                     | 0.46              |
| 16:Q:294:ARG:NH2  | 16:Q:401:GLU:OE2  | 2.48                     | 0.46              |
| 22:Y:97:LEU:HD23  | 43:v:107:ARG:HD2  | 1.98                     | 0.46              |
| 16:Q:432:LEU:HB2  | 16:Q:456:ILE:HD13 | 1.97                     | 0.46              |
| 18:T:37:LYS:HB2   | 18:T:37:LYS:HE3   | 1.54                     | 0.46              |
| 32:i:278:MET:O    | 32:i:282:MET:HG3  | 2.15                     | 0.46              |
| 38:o:117:GLN:OE1  | 38:o:117:GLN:HA   | 2.15                     | 0.46              |
| 41:s:59:GLU:HA    | 41:s:60:PRO:HD3   | 1.76                     | 0.46              |
| 23:Z:63:PHE:CZ    | 35:l:424:THR:HG23 | 2.51                     | 0.46              |
| 40:r:273:SER:HB3  | 40:r:402:ILE:HG21 | 1.97                     | 0.46              |
| 3:C:63:TRP:HH2    | 50:C:304:UQ:H153  | 1.80                     | 0.46              |
| 12:M:260:ASN:HD22 | 12:M:260:ASN:N    | 2.12                     | 0.46              |
| 15:P:161:LYS:HG2  | 16:Q:285:ASN:ND2  | 2.30                     | 0.46              |
| 27:d:61:TYR:CD1   | 27:d:61:TYR:N     | 2.84                     | 0.46              |
| 40:r:203:PHE:O    | 40:r:207:MET:HG2  | 2.15                     | 0.46              |
| 41:s:152:SER:HA   | 41:s:155:LEU:HD12 | 1.97                     | 0.46              |
| 4:E:16:SER:HA     | 11:L:52:LEU:HD13  | 1.97                     | 0.46              |
| 7:H:114:TRP:CD2   | 7:H:115:PRO:HA    | 2.51                     | 0.46              |
| 27:d:37:PHE:CE1   | 35:l:3:PRO:HB3    | 2.51                     | 0.46              |
| 35:l:298:ILE:O    | 35:l:302:VAL:HG23 | 2.16                     | 0.46              |
| 48:l:703:PEE:O5   | 48:l:703:PEE:H1   | 2.15                     | 0.46              |
| 1:A:62:TRP:HZ2    | 1:A:139:VAL:HG12  | 1.81                     | 0.46              |
| 1:A:81:LYS:HG2    | 1:A:96:GLY:HA3    | 1.96                     | 0.46              |
| 3:C:98:ARG:NH2    | 33:j:35:SER:O     | 2.48                     | 0.46              |
| 12:M:257:VAL:O    | 12:M:598:ASN:ND2  | 2.48                     | 0.46              |
| 13:N:129:THR:HA   | 18:T:43:GLN:HG2   | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:o:113:GLU:OE1  | 38:o:113:GLU:HA   | 2.16                     | 0.46              |
| 1:A:63:TYR:CE2    | 14:O:245:VAL:HG21 | 2.50                     | 0.46              |
| 3:C:188:LYS:HG2   | 3:C:191:ARG:NH1   | 2.31                     | 0.46              |
| 50:C:304:UQ:H262  | 50:C:304:UQ:H221  | 1.41                     | 0.46              |
| 48:V:204:PEE:H7   | 48:V:204:PEE:P    | 2.56                     | 0.46              |
| 22:Y:102:ASP:HA   | 43:v:111:ARG:HD3  | 1.97                     | 0.46              |
| 30:g:2:THR:CG2    | 30:g:5:SER:HB2    | 2.45                     | 0.46              |
| 35:l:20:MET:HG2   | 52:l:701:CDL:H821 | 1.97                     | 0.46              |
| 1:A:338:ASP:OD1   | 1:A:338:ASP:N     | 2.49                     | 0.46              |
| 4:E:101:THR:O     | 4:E:105:ARG:HG3   | 2.15                     | 0.46              |
| 9:J:134:TRP:CZ2   | 9:J:311:GLU:HG2   | 2.50                     | 0.46              |
| 12:M:407:PRO:HD2  | 12:M:438:LEU:HD21 | 1.98                     | 0.46              |
| 15:P:164:ASN:ND2  | 15:P:182:PRO:HG2  | 2.31                     | 0.46              |
| 18:T:43:GLN:NE2   | 18:T:60:LYS:HZ1   | 2.14                     | 0.46              |
| 20:V:140:LYS:HB3  | 20:V:140:LYS:HE2  | 1.54                     | 0.46              |
| 22:Y:51:THR:O     | 22:Y:54:GLN:HG2   | 2.15                     | 0.46              |
| 52:l:702:CDL:H592 | 52:l:702:CDL:H361 | 1.98                     | 0.46              |
| 36:m:28:TYR:CE2   | 36:m:82:VAL:HG12  | 2.51                     | 0.46              |
| 1:A:33:GLY:HA2    | 1:A:294:VAL:HB    | 1.98                     | 0.46              |
| 16:Q:58:THR:HG21  | 35:l:579:ASN:ND2  | 2.31                     | 0.46              |
| 18:T:32:SER:OG    | 18:T:36:GLU:O     | 2.29                     | 0.46              |
| 26:c:110:ASP:OD1  | 26:c:110:ASP:N    | 2.44                     | 0.46              |
| 32:i:21:MET:HE3   | 32:i:136:LEU:HB3  | 1.97                     | 0.46              |
| 48:j:201:PEE:H53  | 48:j:201:PEE:O5   | 2.16                     | 0.46              |
| 5:F:45:LYS:HA     | 5:F:45:LYS:HD2    | 1.73                     | 0.45              |
| 7:H:76:GLN:O      | 7:H:78:GLU:N      | 2.49                     | 0.45              |
| 12:M:389:THR:HG21 | 12:M:473:MET:HE2  | 1.98                     | 0.45              |
| 14:O:153:GLN:HG2  | 14:O:158:ILE:O    | 2.15                     | 0.45              |
| 20:V:2:ALA:HB1    | 35:l:605:HIS:CE1  | 2.51                     | 0.45              |
| 6:X:129:GLU:OE2   | 26:c:89:TRP:CZ2   | 2.69                     | 0.45              |
| 35:l:41:SER:O     | 35:l:45:THR:HG22  | 2.16                     | 0.45              |
| 35:l:264:TYR:CD2  | 35:l:265:PRO:HD3  | 2.51                     | 0.45              |
| 35:l:514:LYS:HB3  | 35:l:514:LYS:HE3  | 1.66                     | 0.45              |
| 1:A:62:TRP:CZ2    | 1:A:139:VAL:HG12  | 2.51                     | 0.45              |
| 11:L:140:LYS:NZ   | 15:P:149:GLU:OE2  | 2.48                     | 0.45              |
| 14:O:148:ILE:CG1  | 14:O:184:PRO:CG   | 2.94                     | 0.45              |
| 43:v:66:LEU:HD11  | 43:v:70:LYS:HE3   | 1.98                     | 0.45              |
| 3:C:73:ALA:HB1    | 56:Q:501:UQ1:C11  | 2.43                     | 0.45              |
| 8:I:40:LYS:HG2    | 21:W:6:VAL:HA     | 1.98                     | 0.45              |
| 52:J:404:CDL:H381 | 52:J:404:CDL:H742 | 1.98                     | 0.45              |
| 32:i:289:ASN:HA   | 32:i:292:PHE:CE2  | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:Y:86:TYR:HD1   | 35:l:481:THR:HG22 | 1.81                     | 0.45              |
| 23:Z:14:MET:HE3   | 23:Z:14:MET:HB3   | 1.76                     | 0.45              |
| 27:d:37:PHE:CD1   | 35:l:3:PRO:HB3    | 2.50                     | 0.45              |
| 35:l:66:TRP:CD1   | 48:l:704:PEE:C12  | 2.96                     | 0.45              |
| 1:A:63:TYR:HE2    | 14:O:245:VAL:HG21 | 1.81                     | 0.45              |
| 5:F:61:VAL:O      | 5:F:62:GLN:HG2    | 2.15                     | 0.45              |
| 12:M:208:THR:OG1  | 12:M:210:ILE:O    | 2.34                     | 0.45              |
| 26:c:96:ASP:N     | 26:c:96:ASP:OD1   | 2.50                     | 0.45              |
| 34:k:17:ALA:HB2   | 52:k:101:CDL:H811 | 1.97                     | 0.45              |
| 40:r:210:TYR:CG   | 40:r:268:GLY:HA3  | 2.52                     | 0.45              |
| 4:E:68:MET:HE2    | 4:E:68:MET:HA     | 1.99                     | 0.45              |
| 5:F:65:LEU:HD11   | 5:F:91:LEU:HD13   | 1.98                     | 0.45              |
| 5:F:83:SER:O      | 5:F:87:VAL:HG13   | 2.17                     | 0.45              |
| 8:I:90:THR:OG1    | 8:I:91:GLU:N      | 2.49                     | 0.45              |
| 12:M:137:CYS:HB3  | 12:M:140:GLN:HB2  | 1.98                     | 0.45              |
| 14:O:193:TYR:HD1  | 14:O:219:ARG:HH21 | 1.63                     | 0.45              |
| 17:S:59:ARG:HD2   | 17:S:61:HIS:NE2   | 2.31                     | 0.45              |
| 49:e:201:PLX:H202 | 52:l:701:CDL:H792 | 1.99                     | 0.45              |
| 48:j:202:PEE:H40  | 41:s:77:LEU:CD1   | 2.47                     | 0.45              |
| 1:A:177:TYR:CD2   | 10:K:93:LEU:HD22  | 2.51                     | 0.45              |
| 3:C:94:ARG:HH12   | 50:C:304:UQ:HM51  | 1.81                     | 0.45              |
| 14:O:195:ASP:OD2  | 14:O:220:SER:OG   | 2.28                     | 0.45              |
| 15:P:207:TYR:C    | 15:P:224:VAL:HG23 | 2.41                     | 0.45              |
| 16:Q:188:THR:HB   | 16:Q:200:PHE:HA   | 1.98                     | 0.45              |
| 49:e:201:PLX:H282 | 40:r:446:LEU:HB3  | 1.99                     | 0.45              |
| 39:p:57:MET:O     | 39:p:61:THR:HG23  | 2.16                     | 0.45              |
| 28:e:72:ASP:OD1   | 28:e:72:ASP:N     | 2.50                     | 0.45              |
| 32:i:337:LEU:O    | 32:i:340:THR:OG1  | 2.27                     | 0.45              |
| 1:A:75:TRP:O      | 1:A:79:GLU:HG2    | 2.17                     | 0.45              |
| 3:C:83:ARG:HH22   | 8:I:27:ARG:NH2    | 2.15                     | 0.45              |
| 11:L:168:LYS:N    | 11:L:168:LYS:HD2  | 2.31                     | 0.45              |
| 24:a:66:ARG:NH1   | 28:e:72:ASP:HB2   | 2.32                     | 0.45              |
| 24:a:147:ALA:HB2  | 40:r:173:SER:HB2  | 1.98                     | 0.45              |
| 35:l:233:LEU:HB3  | 35:l:234:PRO:HD3  | 1.99                     | 0.45              |
| 52:r:502:CDL:H381 | 52:r:502:CDL:H352 | 1.77                     | 0.45              |
| 41:s:24:GLU:HA    | 41:s:271:LEU:HD13 | 1.97                     | 0.45              |
| 12:M:197:THR:O    | 14:O:114:GLU:HG2  | 2.17                     | 0.45              |
| 12:M:197:THR:HA   | 12:M:205:GLN:O    | 2.17                     | 0.45              |
| 6:X:88:LYS:HB2    | 6:X:88:LYS:HE3    | 1.59                     | 0.45              |
| 4:E:25:MET:O      | 4:E:29:LYS:HG3    | 2.17                     | 0.44              |
| 12:M:650:SER:OG   | 12:M:652:ASN:OD1  | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:T:43:GLN:C     | 18:T:43:GLN:CD    | 2.85                     | 0.44              |
| 19:U:16:GLU:HG3   | 48:j:201:PEE:C31  | 2.46                     | 0.44              |
| 19:U:30:ILE:HD12  | 48:j:201:PEE:H43  | 1.98                     | 0.44              |
| 35:l:500:LEU:HD11 | 52:l:702:CDL:H352 | 1.98                     | 0.44              |
| 35:l:529:TYR:HB3  | 35:l:530:PRO:HD3  | 1.98                     | 0.44              |
| 38:o:116:ILE:HG13 | 38:o:121:LEU:HD22 | 1.99                     | 0.44              |
| 1:A:43:THR:OG1    | 1:A:59:ARG:HD2    | 2.17                     | 0.44              |
| 12:M:391:ILE:HG13 | 12:M:600:GLU:OE2  | 2.17                     | 0.44              |
| 16:Q:218:SER:OG   | 16:Q:224:ALA:CB   | 2.64                     | 0.44              |
| 17:S:31:ASN:ND2   | 17:S:36:LYS:HB2   | 2.31                     | 0.44              |
| 20:V:110:ILE:CG1  | 48:V:204:PEE:H8   | 2.47                     | 0.44              |
| 26:c:167:TYR:CD2  | 26:c:178:PRO:HG3  | 2.52                     | 0.44              |
| 34:k:21:MET:HE2   | 35:l:592:LEU:CD2  | 2.47                     | 0.44              |
| 36:m:24:PRO:O     | 36:m:81:GLU:HB2   | 2.17                     | 0.44              |
| 2:B:39:LYS:HD2    | 16:Q:335:GLU:HG2  | 1.99                     | 0.44              |
| 3:C:59:ARG:HH12   | 49:C:303:PLX:P1   | 2.40                     | 0.44              |
| 4:E:19:PRO:HB3    | 11:L:53:ILE:HG21  | 1.99                     | 0.44              |
| 7:H:72:LEU:HD13   | 7:H:80:VAL:HG11   | 1.99                     | 0.44              |
| 12:M:402:LEU:HD23 | 12:M:475:VAL:HB   | 1.98                     | 0.44              |
| 12:M:688:GLN:H    | 12:M:688:GLN:HG2  | 1.60                     | 0.44              |
| 16:Q:268:TRP:O    | 16:Q:272:THR:OG1  | 2.30                     | 0.44              |
| 20:V:34:LEU:HD23  | 20:V:34:LEU:HA    | 1.82                     | 0.44              |
| 24:a:78:THR:HG21  | 28:e:96:SER:HA    | 1.99                     | 0.44              |
| 40:r:243:MET:HG2  | 40:r:301:ILE:HG21 | 2.00                     | 0.44              |
| 40:r:259:TYR:O    | 40:r:263:MET:HG2  | 2.16                     | 0.44              |
| 42:u:11:GLU:HG2   | 42:u:14:LYS:NZ    | 2.32                     | 0.44              |
| 6:G:139:MET:CE    | 6:G:139:MET:CA    | 2.93                     | 0.44              |
| 12:M:483:ARG:H    | 12:M:483:ARG:HG2  | 1.57                     | 0.44              |
| 20:V:123:ALA:O    | 20:V:127:MET:HG3  | 2.17                     | 0.44              |
| 48:V:202:PEE:O2P  | 48:V:202:PEE:H12  | 2.17                     | 0.44              |
| 21:W:51:MET:HE2   | 21:W:51:MET:HB3   | 1.84                     | 0.44              |
| 48:W:201:PEE:H50  | 36:m:45:LEU:CD2   | 2.46                     | 0.44              |
| 24:a:170:GLN:CB   | 30:g:6:GLY:O      | 2.54                     | 0.44              |
| 41:s:233:MET:HE3  | 41:s:233:MET:HB3  | 1.82                     | 0.44              |
| 44:w:189:GLU:O    | 44:w:193:VAL:HG22 | 2.18                     | 0.44              |
| 2:B:99:GLY:HA3    | 2:B:170:GLY:O     | 2.17                     | 0.44              |
| 6:G:113:LEU:HD23  | 6:G:113:LEU:HA    | 1.75                     | 0.44              |
| 8:I:39:PRO:HB2    | 8:I:41:LEU:HD13   | 1.99                     | 0.44              |
| 11:L:131:LYS:HD2  | 11:L:147:VAL:HG11 | 1.99                     | 0.44              |
| 13:N:132:LYS:NZ   | 13:N:136:GLU:OE1  | 2.51                     | 0.44              |
| 52:V:201:CDL:H341 | 52:V:201:CDL:H371 | 1.81                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:Y:61:PHE:HA    | 22:Y:64:THR:HG22  | 1.98                     | 0.44              |
| 30:g:33:LEU:HD22  | 30:g:71:VAL:HG13  | 2.00                     | 0.44              |
| 32:i:75:ILE:HD12  | 34:k:40:LEU:HD22  | 2.00                     | 0.44              |
| 39:p:108:HIS:HB3  | 39:p:111:GLU:HG3  | 2.00                     | 0.44              |
| 41:s:81:LEU:HD11  | 41:s:111:LEU:HG   | 1.99                     | 0.44              |
| 44:w:45:LEU:O     | 44:w:45:LEU:HD12  | 2.18                     | 0.44              |
| 12:M:124:HIS:HD2  | 16:Q:375:MET:HE2  | 1.83                     | 0.44              |
| 12:M:167:PRO:HD2  | 12:M:215:MET:HE1  | 2.00                     | 0.44              |
| 22:Y:81:LEU:HD23  | 35:l:488:MET:HE1  | 1.99                     | 0.44              |
| 52:a:201:CDL:H341 | 52:a:201:CDL:H372 | 1.67                     | 0.44              |
| 35:l:566:THR:O    | 35:l:570:GLN:HG2  | 2.17                     | 0.44              |
| 35:l:599:MET:HA   | 35:l:603:ASN:CB   | 2.48                     | 0.44              |
| 43:v:113:LYS:HG3  | 43:v:114:ARG:N    | 2.33                     | 0.44              |
| 1:A:76:ILE:HG23   | 1:A:255:CYS:SG    | 2.58                     | 0.44              |
| 26:c:126:TRP:O    | 26:c:127:ASN:HB2  | 2.18                     | 0.44              |
| 13:N:85:GLU:HG2   | 13:N:86:TRP:H     | 1.83                     | 0.44              |
| 44:w:80:LYS:HB2   | 44:w:270:VAL:HG21 | 2.00                     | 0.44              |
| 3:C:107:GLY:HA2   | 45:C:301:SF4:S1   | 2.58                     | 0.44              |
| 9:J:220:MET:HE2   | 9:J:226:VAL:HG13  | 2.00                     | 0.44              |
| 29:f:47:THR:HG23  | 30:g:65:LEU:HD22  | 1.99                     | 0.44              |
| 52:l:701:CDL:H611 | 52:l:701:CDL:H581 | 1.77                     | 0.44              |
| 42:u:49:GLU:OE1   | 42:u:135:ARG:NH2  | 2.43                     | 0.44              |
| 7:H:40:LYS:HE2    | 7:H:40:LYS:HB2    | 1.90                     | 0.43              |
| 8:I:103:ARG:HH11  | 8:I:103:ARG:HB3   | 1.82                     | 0.43              |
| 23:Z:63:PHE:CE1   | 35:l:424:THR:HG23 | 2.52                     | 0.43              |
| 27:d:99:ASP:HB3   | 28:e:137:MET:CE   | 2.38                     | 0.43              |
| 28:e:125:LEU:HD23 | 28:e:129:ARG:NH2  | 2.33                     | 0.43              |
| 32:i:228:LEU:O    | 32:i:231:SER:OG   | 2.31                     | 0.43              |
| 34:k:23:ARG:HG3   | 36:m:23:LYS:CE    | 2.47                     | 0.43              |
| 40:r:6:ILE:O      | 40:r:10:MET:HG2   | 2.17                     | 0.43              |
| 40:r:22:MET:HE3   | 40:r:22:MET:HB3   | 1.91                     | 0.43              |
| 41:s:209:SER:HB3  | 41:s:213:VAL:CA   | 2.45                     | 0.43              |
| 41:s:313:SER:O    | 41:s:313:SER:OG   | 2.30                     | 0.43              |
| 2:B:184:LEU:HD23  | 11:L:112:MET:HG3  | 2.00                     | 0.43              |
| 15:P:119:VAL:HG12 | 15:P:121:THR:HG22 | 2.00                     | 0.43              |
| 20:V:2:ALA:HB1    | 35:l:605:HIS:HE1  | 1.83                     | 0.43              |
| 25:b:99:GLU:HG2   | 35:l:61:MET:HG2   | 2.00                     | 0.43              |
| 27:d:127:LYS:O    | 27:d:131:GLN:HG3  | 2.18                     | 0.43              |
| 39:p:82:PHE:HB2   | 39:p:85:SER:OG    | 2.19                     | 0.43              |
| 40:r:8:THR:O      | 40:r:11:LEU:HB2   | 2.18                     | 0.43              |
| 41:s:138:GLN:NE2  | 41:s:191:ALA:O    | 2.46                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:72:ARG:O     | 44:w:76:GLU:HG2   | 2.18                     | 0.43              |
| 1:A:115:VAL:HG11  | 1:A:138:LEU:HD11  | 2.00                     | 0.43              |
| 2:B:204:ASN:HD21  | 13:N:93:MET:HE2   | 1.83                     | 0.43              |
| 9:J:222:TRP:CZ3   | 52:J:404:CDL:HA4  | 2.52                     | 0.43              |
| 17:S:64:LYS:HE2   | 17:S:64:LYS:HA    | 2.00                     | 0.43              |
| 18:T:43:GLN:HE21  | 18:T:60:LYS:NZ    | 2.14                     | 0.43              |
| 21:W:81:ARG:NH1   | 42:u:15:VAL:HG11  | 2.33                     | 0.43              |
| 26:c:91:ASP:O     | 38:o:44:LYS:NZ    | 2.51                     | 0.43              |
| 30:g:32:ARG:O     | 30:g:36:MET:HG2   | 2.18                     | 0.43              |
| 32:i:150:ASN:HD22 | 32:i:151:PRO:HD2  | 1.83                     | 0.43              |
| 36:m:163:ILE:HD13 | 36:m:163:ILE:HA   | 1.85                     | 0.43              |
| 40:r:204:MET:HE2  | 40:r:243:MET:SD   | 2.58                     | 0.43              |
| 1:A:145:GLY:O     | 1:A:149:MET:HE3   | 2.18                     | 0.43              |
| 1:A:162:PHE:HB3   | 1:A:165:GLU:HB2   | 1.99                     | 0.43              |
| 6:G:105:MET:CE    | 6:G:139:MET:CE    | 2.84                     | 0.43              |
| 9:J:220:MET:HE3   | 9:J:227:PRO:HD2   | 1.96                     | 0.43              |
| 6:X:125:GLU:OE1   | 35:l:439:PRO:HG3  | 2.18                     | 0.43              |
| 6:X:139:MET:CE    | 6:X:139:MET:CA    | 2.86                     | 0.43              |
| 24:a:139:ILE:HG12 | 40:r:54:LEU:HD23  | 2.00                     | 0.43              |
| 25:b:32:GLU:HB3   | 39:p:115:TYR:HD1  | 1.83                     | 0.43              |
| 52:k:101:CDL:H362 | 52:k:101:CDL:H392 | 1.50                     | 0.43              |
| 42:u:11:GLU:HG2   | 42:u:14:LYS:HZ3   | 1.84                     | 0.43              |
| 44:w:165:SER:O    | 44:w:168:VAL:HG22 | 2.18                     | 0.43              |
| 4:E:35:LEU:HD21   | 4:E:86:GLY:HA3    | 2.00                     | 0.43              |
| 9:J:303:ARG:HB2   | 9:J:316:ARG:HD2   | 2.01                     | 0.43              |
| 12:M:94:MET:HA    | 12:M:95:PRO:HD3   | 1.91                     | 0.43              |
| 15:P:161:LYS:HD3  | 15:P:161:LYS:HA   | 1.77                     | 0.43              |
| 21:W:131:GLU:CD   | 21:W:131:GLU:H    | 2.27                     | 0.43              |
| 6:X:126:PHE:CE2   | 6:X:148:ILE:CD1   | 3.01                     | 0.43              |
| 33:j:27:LEU:CD2   | 41:s:60:PRO:HD2   | 2.48                     | 0.43              |
| 40:r:104:LEU:HG   | 40:r:108:MET:HE2  | 2.01                     | 0.43              |
| 41:s:123:SER:HB3  | 41:s:214:GLU:HG3  | 2.00                     | 0.43              |
| 10:K:105:ARG:NH2  | 12:M:426:ASP:OD1  | 2.51                     | 0.43              |
| 12:M:284:GLU:HG2  | 12:M:284:GLU:O    | 2.17                     | 0.43              |
| 12:M:632:MET:HE2  | 12:M:632:MET:HB3  | 1.76                     | 0.43              |
| 32:i:20:VAL:HG11  | 32:i:137:ALA:HB1  | 1.99                     | 0.43              |
| 35:l:389:PHE:O    | 35:l:393:ASP:HB3  | 2.18                     | 0.43              |
| 40:r:71:TRP:O     | 40:r:74:PRO:HD2   | 2.19                     | 0.43              |
| 40:r:433:GLU:O    | 40:r:437:MET:HG2  | 2.19                     | 0.43              |
| 1:A:446:LEU:O     | 1:A:450:MET:HG3   | 2.19                     | 0.43              |
| 8:I:27:ARG:HB2    | 8:I:30:GLU:OE2    | 2.17                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:8:ARG:HA     | 13:N:11:LEU:HD12  | 2.01                     | 0.43              |
| 14:O:134:VAL:O    | 14:O:134:VAL:HG23 | 2.18                     | 0.43              |
| 16:Q:184:ILE:HG23 | 16:Q:203:MET:HB3  | 1.99                     | 0.43              |
| 49:g:201:PLX:H351 | 32:i:336:VAL:HG22 | 2.01                     | 0.43              |
| 36:m:49:GLY:HA2   | 36:m:139:GLU:OE2  | 2.19                     | 0.43              |
| 41:s:306:SER:O    | 41:s:310:MET:HG3  | 2.18                     | 0.43              |
| 8:I:108:LYS:HD3   | 8:I:108:LYS:HA    | 1.83                     | 0.43              |
| 12:M:339:ALA:HB3  | 12:M:542:PRO:HG3  | 2.00                     | 0.43              |
| 12:M:484:SER:OG   | 12:M:680:LEU:HD11 | 2.19                     | 0.43              |
| 14:O:218:PRO:HD2  | 14:O:223:PHE:HA   | 2.00                     | 0.43              |
| 16:Q:342:ARG:HD2  | 21:W:21:TYR:CZ    | 2.53                     | 0.43              |
| 21:W:7:LYS:HA     | 21:W:7:LYS:HD3    | 1.83                     | 0.43              |
| 32:i:110:PRO:HG3  | 35:l:594:THR:HG21 | 2.01                     | 0.43              |
| 33:j:38:GLU:OE1   | 33:j:43:PRO:HB3   | 2.19                     | 0.43              |
| 2:B:79:ARG:HH11   | 8:I:25:GLN:NE2    | 2.16                     | 0.43              |
| 15:P:152:PRO:HB3  | 15:P:177:PHE:HD2  | 1.84                     | 0.43              |
| 16:Q:106:VAL:HG21 | 16:Q:447:VAL:HG21 | 2.01                     | 0.43              |
| 48:W:201:PEE:H20  | 48:W:201:PEE:H14  | 1.55                     | 0.43              |
| 28:e:55:LEU:HD11  | 44:w:320:GLY:HA2  | 2.00                     | 0.43              |
| 33:j:33:LYS:HD3   | 41:s:61:LEU:HD21  | 2.00                     | 0.43              |
| 44:w:190:VAL:O    | 44:w:194:THR:OG1  | 2.24                     | 0.43              |
| 44:w:245:PHE:O    | 44:w:249:MET:HB2  | 2.19                     | 0.43              |
| 13:N:68:MET:CG    | 13:N:69:ASN:H     | 2.32                     | 0.43              |
| 25:b:101:LYS:HA   | 25:b:102:PRO:HD3  | 1.82                     | 0.43              |
| 30:g:48:ASN:HB3   | 30:g:55:VAL:HA    | 2.01                     | 0.43              |
| 31:h:39:GLU:OE2   | 42:u:144:SER:OG   | 2.31                     | 0.43              |
| 40:r:167:ILE:HD11 | 40:r:195:MET:HE3  | 2.01                     | 0.43              |
| 1:A:201:ALA:HB1   | 14:O:121:MET:HB2  | 2.00                     | 0.42              |
| 12:M:712:LYS:O    | 12:M:716:GLU:HG2  | 2.19                     | 0.42              |
| 31:h:2:PRO:HA     | 32:i:140:SER:HB2  | 2.01                     | 0.42              |
| 32:i:42:PRO:HG3   | 36:m:167:VAL:HG13 | 2.01                     | 0.42              |
| 35:l:331:MET:SD   | 35:l:465:GLY:HA2  | 2.59                     | 0.42              |
| 52:l:701:CDL:H812 | 52:l:701:CDL:H841 | 1.79                     | 0.42              |
| 1:A:56:ALA:O      | 1:A:61:ASP:N      | 2.47                     | 0.42              |
| 1:A:152:ARG:NH2   | 10:K:99:PRO:O     | 2.47                     | 0.42              |
| 8:I:107:SER:HB3   | 8:I:111:PRO:HA    | 2.00                     | 0.42              |
| 12:M:178:GLN:HG2  | 12:M:204:MET:CE   | 2.49                     | 0.42              |
| 12:M:347:ASP:CB   | 12:M:594:ALA:HB1  | 2.49                     | 0.42              |
| 28:e:136:LEU:HD12 | 28:e:136:LEU:HA   | 1.84                     | 0.42              |
| 32:i:261:MET:O    | 32:i:265:MET:HG2  | 2.19                     | 0.42              |
| 38:o:53:ASP:HA    | 38:o:54:PRO:HD3   | 1.75                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:s:245:ALA:HB3  | 41:s:255:TYR:CE2  | 2.54                     | 0.42              |
| 6:G:140:CYS:SG    | 6:G:143:GLU:HG3   | 2.59                     | 0.42              |
| 15:P:132:LEU:HB2  | 15:P:141:ILE:HG22 | 2.01                     | 0.42              |
| 6:X:155:TYR:HA    | 25:b:20:ARG:HG2   | 2.01                     | 0.42              |
| 32:i:41:ILE:HG13  | 34:k:73:LEU:HD21  | 2.01                     | 0.42              |
| 35:l:49:VAL:HB    | 35:l:50:PRO:HD3   | 2.01                     | 0.42              |
| 35:l:125:LEU:O    | 35:l:129:MET:HG2  | 2.20                     | 0.42              |
| 40:r:202:ALA:O    | 40:r:205:VAL:HG12 | 2.18                     | 0.42              |
| 19:U:66:VAL:O     | 42:u:130:LYS:HE3  | 2.20                     | 0.42              |
| 25:b:120:MET:HE3  | 43:v:61:HIS:HB2   | 2.01                     | 0.42              |
| 32:i:31:ILE:HD11  | 34:k:62:ILE:HG21  | 2.01                     | 0.42              |
| 35:l:7:LEU:HD22   | 35:l:46:LEU:HD11  | 2.01                     | 0.42              |
| 35:l:230:HIS:N    | 35:l:231:PRO:HD3  | 2.34                     | 0.42              |
| 40:r:329:LEU:HD23 | 40:r:437:MET:HE3  | 2.01                     | 0.42              |
| 43:v:17:PRO:HB2   | 43:v:22:MET:HE2   | 2.02                     | 0.42              |
| 1:A:292:MET:HE3   | 1:A:292:MET:HB3   | 1.82                     | 0.42              |
| 5:F:27:SER:O      | 5:F:34:ARG:NH2    | 2.44                     | 0.42              |
| 8:I:6:ARG:HA      | 8:I:9:GLN:HG3     | 2.02                     | 0.42              |
| 9:J:132:ARG:NH1   | 53:J:401:NDP:O3X  | 2.51                     | 0.42              |
| 12:M:689:LEU:HD12 | 12:M:689:LEU:HA   | 1.85                     | 0.42              |
| 20:V:36:VAL:HG22  | 52:V:201:CDL:H741 | 2.02                     | 0.42              |
| 25:b:16:ARG:HD2   | 25:b:20:ARG:NH2   | 2.35                     | 0.42              |
| 37:n:25:CYS:O     | 37:n:29:ARG:HG3   | 2.19                     | 0.42              |
| 40:r:189:SER:HA   | 49:r:501:PLX:H1B3 | 2.02                     | 0.42              |
| 52:r:502:CDL:H221 | 52:r:502:CDL:H401 | 2.01                     | 0.42              |
| 42:u:139:GLU:H    | 42:u:139:GLU:CD   | 2.27                     | 0.42              |
| 44:w:350:LYS:HA   | 44:w:350:LYS:HD3  | 1.90                     | 0.42              |
| 1:A:52:ARG:O      | 1:A:53:LEU:C      | 2.62                     | 0.42              |
| 2:B:40:PHE:HB3    | 2:B:43:MET:HB2    | 2.02                     | 0.42              |
| 2:B:74:LEU:HB2    | 41:s:272:TRP:CZ2  | 2.54                     | 0.42              |
| 2:B:122:VAL:HG21  | 16:Q:385:TYR:HD1  | 1.84                     | 0.42              |
| 49:J:403:PLX:H251 | 49:J:403:PLX:H282 | 1.69                     | 0.42              |
| 14:O:154:LYS:HB3  | 14:O:154:LYS:HE3  | 1.78                     | 0.42              |
| 17:S:57:VAL:HG21  | 17:S:62:VAL:HG21  | 2.02                     | 0.42              |
| 30:g:107:ASP:OD1  | 30:g:107:ASP:N    | 2.53                     | 0.42              |
| 49:g:201:PLX:H332 | 32:i:342:ALA:HB3  | 2.01                     | 0.42              |
| 33:j:73:LEU:HD12  | 36:m:55:MET:SD    | 2.60                     | 0.42              |
| 38:o:31:LYS:O     | 38:o:35:GLU:HG3   | 2.20                     | 0.42              |
| 38:o:57:LEU:HD13  | 38:o:58:GLY:N     | 2.35                     | 0.42              |
| 40:r:3:LYS:HB3    | 40:r:3:LYS:HE2    | 1.81                     | 0.42              |
| 41:s:2:PHE:O      | 41:s:6:ILE:HG13   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:339:PHE:CE1   | 1:A:349:LEU:HD23  | 2.55                     | 0.42              |
| 49:C:303:PLX:H21  | 49:C:303:PLX:H1C3 | 1.86                     | 0.42              |
| 9:J:36:LEU:N      | 12:M:304:GLN:HE22 | 2.17                     | 0.42              |
| 12:M:219:SER:OG   | 12:M:288:ASP:OD2  | 2.36                     | 0.42              |
| 16:Q:180:LEU:CB   | 16:Q:210:MET:HE1  | 2.49                     | 0.42              |
| 29:f:70:LYS:HG2   | 29:f:75:LEU:HB2   | 2.01                     | 0.42              |
| 32:i:246:VAL:HG21 | 52:r:502:CDL:H362 | 2.01                     | 0.42              |
| 35:l:152:PHE:CD1  | 35:l:168:ALA:HB1  | 2.54                     | 0.42              |
| 52:l:701:CDL:H342 | 52:l:701:CDL:H372 | 1.65                     | 0.42              |
| 36:m:55:MET:HE1   | 36:m:58:LEU:HD23  | 2.00                     | 0.42              |
| 41:s:106:LEU:HD23 | 41:s:106:LEU:HA   | 1.94                     | 0.42              |
| 42:u:61:LYS:O     | 42:u:65:GLN:HG3   | 2.20                     | 0.42              |
| 43:v:26:PRO:HD2   | 43:v:29:TYR:HB2   | 2.01                     | 0.42              |
| 12:M:277:MET:HG2  | 12:M:283:GLU:O    | 2.19                     | 0.42              |
| 56:Q:502:UQ1:H113 | 56:Q:502:UQ1:H72  | 1.83                     | 0.42              |
| 19:U:50:PRO:HB2   | 21:W:69:ILE:HD11  | 2.01                     | 0.42              |
| 6:X:146:ASP:HB3   | 25:b:16:ARG:NH1   | 2.35                     | 0.42              |
| 24:a:184:LYS:C    | 24:a:186:THR:H    | 2.27                     | 0.42              |
| 52:a:201:CDL:H411 | 52:a:201:CDL:H441 | 1.84                     | 0.42              |
| 32:i:304:MET:HE3  | 40:r:135:ARG:HH22 | 1.84                     | 0.42              |
| 35:l:55:MET:SD    | 35:l:471:ASN:HB3  | 2.59                     | 0.42              |
| 35:l:211:MET:HE3  | 35:l:211:MET:HB2  | 1.91                     | 0.42              |
| 38:o:50:GLN:O     | 38:o:56:ARG:HD3   | 2.19                     | 0.42              |
| 40:r:1:MET:SD     | 40:r:111:THR:HG21 | 2.60                     | 0.42              |
| 1:A:97:LEU:HD23   | 1:A:97:LEU:HA     | 1.92                     | 0.42              |
| 3:C:190:LEU:HD22  | 48:C:302:PEE:H14  | 2.02                     | 0.42              |
| 12:M:81:GLU:OE2   | 12:M:103:LEU:HD12 | 2.20                     | 0.42              |
| 14:O:133:GLN:HG2  | 14:O:172:ILE:HD11 | 2.01                     | 0.42              |
| 56:Q:501:UQ1:HM22 | 56:Q:502:UQ1:H103 | 2.00                     | 0.42              |
| 52:V:203:CDL:H812 | 52:V:203:CDL:H781 | 1.88                     | 0.42              |
| 24:a:60:SER:OG    | 39:p:111:GLU:OE2  | 2.30                     | 0.42              |
| 40:r:233:ALA:HA   | 40:r:320:GLY:HA2  | 2.01                     | 0.42              |
| 41:s:11:ILE:HB    | 41:s:12:PRO:HD3   | 2.02                     | 0.42              |
| 41:s:129:LEU:O    | 41:s:133:LEU:HD23 | 2.19                     | 0.42              |
| 1:A:138:LEU:HD13  | 1:A:245:VAL:HG23  | 2.02                     | 0.42              |
| 9:J:61:ALA:HB3    | 9:J:82:VAL:HG13   | 2.02                     | 0.42              |
| 9:J:313:TRP:CE2   | 50:J:402:UQ:H8    | 2.55                     | 0.42              |
| 12:M:219:SER:O    | 12:M:222:ILE:HG12 | 2.19                     | 0.42              |
| 16:Q:123:LEU:O    | 16:Q:127:LYS:HG2  | 2.19                     | 0.42              |
| 16:Q:404:LYS:HG2  | 16:Q:455:ASP:OD2  | 2.20                     | 0.42              |
| 48:Q:503:PEE:H14  | 48:Q:503:PEE:H1   | 1.92                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:U:16:GLU:CG    | 48:j:201:PEE:H49  | 2.47                     | 0.42              |
| 19:U:38:TYR:HD1   | 19:U:41:TYR:HD2   | 1.68                     | 0.42              |
| 6:X:93:ILE:HG23   | 6:X:108:LEU:HD11  | 2.01                     | 0.42              |
| 24:a:71:MET:HE2   | 24:a:71:MET:HB3   | 1.97                     | 0.42              |
| 27:d:51:PHE:O     | 27:d:55:GLN:HG2   | 2.19                     | 0.42              |
| 27:d:100:GLN:HB3  | 35:l:72:GLN:O     | 2.20                     | 0.42              |
| 31:h:24:GLU:O     | 31:h:24:GLU:HG3   | 2.20                     | 0.42              |
| 32:i:278:MET:HB3  | 32:i:279:PRO:HD3  | 2.02                     | 0.42              |
| 35:l:130:ILE:HD13 | 52:l:701:CDL:H252 | 2.01                     | 0.42              |
| 35:l:214:ILE:HG12 | 35:l:276:MET:HE1  | 2.01                     | 0.42              |
| 48:l:703:PEE:H7   | 48:l:703:PEE:C11  | 2.49                     | 0.42              |
| 40:r:310:MET:HG2  | 40:r:455:LEU:O    | 2.20                     | 0.42              |
| 9:J:208:GLY:H     | 9:J:211:ASP:HB3   | 1.85                     | 0.41              |
| 12:M:215:MET:HG2  | 12:M:714:VAL:HG12 | 2.02                     | 0.41              |
| 12:M:326:VAL:HG13 | 12:M:567:ILE:HD13 | 2.02                     | 0.41              |
| 12:M:354:LEU:HD22 | 12:M:548:LEU:HD22 | 2.01                     | 0.41              |
| 15:P:173:MET:HE3  | 15:P:188:LEU:HB2  | 2.01                     | 0.41              |
| 16:Q:238:LEU:HD23 | 16:Q:238:LEU:HA   | 1.85                     | 0.41              |
| 33:j:73:LEU:O     | 33:j:76:PRO:HD2   | 2.20                     | 0.41              |
| 34:k:48:ILE:HD13  | 34:k:56:ALA:O     | 2.20                     | 0.41              |
| 35:l:599:MET:CA   | 35:l:603:ASN:HB3  | 2.49                     | 0.41              |
| 36:m:24:PRO:HG3   | 36:m:83:TRP:CE2   | 2.54                     | 0.41              |
| 49:r:501:PLX:H111 | 49:r:501:PLX:H141 | 1.88                     | 0.41              |
| 42:u:103:GLN:OE1  | 42:u:103:GLN:N    | 2.52                     | 0.41              |
| 13:N:53:LYS:HD3   | 13:N:53:LYS:HA    | 1.75                     | 0.41              |
| 41:s:185:TRP:O    | 41:s:189:THR:HG23 | 2.20                     | 0.41              |
| 44:w:267:GLU:CD   | 44:w:267:GLU:H    | 2.27                     | 0.41              |
| 1:A:60:GLY:CA     | 14:O:241:PRO:HA   | 2.50                     | 0.41              |
| 2:B:140:ARG:HG3   | 12:M:238:PHE:CG   | 2.55                     | 0.41              |
| 4:E:127:ASP:OD2   | 9:J:45:LYS:HD3    | 2.21                     | 0.41              |
| 8:I:73:GLN:OE1    | 8:I:74:LYS:N      | 2.53                     | 0.41              |
| 9:J:375:VAL:HG23  | 9:J:375:VAL:O     | 2.21                     | 0.41              |
| 12:M:602:ARG:HD3  | 12:M:657:ASP:OD1  | 2.20                     | 0.41              |
| 16:Q:80:LEU:HD11  | 41:s:126:LYS:HE3  | 2.02                     | 0.41              |
| 52:V:203:CDL:H792 | 52:V:203:CDL:H761 | 1.65                     | 0.41              |
| 6:X:132:ASP:OD2   | 39:p:18:ARG:HG2   | 2.20                     | 0.41              |
| 22:Y:97:LEU:HD22  | 43:v:107:ARG:NH1  | 2.35                     | 0.41              |
| 27:d:158:LYS:HG3  | 30:g:118:PHE:CE2  | 2.55                     | 0.41              |
| 49:j:203:PLX:H132 | 49:j:203:PLX:H161 | 1.50                     | 0.41              |
| 35:l:2:ASN:O      | 35:l:4:PHE:N      | 2.52                     | 0.41              |
| 41:s:91:MET:HG2   | 41:s:259:PHE:CE2  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:246:LEU:HB2  | 44:w:247:PRO:HD3  | 2.03                     | 0.41              |
| 12:M:49:VAL:HB    | 12:M:91:ALA:HA    | 2.01                     | 0.41              |
| 20:V:107:SER:HB3  | 20:V:110:ILE:HB   | 2.02                     | 0.41              |
| 6:X:82:ARG:HD2    | 22:Y:44:TYR:CE1   | 2.55                     | 0.41              |
| 27:d:115:GLN:HG2  | 35:l:62:ILE:HG12  | 2.01                     | 0.41              |
| 33:j:80:GLN:HG3   | 41:s:318:SER:HA   | 2.03                     | 0.41              |
| 35:l:166:THR:HG21 | 48:l:703:PEE:H2   | 2.03                     | 0.41              |
| 35:l:535:ARG:NH1  | 38:o:11:LEU:O     | 2.47                     | 0.41              |
| 39:p:97:TYR:HB2   | 39:p:178:PRO:HG2  | 2.01                     | 0.41              |
| 49:r:501:PLX:H22  | 49:r:501:PLX:H1C3 | 1.79                     | 0.41              |
| 1:A:201:ALA:O     | 14:O:119:TYR:HB3  | 2.20                     | 0.41              |
| 50:J:402:UQ:C13   | 50:J:402:UQ:H101  | 2.50                     | 0.41              |
| 16:Q:315:GLU:HA   | 16:Q:315:GLU:OE1  | 2.19                     | 0.41              |
| 24:a:66:ARG:HA    | 24:a:69:LYS:HE3   | 2.02                     | 0.41              |
| 28:e:55:LEU:CD2   | 28:e:57:GLU:HB2   | 2.51                     | 0.41              |
| 32:i:142:LEU:HB3  | 32:i:194:LEU:HD21 | 2.02                     | 0.41              |
| 35:l:124:PHE:CE1  | 35:l:252:MET:HB2  | 2.56                     | 0.41              |
| 35:l:401:MET:HE3  | 35:l:401:MET:HB3  | 1.75                     | 0.41              |
| 52:l:702:CDL:H641 | 52:l:702:CDL:H612 | 1.83                     | 0.41              |
| 36:m:82:VAL:HG23  | 36:m:84:VAL:H     | 1.85                     | 0.41              |
| 8:I:64:MET:HE3    | 15:P:80:CYS:SG    | 2.60                     | 0.41              |
| 48:V:202:PEE:H68  | 48:V:202:PEE:H62  | 1.66                     | 0.41              |
| 26:c:101:TRP:CE3  | 38:o:47:TYR:HB2   | 2.55                     | 0.41              |
| 31:h:87:ILE:HG22  | 31:h:92:TYR:HB3   | 2.01                     | 0.41              |
| 35:l:51:LEU:HD22  | 35:l:91:PRO:HG3   | 2.03                     | 0.41              |
| 35:l:68:TRP:CD2   | 48:l:704:PEE:H42  | 2.56                     | 0.41              |
| 3:C:96:SER:HB2    | 41:s:209:SER:HB2  | 2.03                     | 0.41              |
| 3:C:184:ILE:O     | 3:C:187:GLU:HG2   | 2.21                     | 0.41              |
| 50:C:304:UQ:H152  | 50:C:304:UQ:H121  | 1.82                     | 0.41              |
| 50:C:304:UQ:H222  | 41:s:225:MET:HE3  | 2.02                     | 0.41              |
| 8:I:8:ILE:HD11    | 52:I:201:CDL:H111 | 2.02                     | 0.41              |
| 14:O:148:ILE:HG12 | 14:O:184:PRO:HG3  | 2.01                     | 0.41              |
| 14:O:181:VAL:CG1  | 14:O:222:ARG:NH2  | 2.81                     | 0.41              |
| 16:Q:259:GLU:HG3  | 16:Q:263:THR:OG1  | 2.20                     | 0.41              |
| 48:V:202:PEE:H71  | 48:V:202:PEE:H33  | 2.03                     | 0.41              |
| 26:c:46:GLU:OE1   | 26:c:46:GLU:N     | 2.38                     | 0.41              |
| 35:l:419:THR:HA   | 35:l:422:TYR:CD2  | 2.56                     | 0.41              |
| 43:v:19:PRO:HA    | 43:v:22:MET:HE3   | 2.03                     | 0.41              |
| 44:w:75:ARG:HG3   | 44:w:75:ARG:NH1   | 2.35                     | 0.41              |
| 3:C:98:ARG:HB3    | 41:s:216:ALA:HB2  | 2.01                     | 0.41              |
| 9:J:157:LYS:NZ    | 9:J:197:GLU:OE1   | 2.52                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:74:ASP:OD1   | 16:Q:74:ASP:N     | 2.48                     | 0.41              |
| 52:V:203:CDL:HB4  | 38:o:82:PRO:HB2   | 2.02                     | 0.41              |
| 6:X:120:MET:HE1   | 39:p:24:LEU:HB3   | 2.01                     | 0.41              |
| 27:d:99:ASP:OD2   | 27:d:142:ARG:NH1  | 2.53                     | 0.41              |
| 27:d:142:ARG:HD2  | 28:e:137:MET:HE2  | 2.02                     | 0.41              |
| 28:e:70:ASN:HB3   | 28:e:73:SER:HB2   | 2.03                     | 0.41              |
| 35:l:251:THR:O    | 35:l:254:VAL:HG22 | 2.20                     | 0.41              |
| 35:l:504:LEU:HD23 | 35:l:504:LEU:HA   | 1.85                     | 0.41              |
| 35:l:544:MET:HE1  | 38:o:93:PHE:CE1   | 2.56                     | 0.41              |
| 40:r:118:PHE:O    | 40:r:122:PHE:HB3  | 2.20                     | 0.41              |
| 40:r:257:MET:HE3  | 40:r:257:MET:HB3  | 1.98                     | 0.41              |
| 43:v:35:LYS:H     | 43:v:35:LYS:CE    | 2.32                     | 0.41              |
| 44:w:295:ARG:HA   | 44:w:298:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:70:LEU:HD21   | 1:A:189:SER:HA    | 2.03                     | 0.41              |
| 1:A:367:ILE:O     | 1:A:371:ILE:HG12  | 2.20                     | 0.41              |
| 9:J:171:ASN:HA    | 9:J:327:MET:SD    | 2.61                     | 0.41              |
| 52:J:404:CDL:H122 | 41:s:72:ILE:HD12  | 2.02                     | 0.41              |
| 12:M:61:PRO:HB2   | 12:M:77:MET:HG3   | 2.03                     | 0.41              |
| 15:P:108:PHE:CD2  | 15:P:134:SER:HB2  | 2.56                     | 0.41              |
| 16:Q:404:LYS:HE3  | 16:Q:455:ASP:O    | 2.20                     | 0.41              |
| 21:W:50:MET:HE1   | 41:s:168:THR:O    | 2.21                     | 0.41              |
| 25:b:103:ARG:NH1  | 43:v:67:LEU:HD13  | 2.35                     | 0.41              |
| 26:c:44:THR:OG1   | 26:c:47:GLU:HG3   | 2.21                     | 0.41              |
| 27:d:168:LYS:O    | 27:d:171:LYS:HG3  | 2.21                     | 0.41              |
| 29:f:48:LEU:O     | 29:f:52:VAL:HG23  | 2.20                     | 0.41              |
| 35:l:80:PHE:HB3   | 35:l:82:MET:HE2   | 2.02                     | 0.41              |
| 35:l:176:ARG:NH1  | 40:r:404:ALA:HB2  | 2.36                     | 0.41              |
| 52:l:702:CDL:H112 | 52:l:702:CDL:H322 | 2.02                     | 0.41              |
| 36:m:1:MET:SD     | 36:m:1:MET:N      | 2.93                     | 0.41              |
| 39:p:34:ARG:HD2   | 39:p:34:ARG:HA    | 1.82                     | 0.41              |
| 39:p:108:HIS:ND1  | 39:p:110:SER:OG   | 2.30                     | 0.41              |
| 41:s:90:PRO:HD2   | 41:s:240:ILE:HD13 | 2.03                     | 0.41              |
| 43:v:95:TYR:O     | 43:v:99:MET:HG3   | 2.21                     | 0.41              |
| 44:w:110:GLY:HA2  | 44:w:134:TRP:CE2  | 2.56                     | 0.41              |
| 6:G:104:PHE:CD1   | 6:G:108:LEU:HD12  | 2.52                     | 0.41              |
| 7:H:50:GLN:O      | 7:H:54:GLU:HG3    | 2.20                     | 0.41              |
| 15:P:118:ASP:OD1  | 15:P:125:ARG:HG2  | 2.21                     | 0.41              |
| 5:F:17:ARG:HH21   | 5:F:70:ALA:HB2    | 1.86                     | 0.40              |
| 7:H:33:ASP:OD2    | 44:w:268:LYS:NZ   | 2.54                     | 0.40              |
| 14:O:185:MET:SD   | 14:O:185:MET:O    | 2.79                     | 0.40              |
| 19:U:32:LEU:HD23  | 41:s:310:MET:HE1  | 2.02                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:102:LEU:HD13 | 32:i:142:LEU:HG   | 2.03                     | 0.40              |
| 32:i:245:MET:HE3  | 32:i:245:MET:HB3  | 1.77                     | 0.40              |
| 52:k:101:CDL:H432 | 52:k:101:CDL:H402 | 1.65                     | 0.40              |
| 35:l:293:ILE:HD12 | 52:l:702:CDL:H521 | 2.04                     | 0.40              |
| 52:l:702:CDL:H532 | 52:l:702:CDL:H561 | 1.85                     | 0.40              |
| 42:u:169:PHE:CE1  | 52:u:201:CDL:H561 | 2.57                     | 0.40              |
| 44:w:200:PRO:HG3  | 44:w:252:LYS:HD3  | 2.02                     | 0.40              |
| 12:M:502:LEU:HD12 | 12:M:502:LEU:HA   | 1.90                     | 0.40              |
| 15:P:153:ILE:O    | 15:P:178:PHE:HA   | 2.20                     | 0.40              |
| 24:a:176:LYS:HE3  | 31:h:45:HIS:CD2   | 2.55                     | 0.40              |
| 26:c:160:GLN:OE1  | 26:c:183:HIS:HB3  | 2.22                     | 0.40              |
| 30:g:87:LEU:HD23  | 30:g:87:LEU:HA    | 1.96                     | 0.40              |
| 35:l:338:MET:HE3  | 35:l:372:ALA:O    | 2.21                     | 0.40              |
| 35:l:341:MET:HE1  | 35:l:453:SER:HB3  | 2.03                     | 0.40              |
| 1:A:141:GLY:HA2   | 1:A:252:PRO:HD3   | 2.04                     | 0.40              |
| 1:A:284:HIS:ND1   | 14:O:228:ALA:HB3  | 2.37                     | 0.40              |
| 8:I:34:ARG:HA     | 8:I:34:ARG:HD2    | 1.89                     | 0.40              |
| 52:J:404:CDL:H162 | 52:J:404:CDL:H191 | 1.92                     | 0.40              |
| 12:M:592:LYS:HG3  | 12:M:594:ALA:HB2  | 2.03                     | 0.40              |
| 16:Q:150:ALA:HB2  | 16:Q:400:ILE:HG12 | 2.03                     | 0.40              |
| 23:Z:32:VAL:HG21  | 39:p:35:ASP:HB2   | 2.03                     | 0.40              |
| 26:c:167:TYR:CG   | 26:c:178:PRO:HG3  | 2.56                     | 0.40              |
| 28:e:76:TYR:HB2   | 28:e:83:ASP:OD1   | 2.20                     | 0.40              |
| 32:i:21:MET:CE    | 32:i:136:LEU:HB3  | 2.51                     | 0.40              |
| 32:i:254:LEU:HA   | 32:i:255:PRO:HD3  | 1.97                     | 0.40              |
| 33:j:104:TYR:O    | 33:j:108:GLN:HG2  | 2.20                     | 0.40              |
| 34:k:75:LEU:HD23  | 34:k:75:LEU:HA    | 1.92                     | 0.40              |
| 35:l:332:HIS:HA   | 35:l:335:PHE:CZ   | 2.56                     | 0.40              |
| 35:l:402:SER:O    | 35:l:404:THR:HG22 | 2.21                     | 0.40              |
| 37:n:58:LYS:HE2   | 37:n:58:LYS:HB2   | 1.94                     | 0.40              |
| 40:r:410:MET:HE2  | 40:r:410:MET:HB3  | 1.94                     | 0.40              |
| 42:u:83:THR:HA    | 42:u:86:TRP:NE1   | 2.35                     | 0.40              |
| 1:A:102:MET:HE3   | 1:A:111:LYS:HB3   | 2.03                     | 0.40              |
| 1:A:296:LEU:HD11  | 1:A:317:VAL:HG11  | 2.03                     | 0.40              |
| 5:F:21:ILE:HG12   | 5:F:65:LEU:HD12   | 2.04                     | 0.40              |
| 12:M:257:VAL:C    | 12:M:598:ASN:ND2  | 2.77                     | 0.40              |
| 21:W:91:LEU:HD22  | 42:u:7:LEU:HD12   | 2.03                     | 0.40              |
| 23:Z:18:ASP:O     | 23:Z:21:GLN:HG2   | 2.21                     | 0.40              |
| 27:d:114:GLN:OE1  | 35:l:199:GLN:HG3  | 2.21                     | 0.40              |
| 33:j:18:VAL:HG23  | 41:s:222:MET:SD   | 2.62                     | 0.40              |
| 39:p:27:LEU:HD11  | 39:p:40:PHE:HB3   | 2.04                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 40:r:186:LEU:O   | 40:r:252:PRO:HD2 | 2.21                     | 0.40              |
| 6:G:139:MET:HE2  | 6:G:139:MET:CA   | 2.44                     | 0.40              |
| 8:I:70:MET:SD    | 8:I:70:MET:O     | 2.79                     | 0.40              |
| 9:J:259:LYS:HD3  | 9:J:259:LYS:HA   | 1.87                     | 0.40              |
| 12:M:379:THR:O   | 12:M:379:THR:CG2 | 2.70                     | 0.40              |
| 12:M:467:LYS:HE2 | 12:M:503:SER:HB3 | 2.02                     | 0.40              |
| 16:Q:93:GLY:HA2  | 56:Q:501:UQ1:H71 | 2.04                     | 0.40              |
| 6:X:92:LYS:NZ    | 6:X:114:ASP:OD2  | 2.52                     | 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%) | 416 (96%) | 14 (3%) | 1 (0%)   | 43          | 66  |
| 2   | B     | 174/176 (99%)  | 168 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 3   | C     | 154/156 (99%)  | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | E     | 113/115 (98%)  | 109 (96%) | 3 (3%)  | 1 (1%)   | 14          | 30  |
| 5   | F     | 84/86 (98%)    | 79 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 6   | G     | 86/88 (98%)    | 81 (94%)  | 4 (5%)  | 1 (1%)   | 10          | 23  |
| 6   | X     | 86/88 (98%)    | 81 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 7   | H     | 110/112 (98%)  | 102 (93%) | 7 (6%)  | 1 (1%)   | 14          | 30  |
| 8   | I     | 93/112 (83%)   | 84 (90%)  | 7 (8%)  | 2 (2%)   | 5           | 10  |
| 9   | J     | 340/342 (99%)  | 327 (96%) | 12 (4%) | 1 (0%)   | 36          | 58  |
| 10  | K     | 41/43 (95%)    | 39 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 11  | L     | 123/125 (98%)  | 121 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 12  | M     | 688/690 (100%) | 668 (97%) | 19 (3%) | 1 (0%)   | 48          | 70  |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 13  | N     | 142/144 (99%)  | 139 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 14  | O     | 215/217 (99%)  | 203 (94%) | 11 (5%) | 1 (0%)   | 24          | 46  |
| 15  | P     | 206/208 (99%)  | 199 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 16  | Q     | 427/430 (99%)  | 418 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 17  | S     | 68/70 (97%)    | 66 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 18  | T     | 94/96 (98%)    | 92 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 19  | U     | 81/83 (98%)    | 79 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 20  | V     | 138/140 (99%)  | 134 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 21  | W     | 140/142 (99%)  | 134 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 22  | Y     | 65/67 (97%)    | 62 (95%)  | 3 (5%)  | 0        | 100         | 100 |
| 23  | Z     | 78/80 (98%)    | 73 (94%)  | 5 (6%)  | 0        | 100         | 100 |
| 24  | a     | 136/138 (99%)  | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 25  | b     | 94/126 (75%)   | 86 (92%)  | 8 (8%)  | 0        | 100         | 100 |
| 26  | c     | 154/156 (99%)  | 145 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 27  | d     | 173/175 (99%)  | 169 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 28  | e     | 102/104 (98%)  | 97 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 29  | f     | 47/49 (96%)    | 43 (92%)  | 4 (8%)  | 0        | 100         | 100 |
| 30  | g     | 120/122 (98%)  | 114 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 31  | h     | 103/105 (98%)  | 98 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 32  | i     | 345/347 (99%)  | 329 (95%) | 16 (5%) | 0        | 100         | 100 |
| 33  | j     | 113/115 (98%)  | 109 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 34  | k     | 96/98 (98%)    | 95 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 35  | l     | 604/606 (100%) | 581 (96%) | 23 (4%) | 0        | 100         | 100 |
| 36  | m     | 173/175 (99%)  | 161 (93%) | 12 (7%) | 0        | 100         | 100 |
| 37  | n     | 54/56 (96%)    | 54 (100%) | 0       | 0        | 100         | 100 |
| 38  | o     | 126/128 (98%)  | 125 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 39  | p     | 176/178 (99%)  | 165 (94%) | 10 (6%) | 1 (1%)   | 21          | 42  |
| 40  | r     | 457/459 (100%) | 451 (99%) | 6 (1%)  | 0        | 100         | 100 |
| 41  | s     | 316/318 (99%)  | 304 (96%) | 11 (4%) | 1 (0%)   | 36          | 58  |
| 42  | u     | 169/171 (99%)  | 165 (98%) | 3 (2%)  | 1 (1%)   | 21          | 42  |
| 43  | v     | 122/125 (98%)  | 114 (93%) | 8 (7%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 44  | w     | 318/320 (99%)   | 304 (96%)  | 14 (4%)  | 0        | 100         | 100 |
| All | All   | 8175/8314 (98%) | 7866 (96%) | 297 (4%) | 12 (0%)  | 49          | 70  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | LEU  |
| 6   | G     | 134 | ASP  |
| 7   | H     | 77  | ILE  |
| 8   | I     | 29  | GLN  |
| 14  | O     | 175 | GLU  |
| 9   | J     | 38  | HIS  |
| 12  | M     | 281 | ILE  |
| 8   | I     | 41  | LEU  |
| 41  | s     | 208 | VAL  |
| 42  | u     | 152 | PRO  |
| 39  | p     | 174 | PRO  |
| 4   | E     | 96  | 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          | 81 |
| 2   | B     | 151/151 (100%) | 149 (99%) | 2 (1%)   | 61          | 82 |
| 3   | C     | 132/132 (100%) | 130 (98%) | 2 (2%)   | 57          | 80 |
| 4   | E     | 107/107 (100%) | 106 (99%) | 1 (1%)   | 70          | 87 |
| 5   | F     | 75/76 (99%)    | 74 (99%)  | 1 (1%)   | 61          | 82 |
| 6   | G     | 76/81 (94%)    | 74 (97%)  | 2 (3%)   | 40          | 68 |
| 6   | X     | 79/81 (98%)    | 77 (98%)  | 2 (2%)   | 42          | 69 |
| 7   | H     | 99/99 (100%)   | 98 (99%)  | 1 (1%)   | 68          | 86 |
| 8   | I     | 87/97 (90%)    | 83 (95%)  | 4 (5%)   | 24          | 49 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9   | J     | 296/296 (100%) | 294 (99%)  | 2 (1%)   | 76          | 89  |
| 10  | K     | 42/42 (100%)   | 42 (100%)  | 0        | 100         | 100 |
| 11  | L     | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 87  |
| 12  | M     | 580/580 (100%) | 567 (98%)  | 13 (2%)  | 45          | 72  |
| 13  | N     | 130/130 (100%) | 130 (100%) | 0        | 100         | 100 |
| 14  | O     | 183/183 (100%) | 179 (98%)  | 4 (2%)   | 45          | 72  |
| 15  | P     | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 16  | Q     | 370/370 (100%) | 364 (98%)  | 6 (2%)   | 55          | 79  |
| 17  | S     | 57/58 (98%)    | 57 (100%)  | 0        | 100         | 100 |
| 18  | T     | 79/79 (100%)   | 79 (100%)  | 0        | 100         | 100 |
| 19  | U     | 69/69 (100%)   | 68 (99%)   | 1 (1%)   | 59          | 81  |
| 20  | V     | 101/101 (100%) | 98 (97%)   | 3 (3%)   | 36          | 64  |
| 21  | W     | 122/123 (99%)  | 120 (98%)  | 2 (2%)   | 55          | 79  |
| 22  | Y     | 62/62 (100%)   | 61 (98%)   | 1 (2%)   | 55          | 79  |
| 23  | Z     | 62/62 (100%)   | 62 (100%)  | 0        | 100         | 100 |
| 24  | a     | 121/121 (100%) | 121 (100%) | 0        | 100         | 100 |
| 25  | b     | 90/119 (76%)   | 89 (99%)   | 1 (1%)   | 65          | 84  |
| 26  | c     | 141/141 (100%) | 139 (99%)  | 2 (1%)   | 59          | 81  |
| 27  | d     | 155/155 (100%) | 153 (99%)  | 2 (1%)   | 61          | 82  |
| 28  | e     | 96/96 (100%)   | 93 (97%)   | 3 (3%)   | 35          | 63  |
| 29  | f     | 36/45 (80%)    | 36 (100%)  | 0        | 100         | 100 |
| 30  | g     | 108/109 (99%)  | 107 (99%)  | 1 (1%)   | 70          | 87  |
| 31  | h     | 93/93 (100%)   | 92 (99%)   | 1 (1%)   | 65          | 84  |
| 32  | i     | 311/311 (100%) | 309 (99%)  | 2 (1%)   | 78          | 91  |
| 33  | j     | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 34  | k     | 85/85 (100%)   | 84 (99%)   | 1 (1%)   | 63          | 83  |
| 35  | l     | 540/540 (100%) | 533 (99%)  | 7 (1%)   | 61          | 82  |
| 36  | m     | 129/141 (92%)  | 127 (98%)  | 2 (2%)   | 55          | 79  |
| 37  | n     | 53/53 (100%)   | 52 (98%)   | 1 (2%)   | 50          | 75  |
| 38  | o     | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 87  |
| 39  | p     | 159/159 (100%) | 158 (99%)  | 1 (1%)   | 78          | 91  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 40  | r     | 410/410 (100%)  | 405 (99%)  | 5 (1%)   | 63          | 83  |
| 41  | s     | 275/275 (100%)  | 271 (98%)  | 4 (2%)   | 57          | 80  |
| 42  | u     | 153/153 (100%)  | 151 (99%)  | 2 (1%)   | 61          | 82  |
| 43  | v     | 104/111 (94%)   | 104 (100%) | 0        | 100         | 100 |
| 44  | w     | 281/283 (99%)   | 280 (100%) | 1 (0%)   | 84          | 93  |
| All | All   | 7161/7241 (99%) | 7071 (99%) | 90 (1%)  | 59          | 82  |

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 97  | LEU  |
| 1   | A     | 245 | VAL  |
| 1   | A     | 273 | THR  |
| 1   | A     | 447 | GLU  |
| 1   | A     | 451 | GLN  |
| 2   | B     | 114 | ILE  |
| 2   | B     | 165 | ASP  |
| 3   | C     | 142 | TYR  |
| 3   | C     | 187 | GLU  |
| 4   | E     | 17  | VAL  |
| 5   | F     | 95  | LEU  |
| 6   | G     | 107 | ASP  |
| 6   | G     | 139 | MET  |
| 7   | H     | 104 | VAL  |
| 8   | I     | 25  | GLN  |
| 8   | I     | 27  | ARG  |
| 8   | I     | 90  | THR  |
| 8   | I     | 95  | VAL  |
| 9   | J     | 322 | VAL  |
| 9   | J     | 374 | THR  |
| 11  | L     | 108 | GLU  |
| 12  | M     | 107 | GLU  |
| 12  | M     | 260 | ASN  |
| 12  | M     | 281 | ILE  |
| 12  | M     | 352 | VAL  |
| 12  | M     | 361 | VAL  |
| 12  | M     | 405 | THR  |
| 12  | M     | 450 | LYS  |
| 12  | M     | 483 | ARG  |
| 12  | M     | 598 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | M     | 619 | ASP  |
| 12  | M     | 658 | ASP  |
| 12  | M     | 672 | SER  |
| 12  | M     | 688 | GLN  |
| 14  | O     | 137 | THR  |
| 14  | O     | 144 | ASN  |
| 14  | O     | 186 | VAL  |
| 14  | O     | 231 | LEU  |
| 16  | Q     | 36  | GLN  |
| 16  | Q     | 143 | SER  |
| 16  | Q     | 192 | LEU  |
| 16  | Q     | 217 | VAL  |
| 16  | Q     | 308 | TYR  |
| 16  | Q     | 453 | THR  |
| 19  | U     | 10  | LYS  |
| 20  | V     | 10  | SER  |
| 20  | V     | 63  | SER  |
| 20  | V     | 120 | LEU  |
| 21  | W     | 34  | SER  |
| 21  | W     | 85  | GLN  |
| 6   | X     | 139 | MET  |
| 6   | X     | 156 | GLU  |
| 22  | Y     | 50  | LEU  |
| 25  | b     | 120 | MET  |
| 26  | c     | 33  | THR  |
| 26  | c     | 120 | SER  |
| 27  | d     | 43  | ARG  |
| 27  | d     | 61  | TYR  |
| 28  | e     | 53  | ILE  |
| 28  | e     | 83  | ASP  |
| 28  | e     | 136 | LEU  |
| 30  | g     | 2   | THR  |
| 31  | h     | 77  | SER  |
| 32  | i     | 111 | PHE  |
| 32  | i     | 336 | VAL  |
| 34  | k     | 24  | SER  |
| 35  | l     | 9   | LEU  |
| 35  | l     | 70  | THR  |
| 35  | l     | 72  | GLN  |
| 35  | l     | 73  | THR  |
| 35  | l     | 140 | LEU  |
| 35  | l     | 197 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | l     | 508 | THR  |
| 36  | m     | 95  | SER  |
| 36  | m     | 167 | VAL  |
| 37  | n     | 15  | ILE  |
| 38  | o     | 129 | TYR  |
| 39  | p     | 69  | GLU  |
| 40  | r     | 1   | MET  |
| 40  | r     | 116 | ILE  |
| 40  | r     | 122 | PHE  |
| 40  | r     | 183 | SER  |
| 40  | r     | 269 | MET  |
| 41  | s     | 40  | VAL  |
| 41  | s     | 145 | THR  |
| 41  | s     | 202 | GLU  |
| 41  | s     | 296 | LEU  |
| 42  | u     | 64  | ASN  |
| 42  | u     | 157 | ASP  |
| 44  | w     | 95  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 136 | HIS  |
| 1   | A     | 281 | HIS  |
| 1   | A     | 393 | ASN  |
| 2   | B     | 204 | ASN  |
| 3   | C     | 111 | ASN  |
| 4   | E     | 70  | ASN  |
| 4   | E     | 126 | HIS  |
| 8   | I     | 21  | GLN  |
| 8   | I     | 47  | HIS  |
| 9   | J     | 128 | ASN  |
| 9   | J     | 166 | HIS  |
| 10  | K     | 70  | ASN  |
| 10  | K     | 78  | HIS  |
| 10  | K     | 79  | HIS  |
| 10  | K     | 90  | ASN  |
| 11  | L     | 71  | HIS  |
| 11  | L     | 85  | ASN  |
| 12  | M     | 39  | GLN  |
| 12  | M     | 74  | ASN  |
| 12  | M     | 260 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | M     | 278 | HIS  |
| 12  | M     | 300 | GLN  |
| 12  | M     | 304 | GLN  |
| 12  | M     | 334 | GLN  |
| 12  | M     | 464 | GLN  |
| 12  | M     | 540 | ASN  |
| 12  | M     | 598 | ASN  |
| 12  | M     | 604 | GLN  |
| 13  | N     | 112 | ASN  |
| 13  | N     | 123 | GLN  |
| 14  | O     | 90  | ASN  |
| 14  | O     | 182 | ASN  |
| 15  | P     | 55  | HIS  |
| 15  | P     | 63  | GLN  |
| 15  | P     | 228 | GLN  |
| 16  | Q     | 79  | ASN  |
| 16  | Q     | 285 | ASN  |
| 16  | Q     | 313 | GLN  |
| 17  | S     | 40  | HIS  |
| 17  | S     | 68  | ASN  |
| 18  | T     | 43  | GLN  |
| 18  | T     | 120 | GLN  |
| 20  | V     | 129 | GLN  |
| 21  | W     | 61  | GLN  |
| 21  | W     | 76  | GLN  |
| 26  | c     | 94  | HIS  |
| 29  | f     | 62  | HIS  |
| 30  | g     | 90  | HIS  |
| 31  | h     | 21  | GLN  |
| 31  | h     | 98  | HIS  |
| 32  | i     | 36  | ASN  |
| 32  | i     | 77  | ASN  |
| 32  | i     | 112 | HIS  |
| 32  | i     | 120 | GLN  |
| 32  | i     | 134 | GLN  |
| 32  | i     | 150 | ASN  |
| 32  | i     | 273 | ASN  |
| 34  | k     | 57  | ASN  |
| 34  | k     | 92  | ASN  |
| 35  | l     | 2   | ASN  |
| 35  | l     | 34  | ASN  |
| 35  | l     | 59  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | l     | 447 | ASN  |
| 35  | l     | 579 | ASN  |
| 35  | l     | 605 | HIS  |
| 37  | n     | 6   | GLN  |
| 38  | o     | 79  | ASN  |
| 39  | p     | 12  | HIS  |
| 39  | p     | 33  | HIS  |
| 39  | p     | 51  | HIS  |
| 40  | r     | 43  | ASN  |
| 40  | r     | 251 | ASN  |
| 40  | r     | 304 | GLN  |
| 40  | r     | 374 | ASN  |
| 42  | u     | 163 | HIS  |
| 43  | v     | 85  | HIS  |
| 44  | w     | 132 | GLN  |
| 44  | w     | 235 | GLN  |
| 44  | w     | 239 | ASN  |

### 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     | 2.01 | 1 (10%)     | 5,13,15     | 6.00 | 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 | 5.69 | 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  | 12.07 | 130.55      | 119.48   |
| 16  | Q     | 118 | 2MR  | CD-NE-CZ   | 3.91  | 130.72      | 123.36   |
| 16  | Q     | 118 | 2MR  | CQ2-NH2-CZ | 3.80  | 131.82      | 123.65   |

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 47 ligands modelled in this entry, 2 are monoatomic - leaving 45 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 |
| 47  | NAI  | A     | 503 | -    | 47,48,48     | 3.99 | 22 (46%) | 64,73,73    | 1.72 | 12 (18%) |
| 51  | 8Q1  | X     | 201 | -    | 32,34,34     | 2.29 | 8 (25%)  | 39,43,43    | 1.73 | 10 (25%) |
| 48  | PEE  | C     | 302 | -    | 46,46,50     | 1.23 | 6 (13%)  | 49,51,55    | 1.01 | 2 (4%)   |
| 56  | UQ1  | Q     | 502 | -    | 18,18,18     | 2.28 | 6 (33%)  | 24,25,25    | 1.79 | 5 (20%)  |
| 50  | UQ   | C     | 304 | -    | 38,38,63     | 3.62 | 9 (23%)  | 48,49,79    | 2.78 | 17 (35%) |
| 48  | PEE  | W     | 201 | -    | 40,40,50     | 1.16 | 5 (12%)  | 43,45,55    | 1.04 | 2 (4%)   |
| 49  | PLX  | C     | 303 | -    | 51,51,51     | 1.19 | 3 (5%)   | 53,59,59    | 0.61 | 1 (1%)   |
| 49  | PLX  | g     | 201 | -    | 51,51,51     | 1.19 | 4 (7%)   | 53,59,59    | 0.65 | 1 (1%)   |
| 52  | CDL  | l     | 701 | -    | 98,98,99     | 1.12 | 9 (9%)   | 104,110,111 | 0.88 | 4 (3%)   |
| 52  | CDL  | l     | 702 | -    | 99,99,99     | 0.93 | 4 (4%)   | 105,111,111 | 1.16 | 9 (8%)   |
| 52  | CDL  | u     | 201 | -    | 54,54,99     | 1.22 | 4 (7%)   | 60,66,111   | 1.25 | 5 (8%)   |
| 45  | SF4  | B     | 301 | 2    | 0,12,12      | -    | -        | -           | -    | -        |
| 45  | SF4  | M     | 801 | 12   | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PEE  | l     | 704 | -    | 45,45,50     | 1.25 | 6 (13%)  | 48,50,55    | 1.00 | 2 (4%)   |
| 54  | FES  | O     | 301 | 14   | 0,4,4        | -    | -        | -           | -    | -        |
| 52  | CDL  | I     | 201 | -    | 50,50,99     | 1.29 | 4 (8%)   | 56,62,111   | 1.38 | 7 (12%)  |
| 45  | SF4  | M     | 802 | 12   | 0,12,12      | -    | -        | -           | -    | -        |
| 45  | SF4  | A     | 501 | 1    | 0,12,12      | -    | -        | -           | -    | -        |
| 56  | UQ1  | Q     | 501 | -    | 18,18,18     | 2.30 | 6 (33%)  | 24,25,25    | 2.06 | 8 (33%)  |
| 52  | CDL  | V     | 203 | -    | 99,99,99     | 1.11 | 8 (8%)   | 105,111,111 | 0.90 | 4 (3%)   |
| 52  | CDL  | k     | 101 | -    | 93,93,99     | 1.13 | 8 (8%)   | 99,105,111  | 0.85 | 4 (4%)   |
| 52  | CDL  | J     | 404 | -    | 88,88,99     | 1.15 | 8 (9%)   | 94,100,111  | 0.92 | 4 (4%)   |
| 54  | FES  | M     | 803 | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 48  | PEE  | V     | 204 | -    | 39,39,50     | 1.33 | 6 (15%)  | 42,44,55    | 1.13 | 3 (7%)   |
| 48  | PEE  | V     | 202 | -    | 50,50,50     | 1.18 | 6 (12%)  | 53,55,55    | 0.95 | 2 (3%)   |
| 52  | CDL  | a     | 201 | -    | 99,99,99     | 1.12 | 8 (8%)   | 105,111,111 | 0.90 | 4 (3%)   |
| 45  | SF4  | C     | 301 | 3    | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PEE  | Q     | 503 | -    | 46,46,50     | 1.22 | 6 (13%)  | 49,51,55    | 1.05 | 2 (4%)   |
| 48  | PEE  | l     | 703 | -    | 50,50,50     | 1.17 | 5 (10%)  | 53,55,55    | 0.96 | 2 (3%)   |
| 50  | UQ   | J     | 402 | -    | 33,33,63     | 3.50 | 10 (30%) | 42,43,79    | 2.75 | 14 (33%) |
| 46  | FMN  | A     | 502 | -    | 33,33,33     | 1.08 | 2 (6%)   | 48,50,50    | 1.28 | 8 (16%)  |
| 52  | CDL  | V     | 201 | -    | 93,93,99     | 1.14 | 8 (8%)   | 99,105,111  | 0.85 | 4 (4%)   |
| 48  | PEE  | s     | 401 | -    | 50,50,50     | 1.18 | 5 (10%)  | 53,55,55    | 1.03 | 2 (3%)   |
| 49  | PLX  | e     | 201 | -    | 51,51,51     | 1.20 | 5 (9%)   | 53,59,59    | 0.54 | 1 (1%)   |
| 53  | NDP  | J     | 401 | -    | 51,52,52     | 2.31 | 6 (11%)  | 71,80,80    | 1.53 | 15 (21%) |
| 49  | PLX  | J     | 403 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.62 | 2 (3%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 49  | PLX  | j     | 203 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.65 | 1 (1%)   |
| 45  | SF4  | B     | 302 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 51  | 8Q1  | G     | 201 | -    | 32,34,34     | 2.23 | 7 (21%)  | 39,43,43    | 1.86 | 11 (28%) |
| 58  | ADP  | w     | 401 | -    | 28,29,29     | 3.16 | 9 (32%)  | 43,45,45    | 1.87 | 8 (18%)  |
| 49  | PLX  | a     | 202 | -    | 51,51,51     | 1.22 | 4 (7%)   | 53,59,59    | 0.61 | 1 (1%)   |
| 48  | PEE  | j     | 202 | -    | 40,40,50     | 1.18 | 5 (12%)  | 43,45,55    | 1.06 | 2 (4%)   |
| 48  | PEE  | j     | 201 | -    | 50,50,50     | 1.16 | 6 (12%)  | 53,55,55    | 0.98 | 2 (3%)   |
| 52  | CDL  | r     | 502 | -    | 99,99,99     | 1.11 | 8 (8%)   | 105,111,111 | 0.88 | 4 (3%)   |
| 49  | PLX  | r     | 501 | -    | 51,51,51     | 1.20 | 5 (9%)   | 53,59,59    | 0.64 | 1 (1%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 47  | NAI  | A     | 503 | -    | -       | 5/29/72/72     | 0/5/5/5 |
| 51  | 8Q1  | X     | 201 | -    | -       | 15/41/41/41    | -       |
| 48  | PEE  | C     | 302 | -    | -       | 24/50/50/54    | -       |
| 56  | UQ1  | Q     | 502 | -    | -       | 1/9/33/33      | 0/1/1/1 |
| 50  | UQ   | C     | 304 | -    | -       | 11/33/57/87    | 0/1/1/1 |
| 48  | PEE  | W     | 201 | -    | -       | 19/44/44/54    | -       |
| 49  | PLX  | C     | 303 | -    | -       | 23/55/55/55    | -       |
| 49  | PLX  | g     | 201 | -    | -       | 25/55/55/55    | -       |
| 52  | CDL  | l     | 701 | -    | -       | 64/109/109/110 | -       |
| 52  | CDL  | l     | 702 | -    | -       | 43/110/110/110 | -       |
| 52  | CDL  | u     | 201 | -    | -       | 26/65/65/110   | -       |
| 45  | SF4  | B     | 301 | 2    | -       | -              | 0/6/5/5 |
| 45  | SF4  | M     | 801 | 12   | -       | -              | 0/6/5/5 |
| 48  | PEE  | l     | 704 | -    | -       | 21/49/49/54    | -       |
| 54  | FES  | O     | 301 | 14   | -       | -              | 0/1/1/1 |
| 52  | CDL  | I     | 201 | -    | -       | 25/61/61/110   | -       |
| 45  | SF4  | M     | 802 | 12   | -       | -              | 0/6/5/5 |
| 56  | UQ1  | Q     | 501 | -    | -       | 3/9/33/33      | 0/1/1/1 |
| 45  | SF4  | A     | 501 | 1    | -       | -              | 0/6/5/5 |
| 52  | CDL  | V     | 203 | -    | -       | 55/110/110/110 | -       |
| 52  | CDL  | k     | 101 | -    | -       | 53/104/104/110 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 52  | CDL  | J     | 404 | -    | -       | 47/99/99/110   | -       |
| 54  | FES  | M     | 803 | 12   | -       | -              | 0/1/1/1 |
| 48  | PEE  | V     | 204 | -    | -       | 18/43/43/54    | -       |
| 48  | PEE  | V     | 202 | -    | -       | 27/54/54/54    | -       |
| 52  | CDL  | a     | 201 | -    | -       | 56/110/110/110 | -       |
| 48  | PEE  | Q     | 503 | -    | -       | 22/50/50/54    | -       |
| 45  | SF4  | C     | 301 | 3    | -       | -              | 0/6/5/5 |
| 48  | PEE  | l     | 703 | -    | -       | 23/54/54/54    | -       |
| 50  | UQ   | J     | 402 | -    | -       | 14/27/51/87    | 0/1/1/1 |
| 46  | FMN  | A     | 502 | -    | -       | 11/18/18/18    | 0/3/3/3 |
| 52  | CDL  | V     | 201 | -    | -       | 59/104/104/110 | -       |
| 48  | PEE  | s     | 401 | -    | -       | 19/54/54/54    | -       |
| 49  | PLX  | e     | 201 | -    | -       | 35/55/55/55    | -       |
| 53  | NDP  | J     | 401 | -    | -       | 6/34/77/77     | 0/5/5/5 |
| 49  | PLX  | J     | 403 | -    | -       | 35/55/55/55    | -       |
| 49  | PLX  | j     | 203 | -    | -       | 24/55/55/55    | -       |
| 51  | 8Q1  | G     | 201 | -    | -       | 11/41/41/41    | -       |
| 58  | ADP  | w     | 401 | -    | -       | 6/16/32/32     | 0/3/3/3 |
| 45  | SF4  | B     | 302 | 2    | -       | -              | 0/6/5/5 |
| 49  | PLX  | a     | 202 | -    | -       | 29/55/55/55    | -       |
| 48  | PEE  | j     | 202 | -    | -       | 17/44/44/54    | -       |
| 48  | PEE  | j     | 201 | -    | -       | 22/54/54/54    | -       |
| 52  | CDL  | r     | 502 | -    | -       | 55/110/110/110 | -       |
| 49  | PLX  | r     | 501 | -    | -       | 32/55/55/55    | -       |

All (239) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 53  | J     | 401 | NDP  | P2B-O2B | 13.10  | 1.82        | 1.59     |
| 47  | A     | 503 | NAI  | C3D-C4D | -10.50 | 1.26        | 1.53     |
| 50  | C     | 304 | UQ   | C18-C19 | 10.00  | 1.56        | 1.33     |
| 50  | J     | 402 | UQ   | C18-C19 | 9.93   | 1.55        | 1.33     |
| 50  | C     | 304 | UQ   | C13-C14 | 9.52   | 1.55        | 1.33     |
| 50  | J     | 402 | UQ   | C13-C14 | 9.45   | 1.54        | 1.33     |
| 50  | C     | 304 | UQ   | C23-C24 | 9.43   | 1.54        | 1.33     |
| 50  | C     | 304 | UQ   | C8-C9   | 9.38   | 1.54        | 1.33     |
| 50  | J     | 402 | UQ   | C8-C9   | 9.30   | 1.54        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | A     | 503 | NAI  | O4B-C1B | 9.26  | 1.63        | 1.42     |
| 58  | w     | 401 | ADP  | C3'-C4' | -9.02 | 1.30        | 1.53     |
| 47  | A     | 503 | NAI  | O4B-C4B | -8.42 | 1.26        | 1.45     |
| 51  | X     | 201 | 8Q1  | P24-O27 | 7.81  | 1.85        | 1.60     |
| 58  | w     | 401 | ADP  | O4'-C4' | 7.73  | 1.62        | 1.45     |
| 47  | A     | 503 | NAI  | C2D-C1D | -7.71 | 1.29        | 1.53     |
| 51  | G     | 201 | 8Q1  | P24-O27 | 7.63  | 1.84        | 1.60     |
| 50  | J     | 402 | UQ   | C23-C24 | 7.49  | 1.54        | 1.32     |
| 47  | A     | 503 | NAI  | C2B-C1B | -7.38 | 1.30        | 1.53     |
| 50  | C     | 304 | UQ   | C28-C29 | 7.33  | 1.54        | 1.32     |
| 56  | Q     | 501 | UQ1  | C8-C9   | 6.94  | 1.53        | 1.32     |
| 56  | Q     | 502 | UQ1  | C8-C9   | 6.85  | 1.52        | 1.32     |
| 47  | A     | 503 | NAI  | O4D-C4D | 6.80  | 1.60        | 1.45     |
| 58  | w     | 401 | ADP  | PA-O3A  | 6.26  | 1.66        | 1.59     |
| 47  | A     | 503 | NAI  | PA-O3   | 6.18  | 1.66        | 1.59     |
| 47  | A     | 503 | NAI  | C2D-C3D | 5.95  | 1.69        | 1.53     |
| 58  | w     | 401 | ADP  | C6-N6   | 5.46  | 1.48        | 1.34     |
| 47  | A     | 503 | NAI  | O4D-C1D | 5.43  | 1.54        | 1.42     |
| 47  | A     | 503 | NAI  | C4N-C3N | -5.31 | 1.40        | 1.50     |
| 51  | X     | 201 | 8Q1  | C28-C29 | 5.31  | 1.61        | 1.52     |
| 47  | A     | 503 | NAI  | C7N-N7N | 5.25  | 1.48        | 1.33     |
| 47  | A     | 503 | NAI  | PN-O3   | 5.23  | 1.65        | 1.59     |
| 47  | A     | 503 | NAI  | C6A-N6A | 4.95  | 1.46        | 1.34     |
| 51  | G     | 201 | 8Q1  | C28-C29 | 4.81  | 1.60        | 1.52     |
| 58  | w     | 401 | ADP  | O4'-C1' | -4.55 | 1.31        | 1.42     |
| 53  | J     | 401 | NDP  | PA-O3   | 4.46  | 1.64        | 1.59     |
| 47  | A     | 503 | NAI  | O2B-C2B | 4.35  | 1.53        | 1.43     |
| 52  | I     | 201 | CDL  | OB8-CB7 | 4.33  | 1.46        | 1.33     |
| 52  | u     | 201 | CDL  | OA8-CA7 | 4.33  | 1.46        | 1.33     |
| 52  | I     | 201 | CDL  | OA8-CA7 | 4.28  | 1.45        | 1.33     |
| 52  | l     | 702 | CDL  | OA8-CA7 | 4.27  | 1.45        | 1.33     |
| 52  | l     | 702 | CDL  | OB8-CB7 | 4.22  | 1.45        | 1.33     |
| 52  | l     | 702 | CDL  | OA6-CA5 | 4.14  | 1.46        | 1.34     |
| 52  | I     | 201 | CDL  | OA6-CA5 | 4.11  | 1.45        | 1.34     |
| 52  | u     | 201 | CDL  | OB6-CB5 | 4.08  | 1.45        | 1.34     |
| 52  | l     | 702 | CDL  | OB6-CB5 | 4.08  | 1.45        | 1.34     |
| 51  | X     | 201 | 8Q1  | C1-S44  | 4.05  | 1.85        | 1.76     |
| 52  | u     | 201 | CDL  | OB8-CB7 | 4.05  | 1.45        | 1.33     |
| 51  | G     | 201 | 8Q1  | C1-S44  | 4.00  | 1.85        | 1.76     |
| 52  | u     | 201 | CDL  | OA6-CA5 | 3.99  | 1.45        | 1.34     |
| 52  | I     | 201 | CDL  | OB6-CB5 | 3.94  | 1.45        | 1.34     |
| 51  | G     | 201 | 8Q1  | C6-C1   | 3.87  | 1.54        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 53  | J     | 401 | NDP  | PN-O5D  | 3.87  | 1.74        | 1.59     |
| 48  | C     | 302 | PEE  | C18-C19 | 3.85  | 1.53        | 1.31     |
| 48  | l     | 703 | PEE  | C18-C19 | 3.83  | 1.53        | 1.31     |
| 48  | V     | 204 | PEE  | C18-C19 | 3.83  | 1.53        | 1.31     |
| 48  | l     | 704 | PEE  | C18-C19 | 3.82  | 1.53        | 1.31     |
| 48  | j     | 202 | PEE  | C18-C19 | 3.81  | 1.53        | 1.31     |
| 48  | s     | 401 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | V     | 202 | PEE  | C18-C19 | 3.79  | 1.53        | 1.31     |
| 48  | j     | 201 | PEE  | C18-C19 | 3.79  | 1.53        | 1.31     |
| 48  | W     | 201 | PEE  | C18-C19 | 3.78  | 1.53        | 1.31     |
| 48  | Q     | 503 | PEE  | C18-C19 | 3.75  | 1.53        | 1.31     |
| 48  | V     | 204 | PEE  | C39-C38 | 3.75  | 1.53        | 1.31     |
| 48  | C     | 302 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | V     | 202 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | l     | 704 | PEE  | C39-C38 | 3.71  | 1.52        | 1.31     |
| 48  | s     | 401 | PEE  | C39-C38 | 3.71  | 1.52        | 1.31     |
| 48  | Q     | 503 | PEE  | C39-C38 | 3.71  | 1.52        | 1.31     |
| 48  | l     | 703 | PEE  | C39-C38 | 3.71  | 1.52        | 1.31     |
| 48  | j     | 201 | PEE  | C39-C38 | 3.69  | 1.52        | 1.31     |
| 52  | V     | 203 | CDL  | OA8-CA7 | 3.46  | 1.43        | 1.33     |
| 52  | l     | 701 | CDL  | OA8-CA7 | 3.44  | 1.43        | 1.33     |
| 47  | A     | 503 | NAI  | C7N-C3N | 3.43  | 1.56        | 1.48     |
| 52  | a     | 201 | CDL  | OA8-CA7 | 3.43  | 1.43        | 1.33     |
| 52  | V     | 201 | CDL  | OA8-CA7 | 3.43  | 1.43        | 1.33     |
| 51  | G     | 201 | 8Q1  | O27-C28 | -3.42 | 1.32        | 1.43     |
| 52  | r     | 502 | CDL  | OA8-CA7 | 3.41  | 1.43        | 1.33     |
| 51  | X     | 201 | 8Q1  | C6-C1   | 3.41  | 1.54        | 1.50     |
| 47  | A     | 503 | NAI  | C4N-C5N | -3.40 | 1.40        | 1.49     |
| 52  | k     | 101 | CDL  | OA8-CA7 | 3.38  | 1.43        | 1.33     |
| 58  | w     | 401 | ADP  | C8-N9   | -3.37 | 1.31        | 1.37     |
| 53  | J     | 401 | NDP  | O2B-C2B | -3.35 | 1.32        | 1.44     |
| 52  | J     | 404 | CDL  | OA8-CA7 | 3.34  | 1.43        | 1.33     |
| 46  | A     | 502 | FMN  | C4A-N5  | 3.34  | 1.38        | 1.30     |
| 51  | X     | 201 | 8Q1  | O27-C28 | -3.29 | 1.33        | 1.43     |
| 52  | k     | 101 | CDL  | OA6-CA5 | 3.27  | 1.43        | 1.34     |
| 51  | X     | 201 | 8Q1  | C34-N36 | 3.25  | 1.41        | 1.33     |
| 52  | a     | 201 | CDL  | OB6-CB5 | 3.10  | 1.43        | 1.34     |
| 52  | r     | 502 | CDL  | OB6-CB5 | 3.08  | 1.43        | 1.34     |
| 58  | w     | 401 | ADP  | O2'-C2' | -3.08 | 1.35        | 1.43     |
| 52  | V     | 201 | CDL  | OA6-CA5 | 3.07  | 1.43        | 1.34     |
| 52  | J     | 404 | CDL  | OB6-CB5 | 3.05  | 1.42        | 1.34     |
| 52  | a     | 201 | CDL  | OB8-CB7 | 3.05  | 1.42        | 1.33     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 52  | l     | 701 | CDL  | OB8-CB7 | 3.03  | 1.42        | 1.33     |
| 52  | l     | 701 | CDL  | OB6-CB5 | 3.02  | 1.42        | 1.34     |
| 58  | w     | 401 | ADP  | O3'-C3' | 3.00  | 1.50        | 1.43     |
| 52  | V     | 201 | CDL  | OB8-CB7 | 3.00  | 1.42        | 1.33     |
| 52  | J     | 404 | CDL  | OA6-CA5 | 3.00  | 1.42        | 1.34     |
| 52  | k     | 101 | CDL  | OB6-CB5 | 2.98  | 1.42        | 1.34     |
| 51  | G     | 201 | 8Q1  | C34-N36 | 2.97  | 1.40        | 1.33     |
| 52  | r     | 502 | CDL  | OA6-CA5 | 2.97  | 1.42        | 1.34     |
| 52  | V     | 201 | CDL  | OB6-CB5 | 2.96  | 1.42        | 1.34     |
| 52  | V     | 203 | CDL  | OB6-CB5 | 2.96  | 1.42        | 1.34     |
| 52  | k     | 101 | CDL  | OB8-CB7 | 2.95  | 1.41        | 1.33     |
| 52  | r     | 502 | CDL  | OB8-CB7 | 2.95  | 1.41        | 1.33     |
| 51  | X     | 201 | 8Q1  | C39-N41 | 2.93  | 1.40        | 1.33     |
| 52  | l     | 701 | CDL  | OA6-CA5 | 2.91  | 1.42        | 1.34     |
| 52  | V     | 203 | CDL  | OB8-CB7 | 2.91  | 1.41        | 1.33     |
| 52  | V     | 203 | CDL  | OA6-CA5 | 2.91  | 1.42        | 1.34     |
| 48  | s     | 401 | PEE  | O2-C2   | -2.91 | 1.39        | 1.46     |
| 52  | a     | 201 | CDL  | OA6-CA5 | 2.89  | 1.42        | 1.34     |
| 52  | J     | 404 | CDL  | OB8-CB7 | 2.86  | 1.41        | 1.33     |
| 49  | C     | 303 | PLX  | O6-C4   | -2.86 | 1.41        | 1.44     |
| 49  | g     | 201 | PLX  | O6-C4   | -2.80 | 1.41        | 1.44     |
| 49  | a     | 202 | PLX  | O6-C4   | -2.78 | 1.41        | 1.44     |
| 47  | A     | 503 | NAI  | C8A-N9A | -2.78 | 1.32        | 1.37     |
| 48  | C     | 302 | PEE  | O2-C2   | -2.78 | 1.40        | 1.46     |
| 49  | e     | 201 | PLX  | O6-C4   | -2.77 | 1.41        | 1.44     |
| 49  | j     | 203 | PLX  | O6-C4   | -2.70 | 1.41        | 1.44     |
| 50  | C     | 304 | UQ   | C6-C1   | 2.68  | 1.54        | 1.46     |
| 48  | Q     | 503 | PEE  | O2-C2   | -2.67 | 1.40        | 1.46     |
| 48  | l     | 703 | PEE  | O2-C2   | -2.64 | 1.40        | 1.46     |
| 50  | J     | 402 | UQ   | C6-C1   | 2.64  | 1.53        | 1.46     |
| 52  | a     | 201 | CDL  | OA6-CA4 | -2.62 | 1.40        | 1.46     |
| 49  | J     | 403 | PLX  | O6-C4   | -2.62 | 1.41        | 1.44     |
| 51  | G     | 201 | 8Q1  | C39-N41 | 2.59  | 1.39        | 1.33     |
| 48  | W     | 201 | PEE  | O2-C2   | -2.59 | 1.40        | 1.46     |
| 52  | V     | 203 | CDL  | OA6-CA4 | -2.57 | 1.40        | 1.46     |
| 52  | l     | 701 | CDL  | OA6-CA4 | -2.57 | 1.40        | 1.46     |
| 48  | j     | 202 | PEE  | O3-C30  | 2.57  | 1.40        | 1.33     |
| 48  | j     | 202 | PEE  | O2-C2   | -2.56 | 1.40        | 1.46     |
| 52  | J     | 404 | CDL  | OA6-CA4 | -2.55 | 1.40        | 1.46     |
| 48  | l     | 704 | PEE  | O2-C2   | -2.54 | 1.40        | 1.46     |
| 48  | V     | 204 | PEE  | O3-C30  | 2.53  | 1.40        | 1.33     |
| 56  | Q     | 501 | UQ1  | O2-CM2  | -2.51 | 1.39        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 52  | r     | 502 | CDL  | OA6-CA4 | -2.51 | 1.40        | 1.46     |
| 56  | Q     | 501 | UQ1  | C6-C1   | 2.50  | 1.53        | 1.46     |
| 48  | V     | 204 | PEE  | O2-C2   | -2.49 | 1.40        | 1.46     |
| 48  | l     | 704 | PEE  | O3-C30  | 2.49  | 1.40        | 1.33     |
| 48  | V     | 202 | PEE  | O2-C2   | -2.47 | 1.40        | 1.46     |
| 48  | j     | 201 | PEE  | O3-C30  | 2.46  | 1.40        | 1.33     |
| 49  | a     | 202 | PLX  | C7-C6   | 2.44  | 1.55        | 1.50     |
| 48  | j     | 201 | PEE  | O2-C2   | -2.44 | 1.40        | 1.46     |
| 46  | A     | 502 | FMN  | C10-N1  | 2.44  | 1.38        | 1.33     |
| 49  | j     | 203 | PLX  | C7-C6   | 2.43  | 1.55        | 1.50     |
| 52  | k     | 101 | CDL  | OB6-CB4 | -2.42 | 1.40        | 1.46     |
| 52  | l     | 701 | CDL  | OB6-CB4 | -2.40 | 1.41        | 1.46     |
| 47  | A     | 503 | NAI  | C6N-C5N | 2.39  | 1.40        | 1.33     |
| 49  | r     | 501 | PLX  | O6-C4   | -2.39 | 1.41        | 1.44     |
| 58  | w     | 401 | ADP  | C5-N7   | -2.38 | 1.34        | 1.39     |
| 52  | V     | 203 | CDL  | OB6-CB4 | -2.38 | 1.41        | 1.46     |
| 52  | V     | 201 | CDL  | OB6-CB4 | -2.38 | 1.41        | 1.46     |
| 49  | e     | 201 | PLX  | C7-C6   | 2.37  | 1.55        | 1.50     |
| 56  | Q     | 502 | UQ1  | C6-C1   | 2.37  | 1.53        | 1.46     |
| 47  | A     | 503 | NAI  | PN-O5D  | 2.36  | 1.68        | 1.59     |
| 47  | A     | 503 | NAI  | O3B-C3B | -2.36 | 1.37        | 1.43     |
| 49  | r     | 501 | PLX  | C7-C6   | 2.36  | 1.55        | 1.50     |
| 48  | l     | 703 | PEE  | O3-C30  | 2.36  | 1.40        | 1.33     |
| 48  | V     | 202 | PEE  | O3-C30  | 2.34  | 1.40        | 1.33     |
| 49  | J     | 403 | PLX  | C7-C6   | 2.34  | 1.55        | 1.50     |
| 56  | Q     | 502 | UQ1  | O3-CM3  | -2.33 | 1.40        | 1.45     |
| 52  | J     | 404 | CDL  | OB6-CB4 | -2.32 | 1.41        | 1.46     |
| 50  | C     | 304 | UQ   | C7-C8   | 2.32  | 1.54        | 1.50     |
| 48  | C     | 302 | PEE  | O3-C3   | -2.32 | 1.40        | 1.45     |
| 48  | W     | 201 | PEE  | O3-C30  | 2.32  | 1.40        | 1.33     |
| 49  | g     | 201 | PLX  | C7-C6   | 2.32  | 1.55        | 1.50     |
| 52  | V     | 203 | CDL  | PB2-OB2 | 2.31  | 1.68        | 1.59     |
| 52  | r     | 502 | CDL  | OB6-CB4 | -2.30 | 1.41        | 1.46     |
| 48  | l     | 704 | PEE  | O2-C10  | 2.30  | 1.40        | 1.34     |
| 48  | j     | 202 | PEE  | O2-C10  | 2.29  | 1.40        | 1.34     |
| 56  | Q     | 501 | UQ1  | O1-C1   | -2.28 | 1.18        | 1.23     |
| 48  | C     | 302 | PEE  | O3-C30  | 2.28  | 1.40        | 1.33     |
| 48  | Q     | 503 | PEE  | O3-C30  | 2.28  | 1.40        | 1.33     |
| 49  | C     | 303 | PLX  | C7-C6   | 2.28  | 1.55        | 1.50     |
| 52  | V     | 201 | CDL  | PB2-OB2 | 2.28  | 1.68        | 1.59     |
| 48  | s     | 401 | PEE  | O3-C30  | 2.27  | 1.40        | 1.33     |
| 56  | Q     | 502 | UQ1  | O4-C4   | -2.27 | 1.18        | 1.23     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 52  | a     | 201 | CDL  | PB2-OB5 | 2.27  | 1.68        | 1.59     |
| 48  | V     | 202 | PEE  | O2-C10  | 2.26  | 1.40        | 1.34     |
| 56  | Q     | 502 | UQ1  | O2-CM2  | -2.26 | 1.40        | 1.45     |
| 48  | V     | 202 | PEE  | O3-C3   | -2.26 | 1.40        | 1.45     |
| 48  | W     | 201 | PEE  | O3-C3   | -2.26 | 1.40        | 1.45     |
| 52  | V     | 201 | CDL  | PB2-OB5 | 2.26  | 1.68        | 1.59     |
| 52  | V     | 201 | CDL  | OA6-CA4 | -2.26 | 1.41        | 1.46     |
| 48  | V     | 204 | PEE  | O2-C10  | 2.26  | 1.40        | 1.34     |
| 48  | Q     | 503 | PEE  | O2-C10  | 2.25  | 1.40        | 1.34     |
| 48  | Q     | 503 | PEE  | O3-C3   | -2.25 | 1.40        | 1.45     |
| 52  | r     | 502 | CDL  | PB2-OB2 | 2.23  | 1.68        | 1.59     |
| 48  | j     | 201 | PEE  | O2-C10  | 2.23  | 1.40        | 1.34     |
| 52  | J     | 404 | CDL  | PB2-OB2 | 2.23  | 1.68        | 1.59     |
| 52  | a     | 201 | CDL  | OB6-CB4 | -2.22 | 1.41        | 1.46     |
| 48  | s     | 401 | PEE  | O3-C3   | -2.22 | 1.40        | 1.45     |
| 52  | l     | 701 | CDL  | PB2-OB5 | 2.21  | 1.68        | 1.59     |
| 50  | J     | 402 | UQ   | C7-C8   | 2.21  | 1.54        | 1.50     |
| 56  | Q     | 502 | UQ1  | O1-C1   | -2.21 | 1.18        | 1.23     |
| 52  | l     | 701 | CDL  | PB2-OB2 | 2.20  | 1.68        | 1.59     |
| 48  | W     | 201 | PEE  | O2-C10  | 2.20  | 1.40        | 1.34     |
| 49  | j     | 203 | PLX  | P1-O4   | 2.20  | 1.68        | 1.59     |
| 49  | a     | 202 | PLX  | P1-O4   | 2.20  | 1.68        | 1.59     |
| 52  | V     | 203 | CDL  | PB2-OB5 | 2.19  | 1.68        | 1.59     |
| 47  | A     | 503 | NAI  | C5B-C4B | 2.19  | 1.58        | 1.51     |
| 49  | r     | 501 | PLX  | P1-O4   | 2.19  | 1.68        | 1.59     |
| 52  | a     | 201 | CDL  | PB2-OB2 | 2.18  | 1.67        | 1.59     |
| 52  | r     | 502 | CDL  | PB2-OB5 | 2.17  | 1.67        | 1.59     |
| 49  | g     | 201 | PLX  | P1-O4   | 2.16  | 1.67        | 1.59     |
| 49  | r     | 501 | PLX  | P1-O1   | 2.16  | 1.67        | 1.59     |
| 56  | Q     | 501 | UQ1  | O4-C4   | -2.16 | 1.18        | 1.23     |
| 48  | C     | 302 | PEE  | O2-C10  | 2.15  | 1.40        | 1.34     |
| 47  | A     | 503 | NAI  | C5A-N7A | -2.15 | 1.35        | 1.39     |
| 52  | J     | 404 | CDL  | PB2-OB5 | 2.15  | 1.67        | 1.59     |
| 52  | k     | 101 | CDL  | PB2-OB5 | 2.15  | 1.67        | 1.59     |
| 50  | C     | 304 | UQ   | O4-C4   | -2.15 | 1.18        | 1.23     |
| 56  | Q     | 501 | UQ1  | O3-CM3  | -2.14 | 1.40        | 1.45     |
| 50  | C     | 304 | UQ   | O3-CM3  | -2.12 | 1.40        | 1.45     |
| 49  | e     | 201 | PLX  | P1-O4   | 2.12  | 1.67        | 1.59     |
| 53  | J     | 401 | NDP  | C5A-C4A | 2.12  | 1.42        | 1.39     |
| 48  | l     | 703 | PEE  | O3-C3   | -2.12 | 1.40        | 1.45     |
| 50  | J     | 402 | UQ   | O1-C1   | -2.10 | 1.18        | 1.23     |
| 49  | j     | 203 | PLX  | P1-O1   | 2.10  | 1.67        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | r     | 501 | PLX  | C25-C24 | 2.08  | 1.55        | 1.50     |
| 52  | k     | 101 | CDL  | PB2-OB2 | 2.08  | 1.67        | 1.59     |
| 49  | C     | 303 | PLX  | P1-O4   | 2.08  | 1.67        | 1.59     |
| 49  | a     | 202 | PLX  | P1-O1   | 2.08  | 1.67        | 1.59     |
| 48  | j     | 201 | PEE  | O3-C3   | -2.07 | 1.40        | 1.45     |
| 53  | J     | 401 | NDP  | O5D-C5D | -2.07 | 1.36        | 1.44     |
| 48  | l     | 704 | PEE  | O3-C3   | -2.06 | 1.40        | 1.45     |
| 49  | e     | 201 | PLX  | P1-O1   | 2.06  | 1.67        | 1.59     |
| 52  | k     | 101 | CDL  | OA6-CA4 | -2.06 | 1.41        | 1.46     |
| 50  | J     | 402 | UQ   | O4-C4   | -2.05 | 1.18        | 1.23     |
| 48  | V     | 204 | PEE  | O3-C3   | -2.05 | 1.40        | 1.45     |
| 50  | J     | 402 | UQ   | C5-C4   | 2.04  | 1.54        | 1.47     |
| 50  | J     | 402 | UQ   | O3-CM3  | -2.04 | 1.40        | 1.45     |
| 49  | J     | 403 | PLX  | P1-O4   | 2.04  | 1.67        | 1.59     |
| 49  | J     | 403 | PLX  | P1-O1   | 2.04  | 1.67        | 1.59     |
| 49  | g     | 201 | PLX  | P1-O1   | 2.02  | 1.67        | 1.59     |
| 49  | e     | 201 | PLX  | C1-C2   | 2.01  | 1.57        | 1.51     |
| 48  | j     | 202 | PEE  | O3-C3   | -2.01 | 1.40        | 1.45     |
| 52  | l     | 701 | CDL  | C11-CA5 | 2.01  | 1.56        | 1.50     |
| 51  | X     | 201 | 8Q1  | O33-C32 | -2.00 | 1.38        | 1.42     |

All (186) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 50  | J     | 402 | UQ   | C7-C8-C9    | -8.36 | 112.43      | 126.83   |
| 50  | C     | 304 | UQ   | C7-C8-C9    | -7.91 | 113.20      | 126.83   |
| 50  | J     | 402 | UQ   | C12-C13-C14 | -6.34 | 113.10      | 127.62   |
| 50  | C     | 304 | UQ   | C17-C18-C19 | -6.24 | 113.34      | 127.62   |
| 50  | J     | 402 | UQ   | C17-C18-C19 | -6.18 | 113.47      | 127.62   |
| 50  | C     | 304 | UQ   | C12-C13-C14 | -6.18 | 113.48      | 127.62   |
| 50  | C     | 304 | UQ   | C22-C23-C24 | -5.97 | 113.96      | 127.62   |
| 51  | G     | 201 | 8Q1  | C6-C1-S44   | 5.41  | 119.85      | 113.40   |
| 58  | w     | 401 | ADP  | C5-C4-N3    | -5.41 | 119.27      | 126.72   |
| 47  | A     | 503 | NAI  | C5A-C4A-N3A | -5.40 | 119.28      | 126.72   |
| 56  | Q     | 502 | UQ1  | C7-C8-C9    | -5.27 | 112.33      | 127.25   |
| 56  | Q     | 501 | UQ1  | C7-C6-C1    | 5.09  | 124.42      | 118.52   |
| 52  | l     | 702 | CDL  | OA6-CA5-C11 | 4.82  | 121.92      | 111.48   |
| 52  | l     | 702 | CDL  | OB6-CB5-C51 | 4.65  | 121.55      | 111.48   |
| 58  | w     | 401 | ADP  | N3-C2-N1    | -4.61 | 121.61      | 128.58   |
| 56  | Q     | 501 | UQ1  | C7-C6-C5    | -4.53 | 117.13      | 124.89   |
| 51  | X     | 201 | 8Q1  | C43-S44-C1  | 4.48  | 115.08      | 101.84   |
| 47  | A     | 503 | NAI  | N3A-C2A-N1A | -4.47 | 121.82      | 128.58   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 50  | J     | 402 | UQ   | C22-C23-C24 | -4.39 | 112.99      | 127.64   |
| 50  | J     | 402 | UQ   | C20-C19-C18 | -4.39 | 112.36      | 123.63   |
| 48  | j     | 202 | PEE  | O2-C10-C11  | 4.36  | 120.92      | 111.48   |
| 50  | C     | 304 | UQ   | C27-C28-C29 | -4.32 | 113.25      | 127.64   |
| 50  | C     | 304 | UQ   | C10-C9-C8   | -4.31 | 112.57      | 123.63   |
| 58  | w     | 401 | ADP  | N3-C4-N9    | 4.30  | 134.48      | 127.17   |
| 50  | C     | 304 | UQ   | C25-C24-C23 | -4.27 | 112.66      | 123.63   |
| 52  | a     | 201 | CDL  | OB6-CB5-C51 | 4.26  | 120.69      | 111.48   |
| 52  | I     | 201 | CDL  | OB6-CB5-C51 | 4.17  | 120.50      | 111.48   |
| 48  | V     | 204 | PEE  | O2-C10-C11  | 4.15  | 120.45      | 111.48   |
| 48  | V     | 202 | PEE  | O2-C10-C11  | 4.14  | 120.44      | 111.48   |
| 48  | j     | 201 | PEE  | O2-C10-C11  | 4.13  | 120.42      | 111.48   |
| 53  | J     | 401 | NDP  | P2B-O2B-C2B | -4.13 | 112.41      | 123.43   |
| 52  | r     | 502 | CDL  | OA6-CA5-C11 | 4.11  | 120.37      | 111.48   |
| 50  | J     | 402 | UQ   | C15-C14-C13 | -4.10 | 113.09      | 123.63   |
| 48  | l     | 704 | PEE  | O2-C10-C11  | 4.10  | 120.35      | 111.48   |
| 51  | X     | 201 | 8Q1  | C6-C1-S44   | 4.03  | 118.20      | 113.40   |
| 52  | l     | 701 | CDL  | OA6-CA5-C11 | 4.03  | 120.19      | 111.48   |
| 52  | J     | 404 | CDL  | OB6-CB5-C51 | 4.02  | 120.18      | 111.48   |
| 52  | I     | 201 | CDL  | OA6-CA5-C11 | 4.02  | 120.17      | 111.48   |
| 52  | V     | 203 | CDL  | OA6-CA5-C11 | 4.00  | 120.14      | 111.48   |
| 48  | W     | 201 | PEE  | O2-C10-C11  | 3.97  | 120.07      | 111.48   |
| 51  | G     | 201 | 8Q1  | C43-S44-C1  | 3.97  | 113.57      | 101.84   |
| 52  | u     | 201 | CDL  | OB6-CB5-C51 | 3.97  | 120.06      | 111.48   |
| 52  | V     | 203 | CDL  | OB6-CB5-C51 | 3.94  | 120.00      | 111.48   |
| 50  | J     | 402 | UQ   | C10-C9-C8   | -3.93 | 113.52      | 123.63   |
| 48  | Q     | 503 | PEE  | O2-C10-C11  | 3.93  | 119.98      | 111.48   |
| 50  | C     | 304 | UQ   | C20-C19-C18 | -3.93 | 113.54      | 123.63   |
| 48  | s     | 401 | PEE  | O2-C10-C11  | 3.92  | 119.96      | 111.48   |
| 52  | J     | 404 | CDL  | OA6-CA5-C11 | 3.91  | 119.95      | 111.48   |
| 52  | r     | 502 | CDL  | OB6-CB5-C51 | 3.91  | 119.93      | 111.48   |
| 52  | a     | 201 | CDL  | OA6-CA5-C11 | 3.90  | 119.91      | 111.48   |
| 56  | Q     | 501 | UQ1  | C7-C8-C9    | -3.89 | 116.26      | 127.25   |
| 48  | l     | 703 | PEE  | O2-C10-C11  | 3.87  | 119.86      | 111.48   |
| 48  | C     | 302 | PEE  | O2-C10-C11  | 3.87  | 119.85      | 111.48   |
| 52  | V     | 201 | CDL  | OA6-CA5-C11 | 3.82  | 119.74      | 111.48   |
| 50  | C     | 304 | UQ   | C15-C14-C13 | -3.80 | 113.88      | 123.63   |
| 47  | A     | 503 | NAI  | N3A-C4A-N9A | 3.79  | 133.62      | 127.17   |
| 52  | k     | 101 | CDL  | OB6-CB5-C51 | 3.79  | 119.68      | 111.48   |
| 50  | J     | 402 | UQ   | C21-C19-C18 | -3.76 | 112.73      | 121.17   |
| 50  | J     | 402 | UQ   | C16-C14-C13 | -3.75 | 112.74      | 121.17   |
| 52  | u     | 201 | CDL  | OA6-CA5-C11 | 3.72  | 119.53      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 52  | V     | 201 | CDL  | OB6-CB5-C51 | 3.72  | 119.53      | 111.48   |
| 50  | C     | 304 | UQ   | C21-C19-C18 | -3.71 | 112.83      | 121.17   |
| 47  | A     | 503 | NAI  | C2A-N3A-C4A | 3.71  | 120.89      | 111.83   |
| 52  | l     | 701 | CDL  | OB6-CB5-C51 | 3.69  | 119.47      | 111.48   |
| 50  | C     | 304 | UQ   | C16-C14-C13 | -3.64 | 112.99      | 121.17   |
| 50  | C     | 304 | UQ   | C11-C9-C8   | -3.62 | 113.05      | 121.17   |
| 58  | w     | 401 | ADP  | C2-N3-C4    | 3.55  | 120.50      | 111.83   |
| 50  | J     | 402 | UQ   | C11-C9-C8   | -3.53 | 113.24      | 121.17   |
| 58  | w     | 401 | ADP  | N9-C8-N7    | -3.51 | 108.96      | 113.94   |
| 51  | G     | 201 | 8Q1  | O35-C34-N36 | -3.48 | 115.61      | 122.98   |
| 47  | A     | 503 | NAI  | C4A-C5A-N7A | -3.48 | 106.61      | 110.58   |
| 47  | A     | 503 | NAI  | C5A-N7A-C8A | 3.44  | 108.86      | 103.45   |
| 46  | A     | 502 | FMN  | C4-N3-C2    | -3.42 | 119.56      | 125.64   |
| 53  | J     | 401 | NDP  | O3-PA-O1A   | -3.39 | 100.50      | 110.70   |
| 53  | J     | 401 | NDP  | O2B-P2B-O1X | -3.38 | 97.27       | 109.33   |
| 47  | A     | 503 | NAI  | N9A-C8A-N7A | -3.37 | 109.15      | 113.94   |
| 52  | k     | 101 | CDL  | OA6-CA5-C11 | 3.33  | 118.69      | 111.48   |
| 50  | C     | 304 | UQ   | C26-C24-C23 | -3.32 | 113.71      | 121.17   |
| 52  | u     | 201 | CDL  | OB8-CB7-C71 | 3.32  | 121.96      | 111.83   |
| 47  | A     | 503 | NAI  | C4D-O4D-C1D | -3.28 | 102.22      | 109.47   |
| 48  | s     | 401 | PEE  | O3-C30-C31  | 3.28  | 121.84      | 111.83   |
| 50  | J     | 402 | UQ   | C25-C24-C23 | -3.28 | 112.82      | 122.66   |
| 50  | C     | 304 | UQ   | C30-C29-C28 | -3.26 | 112.87      | 122.66   |
| 58  | w     | 401 | ADP  | C4-N9-C8    | 3.23  | 109.13      | 105.74   |
| 47  | A     | 503 | NAI  | C3D-C2D-C1D | 3.23  | 107.56      | 101.46   |
| 50  | J     | 402 | UQ   | C26-C24-C23 | -3.22 | 112.99      | 122.66   |
| 51  | X     | 201 | 8Q1  | O35-C34-N36 | -3.18 | 116.26      | 122.98   |
| 58  | w     | 401 | ADP  | C5-N7-C8    | 3.18  | 108.44      | 103.45   |
| 50  | C     | 304 | UQ   | C31-C29-C28 | -3.16 | 113.16      | 122.66   |
| 52  | l     | 702 | CDL  | CB4-OB6-CB5 | -3.13 | 110.30      | 117.80   |
| 56  | Q     | 502 | UQ1  | C10-C9-C8   | -3.08 | 113.41      | 122.66   |
| 53  | J     | 401 | NDP  | PA-O5B-C5B  | -3.06 | 103.81      | 121.35   |
| 56  | Q     | 502 | UQ1  | C7-C6-C5    | -3.03 | 119.70      | 124.89   |
| 52  | a     | 201 | CDL  | OB8-CB7-C71 | 3.02  | 121.04      | 111.83   |
| 56  | Q     | 501 | UQ1  | C10-C9-C8   | -3.02 | 113.61      | 122.66   |
| 52  | l     | 702 | CDL  | OA8-CA7-C31 | 3.00  | 120.99      | 111.83   |
| 56  | Q     | 502 | UQ1  | C11-C9-C8   | -3.00 | 113.65      | 122.66   |
| 48  | Q     | 503 | PEE  | O3-C30-C31  | 2.99  | 120.94      | 111.83   |
| 51  | G     | 201 | 8Q1  | C32-C34-N36 | 2.96  | 122.11      | 116.48   |
| 58  | w     | 401 | ADP  | C4-C5-N7    | -2.95 | 107.21      | 110.58   |
| 52  | I     | 201 | CDL  | CA6-CA4-CA3 | -2.90 | 105.03      | 111.78   |
| 52  | I     | 201 | CDL  | OA8-CA7-C31 | 2.89  | 120.64      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 52  | V     | 203 | CDL  | OB8-CB7-C71 | 2.87  | 120.59      | 111.83   |
| 52  | k     | 101 | CDL  | OA8-CA7-C31 | 2.87  | 120.58      | 111.83   |
| 52  | I     | 201 | CDL  | CB4-OB6-CB5 | -2.84 | 111.00      | 117.80   |
| 52  | l     | 702 | CDL  | OB8-CB7-C71 | 2.82  | 120.42      | 111.83   |
| 52  | I     | 201 | CDL  | OB8-CB7-C71 | 2.82  | 120.42      | 111.83   |
| 51  | X     | 201 | 8Q1  | O2-P24-O27  | -2.81 | 99.35       | 106.67   |
| 51  | G     | 201 | 8Q1  | O4-C1-S44   | -2.80 | 119.12      | 122.68   |
| 53  | J     | 401 | NDP  | PN-O5D-C5D  | -2.80 | 105.30      | 121.35   |
| 48  | C     | 302 | PEE  | O3-C30-C31  | 2.78  | 120.32      | 111.83   |
| 52  | u     | 201 | CDL  | OA8-CA7-C31 | 2.78  | 119.59      | 111.15   |
| 52  | V     | 201 | CDL  | OB8-CB7-C71 | 2.78  | 120.30      | 111.83   |
| 48  | W     | 201 | PEE  | O3-C30-C31  | 2.77  | 120.28      | 111.83   |
| 48  | V     | 204 | PEE  | O3-C30-C31  | 2.77  | 120.27      | 111.83   |
| 51  | X     | 201 | 8Q1  | C37-C38-C39 | 2.75  | 116.98      | 112.39   |
| 52  | l     | 701 | CDL  | OA8-CA7-C31 | 2.75  | 120.22      | 111.83   |
| 46  | A     | 502 | FMN  | C4A-C4-N3   | 2.74  | 120.22      | 113.25   |
| 51  | G     | 201 | 8Q1  | O2-P24-O27  | -2.73 | 99.54       | 106.67   |
| 48  | l     | 703 | PEE  | O3-C30-C31  | 2.73  | 120.17      | 111.83   |
| 48  | j     | 201 | PEE  | O3-C30-C31  | 2.73  | 120.17      | 111.83   |
| 48  | j     | 202 | PEE  | O3-C30-C31  | 2.73  | 120.15      | 111.83   |
| 52  | l     | 701 | CDL  | OB8-CB7-C71 | 2.72  | 120.14      | 111.83   |
| 51  | G     | 201 | 8Q1  | C37-C38-C39 | 2.71  | 116.91      | 112.39   |
| 50  | J     | 402 | UQ   | CM5-C5-C6   | -2.71 | 120.00      | 124.45   |
| 52  | V     | 203 | CDL  | OA8-CA7-C31 | 2.70  | 120.08      | 111.83   |
| 52  | J     | 404 | CDL  | OA8-CA7-C31 | 2.70  | 120.07      | 111.83   |
| 52  | r     | 502 | CDL  | OA8-CA7-C31 | 2.69  | 120.02      | 111.83   |
| 51  | G     | 201 | 8Q1  | O40-C39-N41 | -2.67 | 117.79      | 123.03   |
| 52  | k     | 101 | CDL  | OB8-CB7-C71 | 2.67  | 119.97      | 111.83   |
| 53  | J     | 401 | NDP  | O4B-C4B-C3B | 2.62  | 110.35      | 105.15   |
| 46  | A     | 502 | FMN  | C5A-C9A-N10 | 2.61  | 120.33      | 117.97   |
| 51  | X     | 201 | 8Q1  | C32-C34-N36 | 2.61  | 121.44      | 116.48   |
| 52  | V     | 201 | CDL  | OA8-CA7-C31 | 2.59  | 119.75      | 111.83   |
| 49  | r     | 501 | PLX  | C1A-N1-C1   | 2.57  | 120.12      | 109.91   |
| 53  | J     | 401 | NDP  | O2N-PN-O3   | 2.57  | 114.21      | 107.27   |
| 52  | a     | 201 | CDL  | OA8-CA7-C31 | 2.56  | 119.65      | 111.83   |
| 49  | g     | 201 | PLX  | C1A-N1-C1   | 2.56  | 120.09      | 109.91   |
| 51  | G     | 201 | 8Q1  | O4-C1-C6    | -2.56 | 121.03      | 123.98   |
| 46  | A     | 502 | FMN  | O4-C4-C4A   | -2.55 | 119.81      | 126.53   |
| 53  | J     | 401 | NDP  | O3X-P2B-O2X | 2.54  | 117.32      | 107.80   |
| 52  | r     | 502 | CDL  | OB8-CB7-C71 | 2.54  | 119.57      | 111.83   |
| 50  | J     | 402 | UQ   | C7-C6-C5    | -2.53 | 120.56      | 124.89   |
| 48  | V     | 202 | PEE  | O3-C30-C31  | 2.53  | 119.54      | 111.83   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 48  | l     | 704 | PEE  | O3-C30-C31  | 2.51  | 119.49      | 111.83   |
| 50  | C     | 304 | UQ   | C7-C6-C5    | -2.51 | 120.59      | 124.89   |
| 51  | X     | 201 | 8Q1  | O27-P24-O3  | -2.50 | 99.69       | 106.44   |
| 52  | u     | 201 | CDL  | OB8-CB7-OB9 | -2.50 | 117.39      | 123.63   |
| 53  | J     | 401 | NDP  | C2A-N1A-C6A | -2.47 | 114.67      | 118.73   |
| 53  | J     | 401 | NDP  | O2N-PN-O1N  | 2.47  | 123.92      | 112.44   |
| 49  | j     | 203 | PLX  | C1A-N1-C1   | 2.44  | 119.61      | 109.91   |
| 47  | A     | 503 | NAI  | C4A-N9A-C8A | 2.42  | 108.28      | 105.74   |
| 53  | J     | 401 | NDP  | C5B-C4B-C3B | -2.41 | 106.52      | 115.21   |
| 51  | X     | 201 | 8Q1  | O40-C39-N41 | -2.41 | 118.31      | 123.03   |
| 52  | J     | 404 | CDL  | OB8-CB7-C71 | 2.39  | 119.14      | 111.83   |
| 56  | Q     | 501 | UQ1  | C6-C5-C4    | 2.39  | 121.06      | 119.17   |
| 46  | A     | 502 | FMN  | C4A-C10-N10 | 2.37  | 119.88      | 116.48   |
| 56  | Q     | 501 | UQ1  | C11-C9-C8   | -2.36 | 115.58      | 122.66   |
| 53  | J     | 401 | NDP  | N3A-C4A-N9A | 2.34  | 131.15      | 127.17   |
| 49  | a     | 202 | PLX  | C1A-N1-C1   | 2.34  | 119.21      | 109.91   |
| 53  | J     | 401 | NDP  | O5D-PN-O1N  | -2.34 | 99.67       | 108.94   |
| 49  | J     | 403 | PLX  | C1A-N1-C1   | 2.32  | 119.14      | 109.91   |
| 46  | A     | 502 | FMN  | C9A-C5A-N5  | -2.30 | 120.01      | 122.45   |
| 46  | A     | 502 | FMN  | C4A-C10-N1  | -2.29 | 118.96      | 124.59   |
| 49  | C     | 303 | PLX  | C1A-N1-C1   | 2.29  | 119.02      | 109.91   |
| 48  | V     | 204 | PEE  | C20-C19-C18 | -2.29 | 112.64      | 126.42   |
| 56  | Q     | 502 | UQ1  | CM5-C5-C6   | -2.29 | 120.69      | 124.45   |
| 51  | G     | 201 | 8Q1  | O1-P24-O2   | 2.28  | 116.35      | 107.80   |
| 51  | X     | 201 | 8Q1  | O1-P24-O2   | 2.28  | 116.34      | 107.80   |
| 52  | l     | 702 | CDL  | OA6-CA5-OA7 | -2.27 | 118.39      | 123.70   |
| 47  | A     | 503 | NAI  | C6N-N1N-C2N | 2.27  | 121.75      | 119.32   |
| 52  | l     | 702 | CDL  | OB6-CB5-OB7 | -2.26 | 118.43      | 123.70   |
| 50  | C     | 304 | UQ   | CM5-C5-C6   | -2.25 | 120.75      | 124.45   |
| 56  | Q     | 501 | UQ1  | CM5-C5-C6   | -2.19 | 120.85      | 124.45   |
| 52  | l     | 702 | CDL  | CA4-OA6-CA5 | -2.18 | 112.58      | 117.80   |
| 53  | J     | 401 | NDP  | C5A-C4A-N3A | -2.17 | 123.72      | 126.72   |
| 49  | e     | 201 | PLX  | C1A-N1-C1   | 2.17  | 118.55      | 109.91   |
| 46  | A     | 502 | FMN  | C10-C4A-N5  | -2.16 | 120.39      | 124.81   |
| 56  | Q     | 501 | UQ1  | C8-C7-C6    | 2.13  | 117.32      | 112.08   |
| 52  | I     | 201 | CDL  | OB6-CB5-OB7 | -2.11 | 118.76      | 123.70   |
| 47  | A     | 503 | NAI  | C2D-C3D-C4D | 2.10  | 106.67      | 102.61   |
| 49  | J     | 403 | PLX  | C2-C1-N1    | -2.05 | 109.23      | 115.82   |
| 51  | X     | 201 | 8Q1  | O4-C1-C6    | -2.04 | 121.63      | 123.98   |
| 53  | J     | 401 | NDP  | C5D-C4D-C3D | -2.03 | 107.92      | 115.21   |
| 51  | G     | 201 | 8Q1  | C38-C39-N41 | 2.02  | 120.03      | 116.34   |
| 52  | l     | 702 | CDL  | OA8-CA7-OA9 | -2.02 | 118.57      | 123.63   |



There are no chirality outliers.

All (981) 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  | C1'-C2'-C3'-O3' |
| 46  | A     | 502 | FMN  | C1'-C2'-C3'-C4' |
| 46  | A     | 502 | FMN  | C3'-C4'-C5'-O5' |
| 46  | A     | 502 | FMN  | O4'-C4'-C5'-O5' |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O1P   |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O2P   |
| 47  | A     | 503 | NAI  | PN-O3-PA-O5B    |
| 48  | C     | 302 | PEE  | C4-O4P-P-O1P    |
| 48  | C     | 302 | PEE  | O4P-C4-C5-N     |
| 48  | Q     | 503 | PEE  | C11-C10-O2-C2   |
| 48  | Q     | 503 | PEE  | O4-C10-O2-C2    |
| 48  | Q     | 503 | PEE  | C4-O4P-P-O3P    |
| 48  | Q     | 503 | PEE  | C4-O4P-P-O1P    |
| 48  | V     | 202 | PEE  | C5-C4-O4P-P     |
| 48  | V     | 204 | PEE  | O4P-C4-C5-N     |
| 48  | W     | 201 | PEE  | C4-O4P-P-O3P    |
| 48  | W     | 201 | PEE  | C4-O4P-P-O2P    |
| 48  | W     | 201 | PEE  | C4-O4P-P-O1P    |
| 48  | j     | 201 | PEE  | O4P-C4-C5-N     |
| 48  | j     | 202 | PEE  | C11-C10-O2-C2   |
| 48  | j     | 202 | PEE  | O4P-C4-C5-N     |
| 48  | l     | 703 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 703 | PEE  | C4-O4P-P-O3P    |
| 48  | l     | 703 | PEE  | C4-O4P-P-O1P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O2P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O1P    |
| 48  | l     | 704 | PEE  | C1-O3P-P-O4P    |
| 48  | l     | 704 | PEE  | O4P-C4-C5-N     |
| 49  | C     | 303 | PLX  | O6-C6-C7-C8     |
| 49  | J     | 403 | PLX  | O7-C6-O6-C4     |
| 49  | J     | 403 | PLX  | C3-C4-O6-C6     |
| 49  | J     | 403 | PLX  | C2-O1-P1-O4     |
| 49  | J     | 403 | PLX  | C2-O1-P1-O2     |
| 49  | J     | 403 | PLX  | N1-C1-C2-O1     |
| 49  | J     | 403 | PLX  | O8-C24-C25-C26  |
| 49  | a     | 202 | PLX  | O7-C6-O6-C4     |
| 49  | a     | 202 | PLX  | C2-O1-P1-O4     |
| 49  | a     | 202 | PLX  | C2-O1-P1-O2     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | a     | 202 | PLX  | N1-C1-C2-O1     |
| 49  | a     | 202 | PLX  | O9-C24-O8-C5    |
| 49  | a     | 202 | PLX  | O9-C24-C25-C26  |
| 49  | e     | 201 | PLX  | C3-O4-P1-O2     |
| 49  | e     | 201 | PLX  | O9-C24-O8-C5    |
| 49  | g     | 201 | PLX  | C3-O4-P1-O1     |
| 49  | g     | 201 | PLX  | C3-O4-P1-O2     |
| 49  | g     | 201 | PLX  | C2-O1-P1-O4     |
| 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  | r     | 501 | PLX  | C5-C4-O6-C6     |
| 49  | r     | 501 | PLX  | O9-C24-C25-C26  |
| 50  | C     | 304 | UQ   | C7-C8-C9-C10    |
| 50  | C     | 304 | UQ   | C7-C8-C9-C11    |
| 50  | C     | 304 | UQ   | C12-C13-C14-C16 |
| 50  | C     | 304 | UQ   | C22-C23-C24-C25 |
| 50  | J     | 402 | UQ   | C1-C6-C7-C8     |
| 50  | J     | 402 | UQ   | C7-C8-C9-C10    |
| 50  | J     | 402 | UQ   | C12-C13-C14-C15 |
| 50  | J     | 402 | UQ   | C12-C13-C14-C16 |
| 50  | J     | 402 | UQ   | C17-C18-C19-C21 |
| 51  | G     | 201 | 8Q1  | C28-C29-C32-C34 |
| 51  | G     | 201 | 8Q1  | C28-C29-C32-O33 |
| 51  | G     | 201 | 8Q1  | C30-C29-C32-C34 |
| 51  | G     | 201 | 8Q1  | C30-C29-C32-O33 |
| 51  | G     | 201 | 8Q1  | C31-C29-C32-C34 |
| 51  | G     | 201 | 8Q1  | C31-C29-C32-O33 |
| 51  | X     | 201 | 8Q1  | C1-C6-C7-C8     |
| 51  | X     | 201 | 8Q1  | C28-O27-P24-O3  |
| 51  | X     | 201 | 8Q1  | C28-O27-P24-O2  |
| 51  | X     | 201 | 8Q1  | C28-O27-P24-O1  |
| 52  | I     | 201 | CDL  | O1-C1-CA2-OA2   |
| 52  | I     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 52  | I     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | I     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 52  | I     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 52  | I     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | I     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 52  | I     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | I     | 201 | CDL  | CB2-OB2-PB2-OB5 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | I     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | I     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 52  | J     | 404 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | J     | 404 | CDL  | OA5-CA3-CA4-OA6 |
| 52  | J     | 404 | CDL  | OA9-CA7-OA8-CA6 |
| 52  | J     | 404 | CDL  | C31-CA7-OA8-CA6 |
| 52  | V     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 52  | V     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | V     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | V     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | V     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 52  | V     | 203 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | V     | 203 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | V     | 203 | CDL  | CA3-OA5-PA1-OA4 |
| 52  | V     | 203 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | V     | 203 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | V     | 203 | CDL  | CB3-OB5-PB2-OB4 |
| 52  | V     | 203 | CDL  | OB5-CB3-CB4-OB6 |
| 52  | a     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 52  | a     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | a     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 52  | a     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | a     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | a     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | a     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 52  | a     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 52  | a     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 52  | k     | 101 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | k     | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | k     | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | k     | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 52  | k     | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | k     | 101 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | l     | 701 | CDL  | CA2-C1-CB2-OB2  |
| 52  | l     | 701 | CDL  | CA2-OA2-PA1-OA4 |
| 52  | l     | 701 | CDL  | CA2-OA2-PA1-OA5 |
| 52  | l     | 701 | CDL  | C31-CA7-OA8-CA6 |
| 52  | l     | 701 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | l     | 701 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | l     | 701 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | l     | 701 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | l     | 701 | CDL  | CB3-OB5-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | l     | 701 | CDL  | OB5-CB3-CB4-OB6 |
| 52  | l     | 702 | CDL  | CA2-OA2-PA1-OA4 |
| 52  | l     | 702 | CDL  | CA2-OA2-PA1-OA5 |
| 52  | l     | 702 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | l     | 702 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | l     | 702 | CDL  | CA3-OA5-PA1-OA4 |
| 52  | l     | 702 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | l     | 702 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | l     | 702 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | r     | 502 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | r     | 502 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | r     | 502 | CDL  | CB3-OB5-PB2-OB3 |
| 52  | r     | 502 | CDL  | C51-CB5-OB6-CB4 |
| 52  | u     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | u     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 52  | u     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 52  | u     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 52  | u     | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | u     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 52  | u     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | u     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | u     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | u     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 52  | u     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 53  | J     | 401 | NDP  | C5B-O5B-PA-O1A  |
| 53  | J     | 401 | NDP  | O4D-C4D-C5D-O5D |
| 56  | Q     | 501 | UQ1  | C1-C6-C7-C8     |
| 56  | Q     | 501 | UQ1  | C5-C6-C7-C8     |
| 58  | w     | 401 | ADP  | C5'-O5'-PA-O2A  |
| 48  | Q     | 503 | PEE  | O5-C30-O3-C3    |
| 48  | V     | 204 | PEE  | O5-C30-O3-C3    |
| 52  | l     | 701 | CDL  | OA9-CA7-OA8-CA6 |
| 56  | Q     | 501 | UQ1  | C7-C8-C9-C10    |
| 48  | Q     | 503 | PEE  | C31-C30-O3-C3   |
| 48  | j     | 201 | PEE  | O5-C30-O3-C3    |
| 48  | l     | 703 | PEE  | O4-C10-O2-C2    |
| 52  | r     | 502 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | V     | 204 | PEE  | C31-C30-O3-C3   |
| 48  | j     | 201 | PEE  | C31-C30-O3-C3   |
| 50  | J     | 402 | UQ   | C12-C11-C9-C10  |
| 50  | J     | 402 | UQ   | C20-C19-C21-C22 |
| 50  | J     | 402 | UQ   | C12-C11-C9-C8   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 704 | PEE  | C2-C3-O3-C30    |
| 48  | V     | 204 | PEE  | C17-C18-C19-C20 |
| 50  | C     | 304 | UQ   | C17-C18-C19-C21 |
| 48  | j     | 202 | PEE  | O4-C10-O2-C2    |
| 52  | V     | 201 | CDL  | C11-C12-C13-C14 |
| 52  | I     | 201 | CDL  | O1-C1-CB2-OB2   |
| 52  | V     | 201 | CDL  | O1-C1-CB2-OB2   |
| 52  | a     | 201 | CDL  | O1-C1-CA2-OA2   |
| 52  | a     | 201 | CDL  | O1-C1-CB2-OB2   |
| 52  | l     | 702 | CDL  | O1-C1-CA2-OA2   |
| 52  | r     | 502 | CDL  | O1-C1-CA2-OA2   |
| 52  | l     | 701 | CDL  | C71-CB7-OB8-CB6 |
| 52  | V     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 52  | l     | 702 | CDL  | C11-CA5-OA6-CA4 |
| 52  | l     | 701 | CDL  | OB9-CB7-OB8-CB6 |
| 58  | w     | 401 | ADP  | O4'-C4'-C5'-O5' |
| 52  | V     | 201 | CDL  | C62-C63-C64-C65 |
| 50  | J     | 402 | UQ   | C15-C14-C16-C17 |
| 50  | C     | 304 | UQ   | C18-C19-C21-C22 |
| 48  | j     | 201 | PEE  | C17-C18-C19-C20 |
| 48  | s     | 401 | PEE  | C17-C18-C19-C20 |
| 49  | j     | 203 | PLX  | C13-C14-C15-C16 |
| 52  | V     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 52  | V     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 52  | a     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 52  | r     | 502 | CDL  | CB2-C1-CA2-OA2  |
| 48  | W     | 201 | PEE  | C31-C30-O3-C3   |
| 52  | I     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 52  | V     | 201 | CDL  | C31-CA7-OA8-CA6 |
| 52  | V     | 203 | CDL  | C31-CA7-OA8-CA6 |
| 52  | l     | 702 | CDL  | C71-CB7-OB8-CB6 |
| 49  | r     | 501 | PLX  | C11-C12-C13-C14 |
| 49  | g     | 201 | PLX  | C2-C1-N1-C1A    |
| 49  | r     | 501 | PLX  | C9-C10-C11-C12  |
| 49  | r     | 501 | PLX  | C7-C8-C9-C10    |
| 50  | J     | 402 | UQ   | C18-C19-C21-C22 |
| 56  | Q     | 502 | UQ1  | C7-C8-C9-C11    |
| 48  | l     | 704 | PEE  | C34-C35-C36-C37 |
| 52  | l     | 701 | CDL  | CB7-C71-C72-C73 |
| 52  | k     | 101 | CDL  | O1-C1-CB2-OB2   |
| 52  | u     | 201 | CDL  | O1-C1-CA2-OA2   |
| 48  | W     | 201 | PEE  | O5-C30-O3-C3    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | V     | 203 | CDL  | OA9-CA7-OA8-CA6 |
| 52  | k     | 101 | CDL  | C36-C37-C38-C39 |
| 52  | l     | 702 | CDL  | C33-C34-C35-C36 |
| 52  | l     | 702 | CDL  | C31-C32-C33-C34 |
| 52  | J     | 404 | CDL  | CB7-C71-C72-C73 |
| 50  | J     | 402 | UQ   | C22-C23-C24-C26 |
| 52  | V     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 48  | j     | 201 | PEE  | C40-C41-C42-C43 |
| 48  | V     | 202 | PEE  | C10-C11-C12-C13 |
| 52  | k     | 101 | CDL  | CA7-C31-C32-C33 |
| 52  | r     | 502 | CDL  | CB5-C51-C52-C53 |
| 52  | r     | 502 | CDL  | CB7-C71-C72-C73 |
| 48  | l     | 703 | PEE  | C33-C34-C35-C36 |
| 49  | J     | 403 | PLX  | C25-C26-C27-C28 |
| 50  | C     | 304 | UQ   | C27-C28-C29-C31 |
| 52  | l     | 702 | CDL  | OA7-CA5-OA6-CA4 |
| 50  | C     | 304 | UQ   | C14-C16-C17-C18 |
| 52  | J     | 404 | CDL  | CA7-C31-C32-C33 |
| 52  | l     | 701 | CDL  | CB5-C51-C52-C53 |
| 52  | V     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 52  | l     | 702 | CDL  | OB9-CB7-OB8-CB6 |
| 52  | V     | 201 | CDL  | CB7-C71-C72-C73 |
| 52  | l     | 702 | CDL  | CA5-C11-C12-C13 |
| 52  | l     | 701 | CDL  | C58-C59-C60-C61 |
| 52  | a     | 201 | CDL  | C34-C35-C36-C37 |
| 52  | V     | 201 | CDL  | O1-C1-CA2-OA2   |
| 52  | V     | 203 | CDL  | O1-C1-CB2-OB2   |
| 52  | l     | 702 | CDL  | O1-C1-CB2-OB2   |
| 52  | I     | 201 | CDL  | OA9-CA7-OA8-CA6 |
| 52  | r     | 502 | CDL  | CA7-C31-C32-C33 |
| 52  | I     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 48  | V     | 204 | PEE  | C10-C11-C12-C13 |
| 52  | V     | 203 | CDL  | CA5-C11-C12-C13 |
| 52  | l     | 701 | CDL  | C18-C19-C20-C21 |
| 52  | I     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 52  | V     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 52  | V     | 203 | CDL  | CA2-C1-CB2-OB2  |
| 48  | j     | 202 | PEE  | C31-C30-O3-C3   |
| 52  | k     | 101 | CDL  | C71-CB7-OB8-CB6 |
| 48  | l     | 704 | PEE  | C21-C22-C23-C24 |
| 52  | l     | 702 | CDL  | C35-C36-C37-C38 |
| 48  | W     | 201 | PEE  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | g     | 201 | PLX  | C2-C1-N1-C1B    |
| 49  | J     | 403 | PLX  | C34-C35-C36-C37 |
| 48  | s     | 401 | PEE  | C31-C30-O3-C3   |
| 48  | l     | 704 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 704 | PEE  | O4-C10-O2-C2    |
| 48  | l     | 704 | PEE  | C37-C38-C39-C40 |
| 52  | u     | 201 | CDL  | CB5-C51-C52-C53 |
| 52  | l     | 701 | CDL  | O1-C1-CB2-OB2   |
| 48  | j     | 202 | PEE  | O5-C30-O3-C3    |
| 48  | s     | 401 | PEE  | C11-C12-C13-C14 |
| 52  | J     | 404 | CDL  | C33-C34-C35-C36 |
| 52  | l     | 701 | CDL  | C81-C82-C83-C84 |
| 48  | C     | 302 | PEE  | C31-C30-O3-C3   |
| 49  | g     | 201 | PLX  | C2-C1-N1-C1C    |
| 49  | C     | 303 | PLX  | C25-C26-C27-C28 |
| 49  | a     | 202 | PLX  | C9-C10-C11-C12  |
| 49  | j     | 203 | PLX  | C12-C13-C14-C15 |
| 49  | r     | 501 | PLX  | C11-C10-C9-C8   |
| 52  | l     | 701 | CDL  | C75-C76-C77-C78 |
| 48  | C     | 302 | PEE  | C11-C12-C13-C14 |
| 48  | W     | 201 | PEE  | C12-C13-C14-C15 |
| 49  | J     | 403 | PLX  | C31-C32-C33-C34 |
| 49  | a     | 202 | PLX  | C31-C32-C33-C34 |
| 52  | J     | 404 | CDL  | C52-C53-C54-C55 |
| 52  | V     | 201 | CDL  | C73-C74-C75-C76 |
| 52  | k     | 101 | CDL  | C81-C82-C83-C84 |
| 52  | l     | 702 | CDL  | C41-C42-C43-C44 |
| 48  | s     | 401 | PEE  | C37-C38-C39-C40 |
| 48  | l     | 703 | PEE  | C21-C22-C23-C24 |
| 49  | e     | 201 | PLX  | C29-C30-C31-C32 |
| 52  | J     | 404 | CDL  | C51-C52-C53-C54 |
| 52  | V     | 203 | CDL  | C12-C13-C14-C15 |
| 52  | k     | 101 | CDL  | C75-C76-C77-C78 |
| 49  | C     | 303 | PLX  | O7-C6-C7-C8     |
| 49  | J     | 403 | PLX  | O9-C24-C25-C26  |
| 49  | e     | 201 | PLX  | O9-C24-C25-C26  |
| 49  | r     | 501 | PLX  | O7-C6-C7-C8     |
| 49  | C     | 303 | PLX  | C11-C12-C13-C14 |
| 49  | e     | 201 | PLX  | C13-C14-C15-C16 |
| 49  | g     | 201 | PLX  | C27-C28-C29-C30 |
| 51  | G     | 201 | 8Q1  | C11-C12-C13-C14 |
| 52  | V     | 203 | CDL  | C75-C76-C77-C78 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | k     | 101 | CDL  | C20-C21-C22-C23 |
| 52  | l     | 701 | CDL  | C31-C32-C33-C34 |
| 52  | l     | 701 | CDL  | C71-C72-C73-C74 |
| 52  | r     | 502 | CDL  | C14-C15-C16-C17 |
| 48  | j     | 202 | PEE  | C12-C13-C14-C15 |
| 49  | j     | 203 | PLX  | C33-C34-C35-C36 |
| 52  | J     | 404 | CDL  | C71-C72-C73-C74 |
| 49  | C     | 303 | PLX  | C14-C15-C16-C17 |
| 49  | C     | 303 | PLX  | C28-C29-C30-C31 |
| 51  | X     | 201 | 8Q1  | C12-C13-C14-C15 |
| 52  | k     | 101 | CDL  | OB9-CB7-OB8-CB6 |
| 49  | g     | 201 | PLX  | C11-C10-C9-C8   |
| 49  | j     | 203 | PLX  | C14-C15-C16-C17 |
| 52  | V     | 203 | CDL  | C34-C35-C36-C37 |
| 52  | l     | 701 | CDL  | C14-C15-C16-C17 |
| 52  | l     | 701 | CDL  | C74-C75-C76-C77 |
| 52  | r     | 502 | CDL  | C43-C44-C45-C46 |
| 52  | I     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 52  | J     | 404 | CDL  | C51-CB5-OB6-CB4 |
| 52  | a     | 201 | CDL  | C11-C12-C13-C14 |
| 48  | s     | 401 | PEE  | C34-C35-C36-C37 |
| 52  | V     | 201 | CDL  | C37-C38-C39-C40 |
| 52  | l     | 701 | CDL  | C62-C63-C64-C65 |
| 52  | J     | 404 | CDL  | CB5-C51-C52-C53 |
| 53  | J     | 401 | NDP  | C3D-C4D-C5D-O5D |
| 58  | w     | 401 | ADP  | C3'-C4'-C5'-O5' |
| 48  | C     | 302 | PEE  | C34-C35-C36-C37 |
| 49  | j     | 203 | PLX  | C30-C31-C32-C33 |
| 52  | k     | 101 | CDL  | C15-C16-C17-C18 |
| 52  | k     | 101 | CDL  | C32-C33-C34-C35 |
| 52  | l     | 701 | CDL  | C51-C52-C53-C54 |
| 49  | e     | 201 | PLX  | C25-C26-C27-C28 |
| 52  | V     | 201 | CDL  | C55-C56-C57-C58 |
| 52  | a     | 201 | CDL  | C21-C22-C23-C24 |
| 49  | a     | 202 | PLX  | C7-C8-C9-C10    |
| 52  | J     | 404 | CDL  | C32-C33-C34-C35 |
| 52  | l     | 701 | CDL  | C11-C12-C13-C14 |
| 52  | l     | 701 | CDL  | C36-C37-C38-C39 |
| 48  | j     | 202 | PEE  | C23-C24-C25-C26 |
| 49  | r     | 501 | PLX  | C33-C34-C35-C36 |
| 52  | l     | 701 | CDL  | C56-C57-C58-C59 |
| 48  | V     | 204 | PEE  | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | V     | 203 | CDL  | C76-C77-C78-C79 |
| 52  | a     | 201 | CDL  | C62-C63-C64-C65 |
| 48  | V     | 202 | PEE  | C11-C12-C13-C14 |
| 48  | V     | 202 | PEE  | C40-C41-C42-C43 |
| 49  | C     | 303 | PLX  | C10-C11-C12-C13 |
| 52  | l     | 702 | CDL  | C11-C12-C13-C14 |
| 52  | u     | 201 | CDL  | C73-C74-C75-C76 |
| 52  | a     | 201 | CDL  | CA5-C11-C12-C13 |
| 49  | a     | 202 | PLX  | C12-C13-C14-C15 |
| 49  | e     | 201 | PLX  | C14-C15-C16-C17 |
| 49  | g     | 201 | PLX  | C10-C11-C12-C13 |
| 49  | j     | 203 | PLX  | C7-C8-C9-C10    |
| 51  | X     | 201 | 8Q1  | C10-C11-C12-C13 |
| 52  | V     | 201 | CDL  | C56-C57-C58-C59 |
| 52  | V     | 203 | CDL  | C17-C18-C19-C20 |
| 52  | V     | 203 | CDL  | C40-C41-C42-C43 |
| 52  | k     | 101 | CDL  | C21-C22-C23-C24 |
| 52  | r     | 502 | CDL  | C34-C35-C36-C37 |
| 48  | V     | 202 | PEE  | C31-C32-C33-C34 |
| 52  | a     | 201 | CDL  | C51-C52-C53-C54 |
| 52  | k     | 101 | CDL  | C71-C72-C73-C74 |
| 52  | k     | 101 | CDL  | C78-C79-C80-C81 |
| 52  | r     | 502 | CDL  | C75-C76-C77-C78 |
| 48  | j     | 201 | PEE  | C34-C35-C36-C37 |
| 49  | g     | 201 | PLX  | C28-C29-C30-C31 |
| 48  | V     | 202 | PEE  | C33-C34-C35-C36 |
| 49  | C     | 303 | PLX  | C33-C34-C35-C36 |
| 49  | a     | 202 | PLX  | C13-C14-C15-C16 |
| 52  | J     | 404 | CDL  | C35-C36-C37-C38 |
| 52  | J     | 404 | CDL  | C75-C76-C77-C78 |
| 52  | a     | 201 | CDL  | C54-C55-C56-C57 |
| 52  | k     | 101 | CDL  | C16-C17-C18-C19 |
| 52  | r     | 502 | CDL  | C57-C58-C59-C60 |
| 48  | s     | 401 | PEE  | O5-C30-O3-C3    |
| 49  | a     | 202 | PLX  | C14-C15-C16-C17 |
| 52  | r     | 502 | CDL  | C41-C42-C43-C44 |
| 46  | A     | 502 | FMN  | O2'-C2'-C3'-C4' |
| 48  | W     | 201 | PEE  | C24-C25-C26-C27 |
| 48  | V     | 202 | PEE  | C17-C18-C19-C20 |
| 48  | l     | 704 | PEE  | C20-C21-C22-C23 |
| 49  | r     | 501 | PLX  | C18-C19-C20-C21 |
| 49  | r     | 501 | PLX  | C28-C29-C30-C31 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | a     | 201 | CDL  | C22-C23-C24-C25 |
| 52  | V     | 203 | CDL  | C42-C43-C44-C45 |
| 52  | l     | 701 | CDL  | C35-C36-C37-C38 |
| 52  | l     | 702 | CDL  | CB5-C51-C52-C53 |
| 48  | l     | 703 | PEE  | C44-C45-C46-C47 |
| 49  | J     | 403 | PLX  | C14-C15-C16-C17 |
| 49  | g     | 201 | PLX  | C30-C31-C32-C33 |
| 49  | r     | 501 | PLX  | C27-C28-C29-C30 |
| 48  | C     | 302 | PEE  | O5-C30-O3-C3    |
| 52  | J     | 404 | CDL  | OB7-CB5-OB6-CB4 |
| 52  | V     | 201 | CDL  | C75-C76-C77-C78 |
| 52  | V     | 203 | CDL  | C32-C33-C34-C35 |
| 48  | V     | 202 | PEE  | C20-C21-C22-C23 |
| 49  | J     | 403 | PLX  | C10-C11-C12-C13 |
| 49  | J     | 403 | PLX  | C7-C8-C9-C10    |
| 52  | J     | 404 | CDL  | C14-C15-C16-C17 |
| 52  | a     | 201 | CDL  | C60-C61-C62-C63 |
| 52  | k     | 101 | CDL  | C37-C38-C39-C40 |
| 48  | V     | 202 | PEE  | C21-C22-C23-C24 |
| 49  | J     | 403 | PLX  | C27-C28-C29-C30 |
| 52  | l     | 701 | CDL  | C37-C38-C39-C40 |
| 52  | V     | 203 | CDL  | C59-C60-C61-C62 |
| 52  | k     | 101 | CDL  | C53-C54-C55-C56 |
| 49  | g     | 201 | PLX  | C14-C15-C16-C17 |
| 52  | J     | 404 | CDL  | C73-C74-C75-C76 |
| 52  | k     | 101 | CDL  | C33-C34-C35-C36 |
| 49  | J     | 403 | PLX  | C33-C34-C35-C36 |
| 49  | g     | 201 | PLX  | C25-C26-C27-C28 |
| 52  | a     | 201 | CDL  | C71-C72-C73-C74 |
| 49  | g     | 201 | PLX  | C32-C33-C34-C35 |
| 49  | j     | 203 | PLX  | C10-C11-C12-C13 |
| 52  | V     | 201 | CDL  | C31-C32-C33-C34 |
| 52  | r     | 502 | CDL  | C60-C61-C62-C63 |
| 48  | C     | 302 | PEE  | C11-C10-O2-C2   |
| 48  | s     | 401 | PEE  | C11-C10-O2-C2   |
| 52  | J     | 404 | CDL  | C11-CA5-OA6-CA4 |
| 52  | l     | 701 | CDL  | C11-CA5-OA6-CA4 |
| 52  | l     | 702 | CDL  | C51-CB5-OB6-CB4 |
| 52  | u     | 201 | CDL  | CB7-C71-C72-C73 |
| 48  | C     | 302 | PEE  | O4-C10-O2-C2    |
| 48  | s     | 401 | PEE  | O4-C10-O2-C2    |
| 52  | I     | 201 | CDL  | OB7-CB5-OB6-CB4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | J     | 404 | CDL  | C82-C83-C84-C85 |
| 52  | V     | 201 | CDL  | C40-C41-C42-C43 |
| 48  | W     | 201 | PEE  | C19-C20-C21-C22 |
| 48  | l     | 704 | PEE  | C15-C16-C17-C18 |
| 52  | k     | 101 | CDL  | C34-C35-C36-C37 |
| 50  | J     | 402 | UQ   | C5-C6-C7-C8     |
| 50  | C     | 304 | UQ   | C27-C28-C29-C30 |
| 48  | V     | 202 | PEE  | C13-C14-C15-C16 |
| 48  | l     | 704 | PEE  | C30-C31-C32-C33 |
| 52  | V     | 201 | CDL  | CB5-C51-C52-C53 |
| 48  | j     | 201 | PEE  | C41-C42-C43-C44 |
| 49  | e     | 201 | PLX  | C11-C10-C9-C8   |
| 52  | J     | 404 | CDL  | C59-C60-C61-C62 |
| 52  | l     | 702 | CDL  | C72-C73-C74-C75 |
| 48  | l     | 703 | PEE  | C15-C16-C17-C18 |
| 52  | J     | 404 | CDL  | OB6-CB4-CB6-OB8 |
| 52  | V     | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | l     | 704 | PEE  | C13-C14-C15-C16 |
| 49  | e     | 201 | PLX  | C10-C11-C12-C13 |
| 48  | V     | 202 | PEE  | C36-C37-C38-C39 |
| 48  | V     | 202 | PEE  | C38-C39-C40-C41 |
| 48  | j     | 201 | PEE  | C38-C39-C40-C41 |
| 52  | l     | 701 | CDL  | C52-C53-C54-C55 |
| 52  | r     | 502 | CDL  | C32-C33-C34-C35 |
| 52  | V     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 49  | a     | 202 | PLX  | C27-C28-C29-C30 |
| 49  | e     | 201 | PLX  | C28-C29-C30-C31 |
| 51  | X     | 201 | 8Q1  | C11-C12-C13-C14 |
| 49  | e     | 201 | PLX  | C33-C34-C35-C36 |
| 52  | V     | 203 | CDL  | C37-C38-C39-C40 |
| 52  | k     | 101 | CDL  | C40-C41-C42-C43 |
| 52  | l     | 701 | CDL  | C82-C83-C84-C85 |
| 49  | e     | 201 | PLX  | C12-C13-C14-C15 |
| 52  | J     | 404 | CDL  | C37-C38-C39-C40 |
| 52  | l     | 701 | CDL  | C40-C41-C42-C43 |
| 52  | V     | 203 | CDL  | C14-C15-C16-C17 |
| 48  | j     | 201 | PEE  | C22-C23-C24-C25 |
| 49  | g     | 201 | PLX  | C33-C34-C35-C36 |
| 49  | J     | 403 | PLX  | C18-C19-C20-C21 |
| 49  | J     | 403 | PLX  | C26-C27-C28-C29 |
| 49  | a     | 202 | PLX  | C25-C26-C27-C28 |
| 52  | r     | 502 | CDL  | C62-C63-C64-C65 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | r     | 502 | CDL  | C54-C55-C56-C57 |
| 52  | V     | 201 | CDL  | C14-C15-C16-C17 |
| 52  | l     | 701 | CDL  | C16-C17-C18-C19 |
| 52  | k     | 101 | CDL  | C58-C59-C60-C61 |
| 49  | C     | 303 | PLX  | C11-C10-C9-C8   |
| 52  | V     | 201 | CDL  | C51-C52-C53-C54 |
| 52  | l     | 701 | CDL  | OB5-CB3-CB4-CB6 |
| 52  | J     | 404 | CDL  | OA7-CA5-OA6-CA4 |
| 48  | j     | 202 | PEE  | C11-C12-C13-C14 |
| 49  | a     | 202 | PLX  | C11-C12-C13-C14 |
| 49  | j     | 203 | PLX  | C11-C12-C13-C14 |
| 52  | a     | 201 | CDL  | C35-C36-C37-C38 |
| 48  | j     | 202 | PEE  | C13-C14-C15-C16 |
| 49  | r     | 501 | PLX  | C30-C31-C32-C33 |
| 52  | V     | 201 | CDL  | C71-C72-C73-C74 |
| 52  | V     | 201 | CDL  | C32-C33-C34-C35 |
| 52  | r     | 502 | CDL  | C76-C77-C78-C79 |
| 52  | r     | 502 | CDL  | C84-C85-C86-C87 |
| 48  | l     | 703 | PEE  | C2-C3-O3-C30    |
| 52  | l     | 701 | CDL  | CA7-C31-C32-C33 |
| 52  | V     | 203 | CDL  | C74-C75-C76-C77 |
| 52  | l     | 701 | CDL  | C34-C35-C36-C37 |
| 49  | a     | 202 | PLX  | O6-C6-C7-C8     |
| 49  | r     | 501 | PLX  | O6-C6-C7-C8     |
| 48  | Q     | 503 | PEE  | C34-C35-C36-C37 |
| 48  | j     | 201 | PEE  | C21-C22-C23-C24 |
| 49  | g     | 201 | PLX  | C9-C10-C11-C12  |
| 49  | r     | 501 | PLX  | C13-C14-C15-C16 |
| 52  | l     | 701 | CDL  | C59-C60-C61-C62 |
| 52  | r     | 502 | CDL  | C71-C72-C73-C74 |
| 52  | a     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 52  | V     | 203 | CDL  | C60-C61-C62-C63 |
| 52  | l     | 702 | CDL  | OB7-CB5-OB6-CB4 |
| 52  | u     | 201 | CDL  | C52-C53-C54-C55 |
| 48  | C     | 302 | PEE  | C10-C11-C12-C13 |
| 52  | J     | 404 | CDL  | CB3-CB4-CB6-OB8 |
| 52  | k     | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 52  | l     | 702 | CDL  | CA3-CA4-CA6-OA8 |
| 52  | V     | 203 | CDL  | C54-C55-C56-C57 |
| 48  | C     | 302 | PEE  | C19-C20-C21-C22 |
| 48  | C     | 302 | PEE  | C35-C36-C37-C38 |
| 48  | W     | 201 | PEE  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | j     | 201 | PEE  | C19-C20-C21-C22 |
| 48  | s     | 401 | PEE  | C13-C14-C15-C16 |
| 51  | G     | 201 | 8Q1  | C9-C10-C11-C12  |
| 52  | a     | 201 | CDL  | C33-C34-C35-C36 |
| 52  | k     | 101 | CDL  | C52-C53-C54-C55 |
| 49  | J     | 403 | PLX  | C13-C14-C15-C16 |
| 52  | r     | 502 | CDL  | C83-C84-C85-C86 |
| 52  | J     | 404 | CDL  | C17-C18-C19-C20 |
| 48  | j     | 201 | PEE  | C14-C15-C16-C17 |
| 49  | r     | 501 | PLX  | C14-C15-C16-C17 |
| 49  | e     | 201 | PLX  | C27-C28-C29-C30 |
| 49  | r     | 501 | PLX  | C31-C32-C33-C34 |
| 49  | a     | 202 | PLX  | C15-C16-C17-C18 |
| 48  | V     | 202 | PEE  | C14-C15-C16-C17 |
| 51  | X     | 201 | 8Q1  | C7-C8-C9-C10    |
| 52  | I     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 52  | V     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 52  | V     | 201 | CDL  | C52-C53-C54-C55 |
| 52  | k     | 101 | CDL  | C42-C43-C44-C45 |
| 48  | C     | 302 | PEE  | C15-C16-C17-C18 |
| 48  | s     | 401 | PEE  | C35-C36-C37-C38 |
| 52  | l     | 702 | CDL  | C51-C52-C53-C54 |
| 48  | j     | 201 | PEE  | C36-C37-C38-C39 |
| 52  | a     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 52  | k     | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 47  | A     | 503 | NAI  | C3D-C4D-C5D-O5D |
| 48  | s     | 401 | PEE  | C23-C24-C25-C26 |
| 52  | r     | 502 | CDL  | C37-C38-C39-C40 |
| 48  | l     | 703 | PEE  | C11-C12-C13-C14 |
| 49  | C     | 303 | PLX  | C13-C14-C15-C16 |
| 52  | r     | 502 | CDL  | C12-C13-C14-C15 |
| 52  | r     | 502 | CDL  | C64-C65-C66-C67 |
| 52  | V     | 201 | CDL  | C44-C45-C46-C47 |
| 49  | j     | 203 | PLX  | C31-C32-C33-C34 |
| 49  | C     | 303 | PLX  | C7-C8-C9-C10    |
| 49  | C     | 303 | PLX  | C31-C32-C33-C34 |
| 49  | e     | 201 | PLX  | C11-C12-C13-C14 |
| 49  | g     | 201 | PLX  | C13-C14-C15-C16 |
| 52  | J     | 404 | CDL  | C11-C12-C13-C14 |
| 52  | a     | 201 | CDL  | C52-C53-C54-C55 |
| 48  | l     | 703 | PEE  | O2-C2-C3-O3     |
| 49  | C     | 303 | PLX  | O6-C4-C5-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | a     | 202 | PLX  | O6-C4-C5-O8     |
| 52  | k     | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 51  | X     | 201 | 8Q1  | C13-C14-C15-C16 |
| 48  | W     | 201 | PEE  | C20-C21-C22-C23 |
| 52  | V     | 203 | CDL  | C16-C17-C18-C19 |
| 52  | k     | 101 | CDL  | C43-C44-C45-C46 |
| 52  | V     | 201 | CDL  | C59-C60-C61-C62 |
| 48  | s     | 401 | PEE  | C38-C39-C40-C41 |
| 49  | J     | 403 | PLX  | C30-C31-C32-C33 |
| 48  | Q     | 503 | PEE  | C35-C36-C37-C38 |
| 52  | a     | 201 | CDL  | C23-C24-C25-C26 |
| 52  | l     | 701 | CDL  | C78-C79-C80-C81 |
| 52  | a     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 52  | V     | 201 | CDL  | C19-C20-C21-C22 |
| 52  | V     | 203 | CDL  | C84-C85-C86-C87 |
| 48  | C     | 302 | PEE  | C13-C14-C15-C16 |
| 48  | C     | 302 | PEE  | C42-C43-C44-C45 |
| 52  | a     | 201 | CDL  | C37-C38-C39-C40 |
| 52  | a     | 201 | CDL  | C82-C83-C84-C85 |
| 52  | l     | 701 | CDL  | OA7-CA5-OA6-CA4 |
| 49  | J     | 403 | PLX  | C35-C36-C37-C38 |
| 52  | l     | 701 | CDL  | C73-C74-C75-C76 |
| 49  | J     | 403 | PLX  | C12-C13-C14-C15 |
| 52  | J     | 404 | CDL  | C55-C56-C57-C58 |
| 52  | r     | 502 | CDL  | C11-C12-C13-C14 |
| 52  | r     | 502 | CDL  | C52-C53-C54-C55 |
| 52  | k     | 101 | CDL  | C12-C13-C14-C15 |
| 52  | l     | 702 | CDL  | C14-C15-C16-C17 |
| 52  | V     | 201 | CDL  | C74-C75-C76-C77 |
| 52  | u     | 201 | CDL  | C72-C73-C74-C75 |
| 48  | j     | 201 | PEE  | C44-C45-C46-C47 |
| 52  | l     | 701 | CDL  | C63-C64-C65-C66 |
| 48  | V     | 202 | PEE  | C24-C25-C26-C27 |
| 52  | J     | 404 | CDL  | C54-C55-C56-C57 |
| 52  | a     | 201 | CDL  | C17-C18-C19-C20 |
| 52  | V     | 203 | CDL  | C31-C32-C33-C34 |
| 49  | e     | 201 | PLX  | C7-C8-C9-C10    |
| 52  | a     | 201 | CDL  | C44-C45-C46-C47 |
| 52  | k     | 101 | CDL  | C11-C12-C13-C14 |
| 52  | l     | 702 | CDL  | C39-C40-C41-C42 |
| 52  | k     | 101 | CDL  | CA5-C11-C12-C13 |
| 52  | V     | 203 | CDL  | C39-C40-C41-C42 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | C     | 302 | PEE  | C1-C2-C3-O3     |
| 48  | l     | 704 | PEE  | C1-C2-C3-O3     |
| 49  | J     | 403 | PLX  | C3-C4-C5-O8     |
| 49  | a     | 202 | PLX  | C3-C4-C5-O8     |
| 49  | e     | 201 | PLX  | C3-C4-C5-O8     |
| 49  | j     | 203 | PLX  | C3-C4-C5-O8     |
| 49  | r     | 501 | PLX  | C3-C4-C5-O8     |
| 52  | V     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 52  | V     | 203 | CDL  | CB3-CB4-CB6-OB8 |
| 52  | r     | 502 | CDL  | C33-C34-C35-C36 |
| 49  | a     | 202 | PLX  | C34-C35-C36-C37 |
| 49  | g     | 201 | PLX  | C12-C13-C14-C15 |
| 49  | r     | 501 | PLX  | C16-C17-C18-C19 |
| 49  | r     | 501 | PLX  | C12-C13-C14-C15 |
| 49  | g     | 201 | PLX  | C20-C21-C22-C23 |
| 49  | g     | 201 | PLX  | C17-C18-C19-C20 |
| 50  | J     | 402 | UQ   | C3-C2-O2-CM2    |
| 52  | a     | 201 | CDL  | C42-C43-C44-C45 |
| 52  | a     | 201 | CDL  | C53-C54-C55-C56 |
| 52  | V     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 52  | a     | 201 | CDL  | C32-C33-C34-C35 |
| 52  | V     | 203 | CDL  | C1-CB2-OB2-PB2  |
| 48  | l     | 704 | PEE  | C11-C12-C13-C14 |
| 52  | l     | 701 | CDL  | C21-C22-C23-C24 |
| 52  | u     | 201 | CDL  | C74-C75-C76-C77 |
| 48  | C     | 302 | PEE  | O2-C2-C3-O3     |
| 48  | V     | 204 | PEE  | O2-C2-C3-O3     |
| 48  | W     | 201 | PEE  | O2-C2-C3-O3     |
| 52  | V     | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | l     | 701 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | l     | 701 | CDL  | OB6-CB4-CB6-OB8 |
| 52  | l     | 702 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | r     | 502 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | k     | 101 | CDL  | C84-C85-C86-C87 |
| 52  | r     | 502 | CDL  | C63-C64-C65-C66 |
| 49  | e     | 201 | PLX  | O8-C24-C25-C26  |
| 49  | r     | 501 | PLX  | O8-C24-C25-C26  |
| 51  | X     | 201 | 8Q1  | C11-C10-C9-C8   |
| 48  | Q     | 503 | PEE  | C30-C31-C32-C33 |
| 48  | V     | 204 | PEE  | C36-C37-C38-C39 |
| 49  | r     | 501 | PLX  | C25-C26-C27-C28 |
| 48  | V     | 204 | PEE  | C11-C10-O2-C2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | C     | 302 | PEE  | C12-C13-C14-C15 |
| 48  | C     | 302 | PEE  | C41-C42-C43-C44 |
| 52  | V     | 203 | CDL  | CB2-C1-CA2-OA2  |
| 52  | l     | 702 | CDL  | CB2-C1-CA2-OA2  |
| 52  | V     | 201 | CDL  | C72-C73-C74-C75 |
| 48  | j     | 202 | PEE  | C24-C25-C26-C27 |
| 52  | r     | 502 | CDL  | C17-C18-C19-C20 |
| 49  | J     | 403 | PLX  | O4-C3-C4-C5     |
| 52  | V     | 203 | CDL  | OB5-CB3-CB4-CB6 |
| 52  | a     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 48  | l     | 703 | PEE  | C24-C25-C26-C27 |
| 52  | r     | 502 | CDL  | C59-C60-C61-C62 |
| 48  | Q     | 503 | PEE  | C24-C25-C26-C27 |
| 51  | G     | 201 | 8Q1  | C11-C10-C9-C8   |
| 52  | V     | 201 | CDL  | C54-C55-C56-C57 |
| 52  | V     | 203 | CDL  | C64-C65-C66-C67 |
| 52  | J     | 404 | CDL  | C12-C13-C14-C15 |
| 52  | J     | 404 | CDL  | C36-C37-C38-C39 |
| 49  | e     | 201 | PLX  | C24-C25-C26-C27 |
| 48  | j     | 201 | PEE  | C13-C14-C15-C16 |
| 52  | r     | 502 | CDL  | C21-C22-C23-C24 |
| 46  | A     | 502 | FMN  | O2'-C2'-C3'-O3' |
| 52  | r     | 502 | CDL  | C74-C75-C76-C77 |
| 52  | r     | 502 | CDL  | C44-C45-C46-C47 |
| 52  | k     | 101 | CDL  | C73-C74-C75-C76 |
| 52  | l     | 702 | CDL  | C61-C62-C63-C64 |
| 52  | V     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 52  | u     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 52  | V     | 201 | CDL  | C33-C34-C35-C36 |
| 48  | W     | 201 | PEE  | C1-C2-C3-O3     |
| 48  | l     | 703 | PEE  | C1-C2-C3-O3     |
| 52  | r     | 502 | CDL  | CA3-CA4-CA6-OA8 |
| 48  | j     | 202 | PEE  | C34-C35-C36-C37 |
| 49  | J     | 403 | PLX  | C11-C10-C9-C8   |
| 49  | C     | 303 | PLX  | C27-C28-C29-C30 |
| 52  | l     | 701 | CDL  | C55-C56-C57-C58 |
| 48  | l     | 704 | PEE  | C5-C4-O4P-P     |
| 49  | J     | 403 | PLX  | C1-C2-O1-P1     |
| 52  | V     | 201 | CDL  | C34-C35-C36-C37 |
| 49  | J     | 403 | PLX  | O6-C4-C5-O8     |
| 49  | j     | 203 | PLX  | O6-C4-C5-O8     |
| 49  | r     | 501 | PLX  | O6-C4-C5-O8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 703 | PEE  | C13-C14-C15-C16 |
| 52  | a     | 201 | CDL  | C81-C82-C83-C84 |
| 52  | V     | 203 | CDL  | C24-C25-C26-C27 |
| 52  | k     | 101 | CDL  | C39-C40-C41-C42 |
| 52  | r     | 502 | CDL  | C35-C36-C37-C38 |
| 53  | J     | 401 | NDP  | O4D-C1D-N1N-C6N |
| 52  | V     | 201 | CDL  | C53-C54-C55-C56 |
| 48  | j     | 201 | PEE  | C32-C33-C34-C35 |
| 49  | C     | 303 | PLX  | N1-C1-C2-O1     |
| 52  | J     | 404 | CDL  | C34-C35-C36-C37 |
| 52  | l     | 701 | CDL  | C54-C55-C56-C57 |
| 52  | r     | 502 | CDL  | C77-C78-C79-C80 |
| 52  | l     | 702 | CDL  | CA2-C1-CB2-OB2  |
| 52  | V     | 203 | CDL  | O1-C1-CA2-OA2   |
| 49  | e     | 201 | PLX  | C9-C10-C11-C12  |
| 52  | l     | 702 | CDL  | C40-C41-C42-C43 |
| 52  | k     | 101 | CDL  | C54-C55-C56-C57 |
| 49  | C     | 303 | PLX  | C25-C24-O8-C5   |
| 49  | e     | 201 | PLX  | C18-C19-C20-C21 |
| 49  | j     | 203 | PLX  | C36-C37-C38-C39 |
| 49  | j     | 203 | PLX  | C9-C10-C11-C12  |
| 52  | a     | 201 | CDL  | C64-C65-C66-C67 |
| 52  | J     | 404 | CDL  | OA5-CA3-CA4-CA6 |
| 52  | V     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 52  | V     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 49  | a     | 202 | PLX  | C29-C30-C31-C32 |
| 52  | V     | 201 | CDL  | C22-C23-C24-C25 |
| 48  | V     | 204 | PEE  | O4-C10-O2-C2    |
| 51  | X     | 201 | 8Q1  | O27-C28-C29-C31 |
| 48  | V     | 204 | PEE  | C33-C34-C35-C36 |
| 52  | a     | 201 | CDL  | C14-C15-C16-C17 |
| 49  | a     | 202 | PLX  | C16-C17-C18-C19 |
| 52  | V     | 203 | CDL  | C33-C34-C35-C36 |
| 52  | u     | 201 | CDL  | C71-C72-C73-C74 |
| 52  | V     | 201 | CDL  | C64-C65-C66-C67 |
| 49  | a     | 202 | PLX  | O8-C24-C25-C26  |
| 49  | j     | 203 | PLX  | O6-C6-C7-C8     |
| 49  | J     | 403 | PLX  | O4-C3-C4-O6     |
| 52  | V     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 52  | a     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 52  | l     | 701 | CDL  | C51-CB5-OB6-CB4 |
| 48  | Q     | 503 | PEE  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | e     | 201 | PLX  | C32-C33-C34-C35 |
| 52  | k     | 101 | CDL  | C23-C24-C25-C26 |
| 49  | e     | 201 | PLX  | O6-C4-C5-O8     |
| 52  | J     | 404 | CDL  | CA2-C1-CB2-OB2  |
| 49  | C     | 303 | PLX  | C3-C4-C5-O8     |
| 52  | l     | 701 | CDL  | CB3-CB4-CB6-OB8 |
| 49  | e     | 201 | PLX  | C16-C17-C18-C19 |
| 52  | l     | 702 | CDL  | C15-C16-C17-C18 |
| 51  | X     | 201 | 8Q1  | O27-C28-C29-C32 |
| 48  | Q     | 503 | PEE  | C18-C19-C20-C21 |
| 52  | k     | 101 | CDL  | C14-C15-C16-C17 |
| 52  | l     | 701 | CDL  | C24-C25-C26-C27 |
| 49  | j     | 203 | PLX  | C34-C35-C36-C37 |
| 52  | V     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 51  | G     | 201 | 8Q1  | C13-C14-C15-C16 |
| 52  | r     | 502 | CDL  | C15-C16-C17-C18 |
| 48  | C     | 302 | PEE  | C4-O4P-P-O3P    |
| 48  | C     | 302 | PEE  | C4-O4P-P-O2P    |
| 48  | Q     | 503 | PEE  | C1-O3P-P-O1P    |
| 48  | Q     | 503 | PEE  | C1-O3P-P-O4P    |
| 48  | Q     | 503 | PEE  | C4-O4P-P-O2P    |
| 48  | V     | 202 | PEE  | C1-O3P-P-O1P    |
| 48  | V     | 202 | PEE  | C1-O3P-P-O4P    |
| 48  | l     | 703 | PEE  | C4-O4P-P-O2P    |
| 48  | l     | 704 | PEE  | C4-O4P-P-O1P    |
| 48  | s     | 401 | PEE  | C1-O3P-P-O1P    |
| 49  | C     | 303 | PLX  | C2-O1-P1-O3     |
| 49  | J     | 403 | PLX  | C2-O1-P1-O3     |
| 49  | e     | 201 | PLX  | C3-O4-P1-O1     |
| 49  | e     | 201 | PLX  | C2-O1-P1-O4     |
| 49  | g     | 201 | PLX  | C3-O4-P1-O3     |
| 49  | r     | 501 | PLX  | C3-O4-P1-O1     |
| 49  | r     | 501 | PLX  | C3-O4-P1-O2     |
| 49  | r     | 501 | PLX  | C3-O4-P1-O3     |
| 49  | r     | 501 | PLX  | C2-O1-P1-O4     |
| 49  | r     | 501 | PLX  | C2-O1-P1-O3     |
| 52  | J     | 404 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | J     | 404 | CDL  | CB3-OB5-PB2-OB3 |
| 52  | V     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | V     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 52  | V     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 52  | a     | 201 | CDL  | CB2-OB2-PB2-OB4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | a     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 52  | k     | 101 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | l     | 701 | CDL  | CA2-OA2-PA1-OA3 |
| 52  | l     | 701 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | l     | 701 | CDL  | CB3-OB5-PB2-OB4 |
| 52  | r     | 502 | CDL  | CA3-OA5-PA1-OA3 |
| 52  | r     | 502 | CDL  | CB2-OB2-PB2-OB3 |
| 52  | r     | 502 | CDL  | CB2-OB2-PB2-OB4 |
| 52  | r     | 502 | CDL  | CB2-OB2-PB2-OB5 |
| 52  | r     | 502 | CDL  | CB3-OB5-PB2-OB4 |
| 58  | w     | 401 | ADP  | C5'-O5'-PA-O1A  |
| 58  | w     | 401 | ADP  | C5'-O5'-PA-O3A  |
| 49  | e     | 201 | PLX  | C26-C27-C28-C29 |
| 52  | J     | 404 | CDL  | C31-C32-C33-C34 |
| 52  | r     | 502 | CDL  | C1-CB2-OB2-PB2  |
| 48  | j     | 202 | PEE  | C21-C22-C23-C24 |
| 52  | V     | 203 | CDL  | C55-C56-C57-C58 |
| 49  | C     | 303 | PLX  | C16-C17-C18-C19 |
| 48  | l     | 703 | PEE  | C40-C41-C42-C43 |
| 48  | C     | 302 | PEE  | C20-C21-C22-C23 |
| 48  | s     | 401 | PEE  | C24-C25-C26-C27 |
| 52  | r     | 502 | CDL  | C72-C71-CB7-OB8 |
| 52  | V     | 203 | CDL  | C83-C84-C85-C86 |
| 48  | Q     | 503 | PEE  | O3P-C1-C2-C3    |
| 52  | k     | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 52  | u     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 52  | V     | 201 | CDL  | C12-C13-C14-C15 |
| 52  | l     | 702 | CDL  | C38-C39-C40-C41 |
| 52  | k     | 101 | CDL  | CA2-C1-CB2-OB2  |
| 48  | V     | 202 | PEE  | C34-C35-C36-C37 |
| 52  | a     | 201 | CDL  | CB5-C51-C52-C53 |
| 49  | r     | 501 | PLX  | C19-C20-C21-C22 |
| 52  | V     | 203 | CDL  | C77-C78-C79-C80 |
| 48  | W     | 201 | PEE  | O4-C10-O2-C2    |
| 52  | l     | 701 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | l     | 704 | PEE  | O2-C2-C3-O3     |
| 48  | V     | 204 | PEE  | C18-C19-C20-C21 |
| 48  | W     | 201 | PEE  | C11-C10-O2-C2   |
| 52  | I     | 201 | CDL  | C51-C52-C53-C54 |
| 49  | g     | 201 | PLX  | C6-C7-C8-C9     |
| 48  | j     | 201 | PEE  | C23-C24-C25-C26 |
| 52  | k     | 101 | CDL  | C44-C45-C46-C47 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | V     | 201 | CDL  | C36-C37-C38-C39 |
| 52  | a     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 52  | I     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 52  | u     | 201 | CDL  | CB2-C1-CA2-OA2  |
| 48  | V     | 204 | PEE  | C2-C1-O3P-P     |
| 51  | X     | 201 | 8Q1  | C6-C7-C8-C9     |
| 48  | W     | 201 | PEE  | C10-C11-C12-C13 |
| 52  | a     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 52  | l     | 702 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | V     | 204 | PEE  | C30-C31-C32-C33 |
| 52  | l     | 702 | CDL  | C12-C13-C14-C15 |
| 49  | a     | 202 | PLX  | C35-C36-C37-C38 |
| 52  | a     | 201 | CDL  | C18-C19-C20-C21 |
| 48  | j     | 202 | PEE  | O2-C2-C3-O3     |
| 49  | C     | 303 | PLX  | C9-C10-C11-C12  |
| 52  | V     | 203 | CDL  | C53-C54-C55-C56 |
| 48  | j     | 201 | PEE  | C33-C34-C35-C36 |
| 48  | V     | 202 | PEE  | O4-C10-O2-C2    |
| 52  | J     | 404 | CDL  | C84-C85-C86-C87 |
| 52  | r     | 502 | CDL  | C13-C14-C15-C16 |
| 49  | e     | 201 | PLX  | C17-C18-C19-C20 |
| 48  | Q     | 503 | PEE  | C12-C13-C14-C15 |
| 49  | C     | 303 | PLX  | C26-C27-C28-C29 |
| 48  | Q     | 503 | PEE  | C14-C15-C16-C17 |
| 52  | V     | 201 | CDL  | C43-C44-C45-C46 |
| 48  | l     | 704 | PEE  | C38-C39-C40-C41 |
| 51  | X     | 201 | 8Q1  | O33-C32-C34-N36 |
| 49  | J     | 403 | PLX  | C36-C37-C38-C39 |
| 52  | J     | 404 | CDL  | C15-C16-C17-C18 |
| 53  | J     | 401 | NDP  | O4B-C4B-C5B-O5B |
| 48  | l     | 703 | PEE  | C1-C2-O2-C10    |
| 52  | k     | 101 | CDL  | CA6-CA4-OA6-CA5 |
| 52  | l     | 702 | CDL  | CB7-C71-C72-C73 |
| 47  | A     | 503 | NAI  | O4D-C1D-N1N-C2N |
| 52  | J     | 404 | CDL  | C56-C57-C58-C59 |
| 52  | l     | 701 | CDL  | OA5-CA3-CA4-OA6 |
| 49  | j     | 203 | PLX  | C28-C29-C30-C31 |
| 52  | V     | 203 | CDL  | CA7-C31-C32-C33 |
| 48  | l     | 704 | PEE  | C2-C1-O3P-P     |
| 52  | l     | 702 | CDL  | C53-C54-C55-C56 |
| 48  | j     | 202 | PEE  | C18-C19-C20-C21 |
| 52  | k     | 101 | CDL  | OA6-CA4-CA6-OA8 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | u     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 52  | a     | 201 | CDL  | C61-C62-C63-C64 |
| 49  | J     | 403 | PLX  | C28-C29-C30-C31 |
| 52  | u     | 201 | CDL  | C55-C56-C57-C58 |
| 49  | g     | 201 | PLX  | C15-C16-C17-C18 |
| 52  | k     | 101 | CDL  | C76-C77-C78-C79 |
| 53  | J     | 401 | NDP  | C2B-O2B-P2B-O1X |
| 52  | J     | 404 | CDL  | C72-C71-CB7-OB8 |
| 49  | J     | 403 | PLX  | C19-C20-C21-C22 |
| 49  | j     | 203 | PLX  | C25-C26-C27-C28 |
| 49  | e     | 201 | PLX  | C15-C16-C17-C18 |
| 48  | j     | 201 | PEE  | C11-C12-C13-C14 |
| 48  | W     | 201 | PEE  | C22-C23-C24-C25 |
| 52  | a     | 201 | CDL  | C56-C57-C58-C59 |
| 52  | l     | 702 | CDL  | C22-C23-C24-C25 |
| 48  | j     | 202 | PEE  | C32-C33-C34-C35 |
| 49  | r     | 501 | PLX  | C4-C3-O4-P1     |
| 52  | k     | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 52  | l     | 701 | CDL  | CB4-CB3-OB5-PB2 |
| 48  | Q     | 503 | PEE  | C11-C12-C13-C14 |
| 52  | a     | 201 | CDL  | C84-C85-C86-C87 |
| 49  | e     | 201 | PLX  | C31-C32-C33-C34 |
| 49  | C     | 303 | PLX  | O9-C24-C25-C26  |
| 48  | Q     | 503 | PEE  | O3P-C1-C2-O2    |
| 48  | s     | 401 | PEE  | O3P-C1-C2-O2    |
| 48  | j     | 201 | PEE  | C43-C44-C45-C46 |
| 52  | l     | 701 | CDL  | C12-C11-CA5-OA6 |
| 52  | V     | 201 | CDL  | C32-C31-CA7-OA8 |
| 48  | j     | 201 | PEE  | C37-C38-C39-C40 |
| 48  | C     | 302 | PEE  | C44-C45-C46-C47 |
| 52  | r     | 502 | CDL  | OB5-CB3-CB4-CB6 |
| 52  | I     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 52  | V     | 203 | CDL  | C13-C14-C15-C16 |
| 47  | A     | 503 | NAI  | C2D-C1D-N1N-C2N |
| 46  | A     | 502 | FMN  | C5'-O5'-P-O3P   |
| 49  | e     | 201 | PLX  | C36-C37-C38-C39 |
| 49  | C     | 303 | PLX  | C15-C16-C17-C18 |
| 52  | V     | 203 | CDL  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C3-C2-O2-C10    |
| 48  | C     | 302 | PEE  | C18-C19-C20-C21 |
| 48  | V     | 202 | PEE  | C16-C17-C18-C19 |
| 48  | V     | 204 | PEE  | C16-C17-C18-C19 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | W     | 201 | PEE  | C18-C19-C20-C21 |
| 48  | j     | 201 | PEE  | C16-C17-C18-C19 |
| 52  | J     | 404 | CDL  | O1-C1-CB2-OB2   |
| 48  | s     | 401 | PEE  | C18-C19-C20-C21 |
| 52  | V     | 201 | CDL  | CA4-CA3-OA5-PA1 |
| 52  | I     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 52  | r     | 502 | CDL  | OB5-CB3-CB4-OB6 |
| 48  | V     | 204 | PEE  | C1-C2-C3-O3     |
| 52  | l     | 701 | CDL  | CA3-CA4-CA6-OA8 |
| 52  | J     | 404 | CDL  | OB9-CB7-OB8-CB6 |
| 49  | r     | 501 | PLX  | C36-C37-C38-C39 |
| 48  | Q     | 503 | PEE  | C38-C39-C40-C41 |
| 48  | l     | 703 | PEE  | C36-C37-C38-C39 |
| 49  | a     | 202 | PLX  | C30-C31-C32-C33 |
| 52  | a     | 201 | CDL  | C38-C39-C40-C41 |
| 52  | V     | 201 | CDL  | CA7-C31-C32-C33 |
| 48  | V     | 202 | PEE  | O2-C10-C11-C12  |
| 52  | l     | 701 | CDL  | C39-C40-C41-C42 |
| 48  | C     | 302 | PEE  | C36-C37-C38-C39 |
| 48  | l     | 703 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C16-C17-C18-C19 |
| 52  | a     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 52  | l     | 702 | CDL  | OA5-CA3-CA4-CA6 |
| 49  | j     | 203 | PLX  | C7-C6-O6-C4     |
| 49  | j     | 203 | PLX  | C24-C25-C26-C27 |
| 52  | a     | 201 | CDL  | C41-C42-C43-C44 |
| 52  | u     | 201 | CDL  | C51-C52-C53-C54 |
| 52  | J     | 404 | CDL  | C74-C75-C76-C77 |
| 48  | V     | 202 | PEE  | C11-C10-O2-C2   |
| 48  | W     | 201 | PEE  | C16-C17-C18-C19 |
| 49  | j     | 203 | PLX  | C32-C33-C34-C35 |
| 58  | w     | 401 | ADP  | PB-O3A-PA-O2A   |
| 52  | V     | 203 | CDL  | C71-C72-C73-C74 |
| 48  | V     | 204 | PEE  | C38-C39-C40-C41 |
| 48  | V     | 202 | PEE  | C22-C23-C24-C25 |
| 48  | s     | 401 | PEE  | O2-C10-C11-C12  |
| 49  | j     | 203 | PLX  | C29-C30-C31-C32 |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1B    |
| 52  | k     | 101 | CDL  | CB5-C51-C52-C53 |
| 48  | l     | 703 | PEE  | C10-C11-C12-C13 |
| 48  | V     | 202 | PEE  | C41-C42-C43-C44 |
| 50  | J     | 402 | UQ   | C22-C23-C24-C25 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 52  | k     | 101 | CDL  | C41-C42-C43-C44 |
| 48  | Q     | 503 | PEE  | C2-C1-O3P-P     |
| 52  | a     | 201 | CDL  | C12-C11-CA5-OA6 |
| 49  | a     | 202 | PLX  | C10-C11-C12-C13 |
| 48  | j     | 202 | PEE  | C1-C2-C3-O3     |
| 49  | J     | 403 | PLX  | C25-C24-O8-C5   |
| 49  | a     | 202 | PLX  | C25-C24-O8-C5   |
| 49  | j     | 203 | PLX  | C25-C24-O8-C5   |
| 52  | V     | 203 | CDL  | C19-C20-C21-C22 |
| 50  | C     | 304 | UQ   | C25-C24-C26-C27 |
| 52  | V     | 203 | CDL  | C52-C51-CB5-OB6 |
| 52  | l     | 702 | CDL  | C18-C19-C20-C21 |
| 52  | r     | 502 | CDL  | C53-C54-C55-C56 |
| 48  | l     | 703 | PEE  | C14-C15-C16-C17 |
| 48  | V     | 204 | PEE  | C32-C33-C34-C35 |
| 52  | V     | 203 | CDL  | C82-C83-C84-C85 |
| 49  | a     | 202 | PLX  | O4-C3-C4-C5     |
| 52  | I     | 201 | CDL  | C72-C71-CB7-OB8 |
| 52  | a     | 201 | CDL  | C12-C13-C14-C15 |
| 51  | X     | 201 | 8Q1  | O27-C28-C29-C30 |
| 52  | l     | 701 | CDL  | C84-C85-C86-C87 |
| 49  | J     | 403 | PLX  | C24-C25-C26-C27 |
| 49  | e     | 201 | PLX  | C30-C31-C32-C33 |
| 52  | J     | 404 | CDL  | CA6-CA4-OA6-CA5 |
| 49  | J     | 403 | PLX  | C2-C1-N1-C1A    |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1C    |
| 48  | j     | 202 | PEE  | O3-C30-C31-C32  |
| 48  | V     | 202 | PEE  | C12-C13-C14-C15 |
| 52  | J     | 404 | CDL  | C19-C20-C21-C22 |
| 52  | l     | 702 | CDL  | C13-C14-C15-C16 |
| 47  | A     | 503 | NAI  | O4D-C4D-C5D-O5D |
| 52  | J     | 404 | CDL  | C71-CB7-OB8-CB6 |
| 49  | a     | 202 | PLX  | C19-C20-C21-C22 |
| 52  | V     | 201 | CDL  | C21-C22-C23-C24 |
| 50  | C     | 304 | UQ   | C15-C14-C16-C17 |
| 48  | s     | 401 | PEE  | C20-C21-C22-C23 |
| 49  | e     | 201 | PLX  | O4-C3-C4-O6     |
| 48  | V     | 202 | PEE  | C15-C16-C17-C18 |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1A    |
| 52  | u     | 201 | CDL  | O1-C1-CB2-OB2   |
| 49  | r     | 501 | PLX  | O9-C24-O8-C5    |
| 52  | V     | 203 | CDL  | C52-C51-CB5-OB7 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | V     | 202 | PEE  | O4-C10-C11-C12  |
| 49  | r     | 501 | PLX  | C6-C7-C8-C9     |
| 48  | V     | 202 | PEE  | C30-C31-C32-C33 |
| 52  | l     | 701 | CDL  | C72-C71-CB7-OB8 |
| 52  | V     | 203 | CDL  | C72-C73-C74-C75 |
| 52  | r     | 502 | CDL  | CA5-C11-C12-C13 |
| 52  | r     | 502 | CDL  | C79-C80-C81-C82 |
| 52  | r     | 502 | CDL  | C23-C24-C25-C26 |
| 51  | G     | 201 | 8Q1  | C6-C7-C8-C9     |
| 52  | I     | 201 | CDL  | C72-C71-CB7-OB9 |
| 52  | l     | 701 | CDL  | C52-C51-CB5-OB6 |
| 52  | k     | 101 | CDL  | C82-C83-C84-C85 |
| 52  | a     | 201 | CDL  | C32-C31-CA7-OA8 |
| 49  | J     | 403 | PLX  | C29-C30-C31-C32 |
| 52  | V     | 203 | CDL  | C32-C31-CA7-OA8 |
| 52  | k     | 101 | CDL  | C12-C11-CA5-OA6 |
| 48  | s     | 401 | PEE  | C41-C42-C43-C44 |

There are no ring outliers.

40 monomers are involved in 217 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 47  | A     | 503 | NAI  | 4       | 0            |
| 51  | X     | 201 | 8Q1  | 3       | 0            |
| 48  | C     | 302 | PEE  | 6       | 0            |
| 56  | Q     | 502 | UQ1  | 4       | 0            |
| 50  | C     | 304 | UQ   | 7       | 0            |
| 48  | W     | 201 | PEE  | 8       | 0            |
| 49  | C     | 303 | PLX  | 7       | 0            |
| 49  | g     | 201 | PLX  | 3       | 0            |
| 52  | l     | 701 | CDL  | 13      | 0            |
| 52  | l     | 702 | CDL  | 20      | 0            |
| 52  | u     | 201 | CDL  | 3       | 0            |
| 48  | l     | 704 | PEE  | 7       | 0            |
| 54  | O     | 301 | FES  | 3       | 0            |
| 52  | I     | 201 | CDL  | 2       | 0            |
| 45  | M     | 802 | SF4  | 3       | 0            |
| 45  | A     | 501 | SF4  | 2       | 0            |
| 56  | Q     | 501 | UQ1  | 4       | 0            |
| 52  | V     | 203 | CDL  | 6       | 0            |
| 52  | k     | 101 | CDL  | 7       | 0            |
| 52  | J     | 404 | CDL  | 8       | 0            |

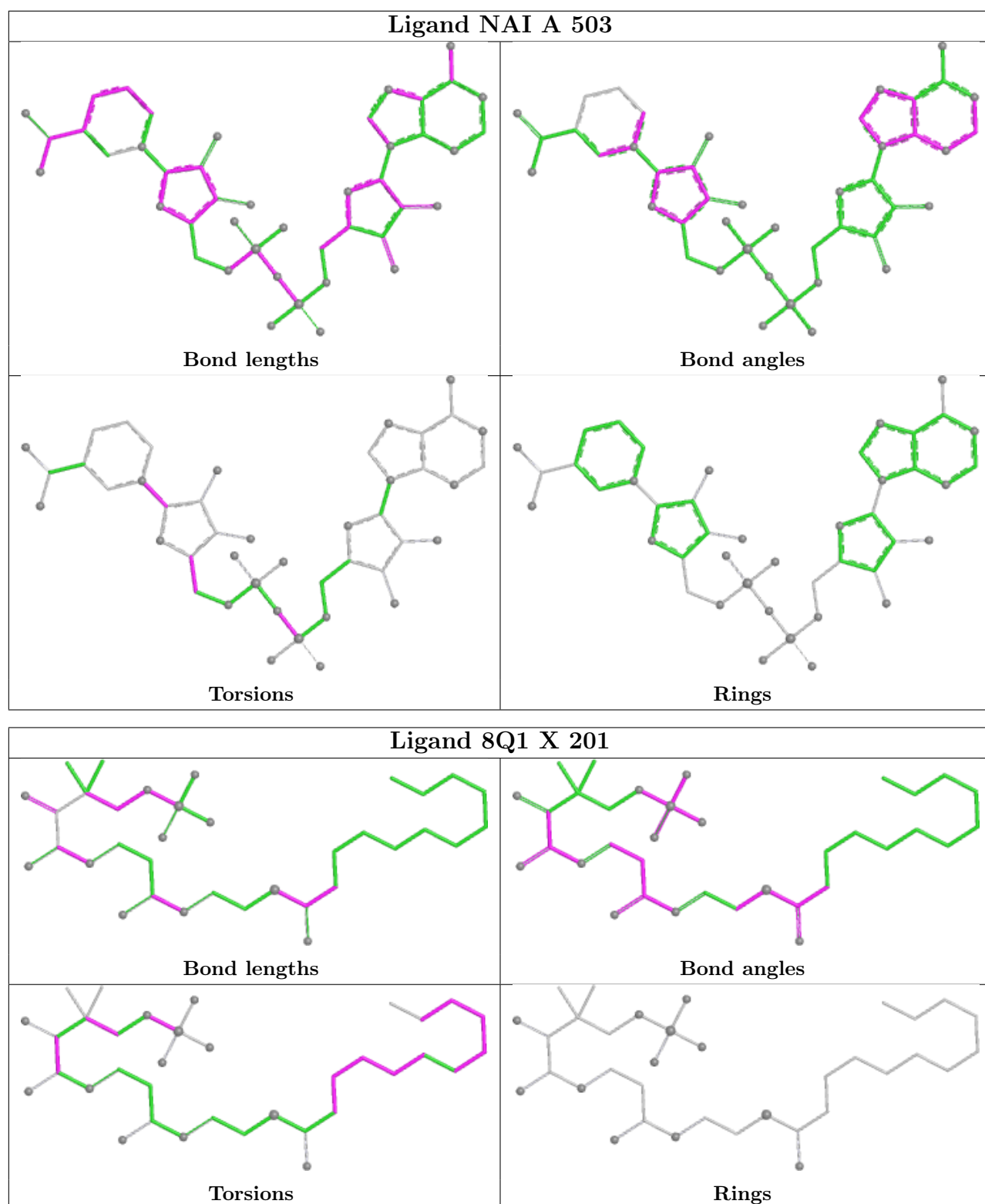
*Continued on next page...*

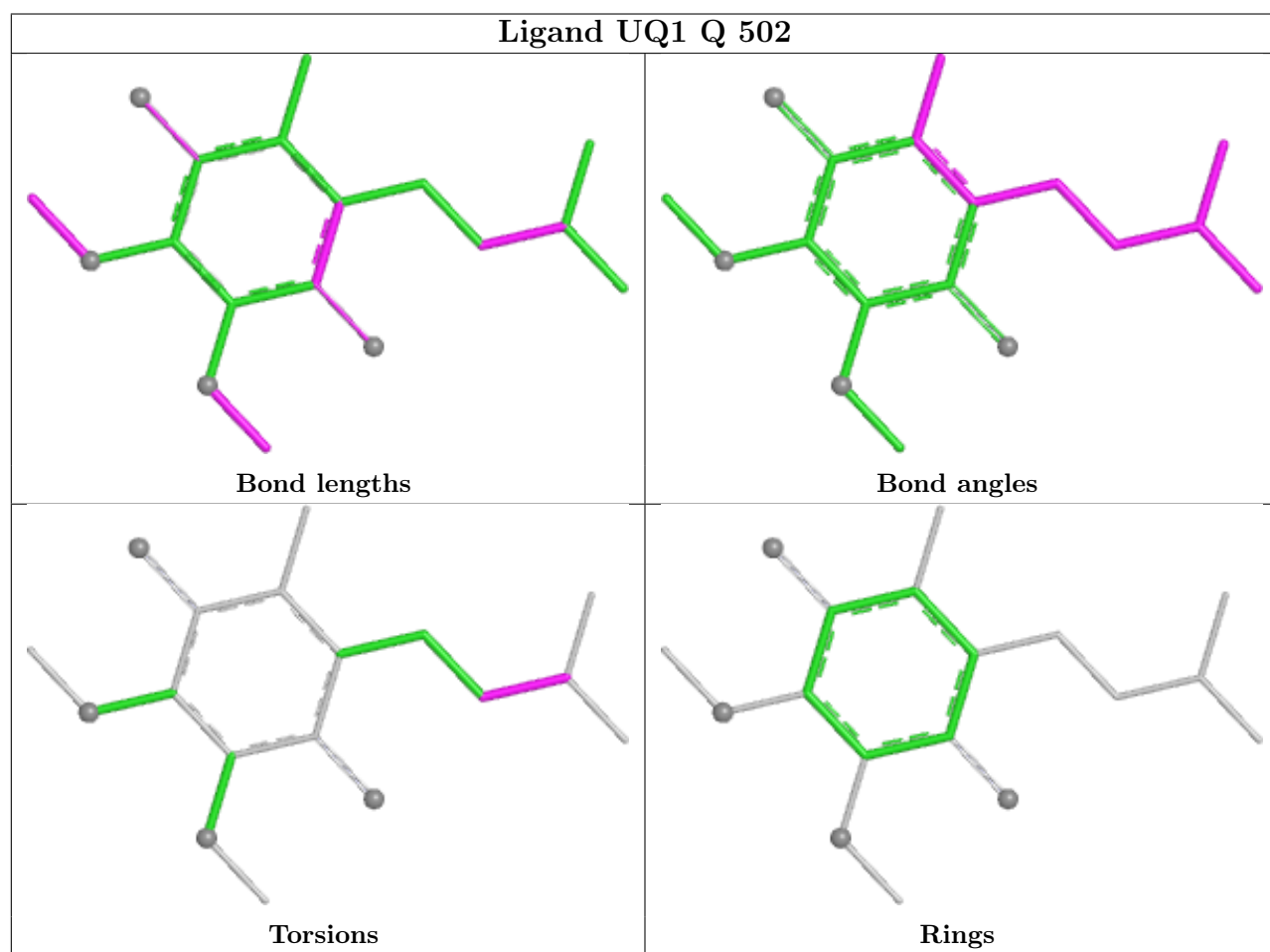
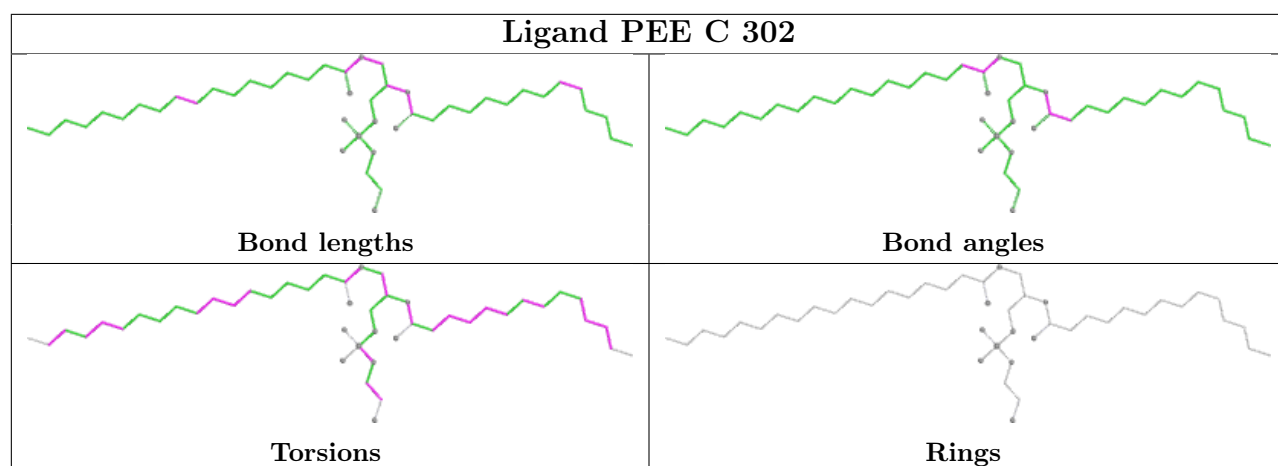


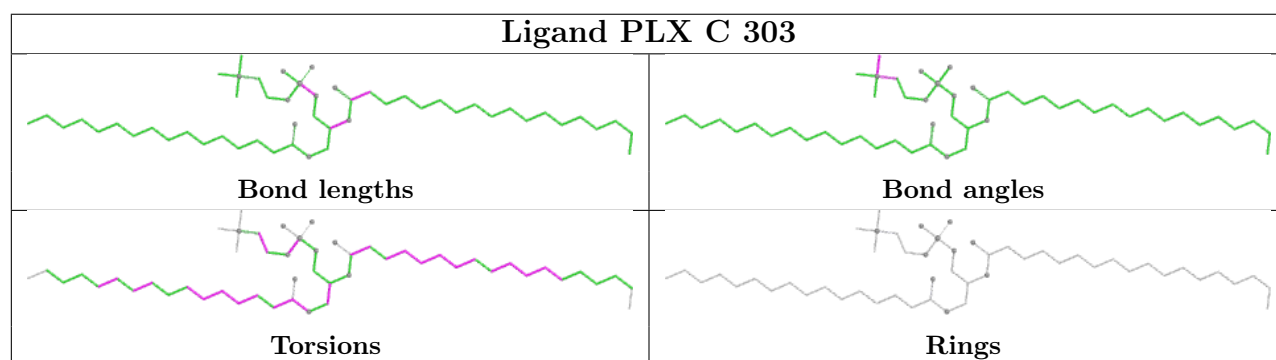
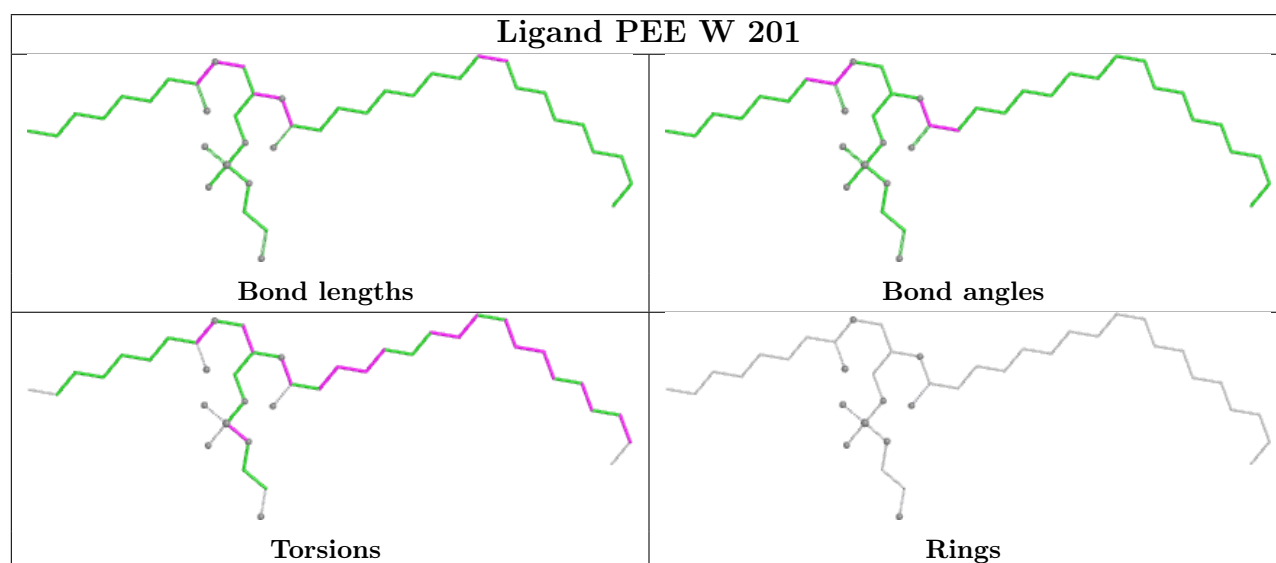
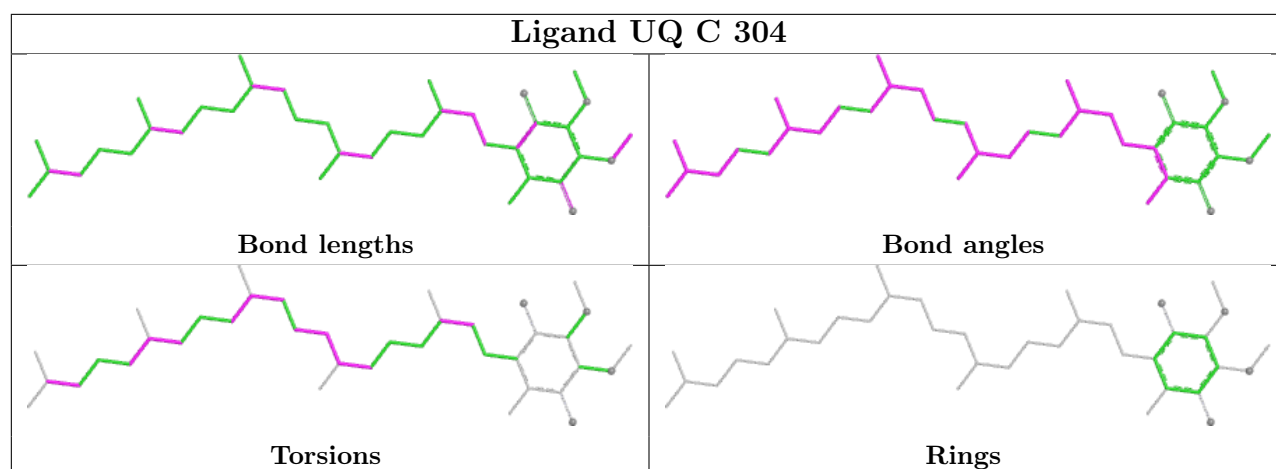
*Continued from previous page...*

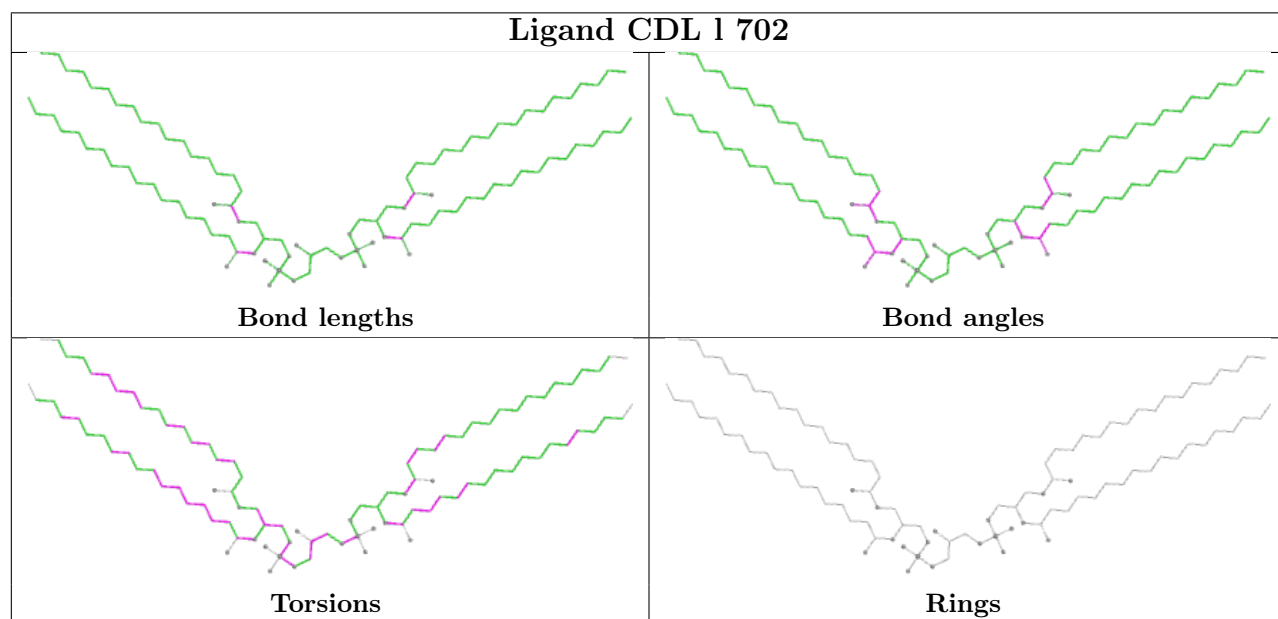
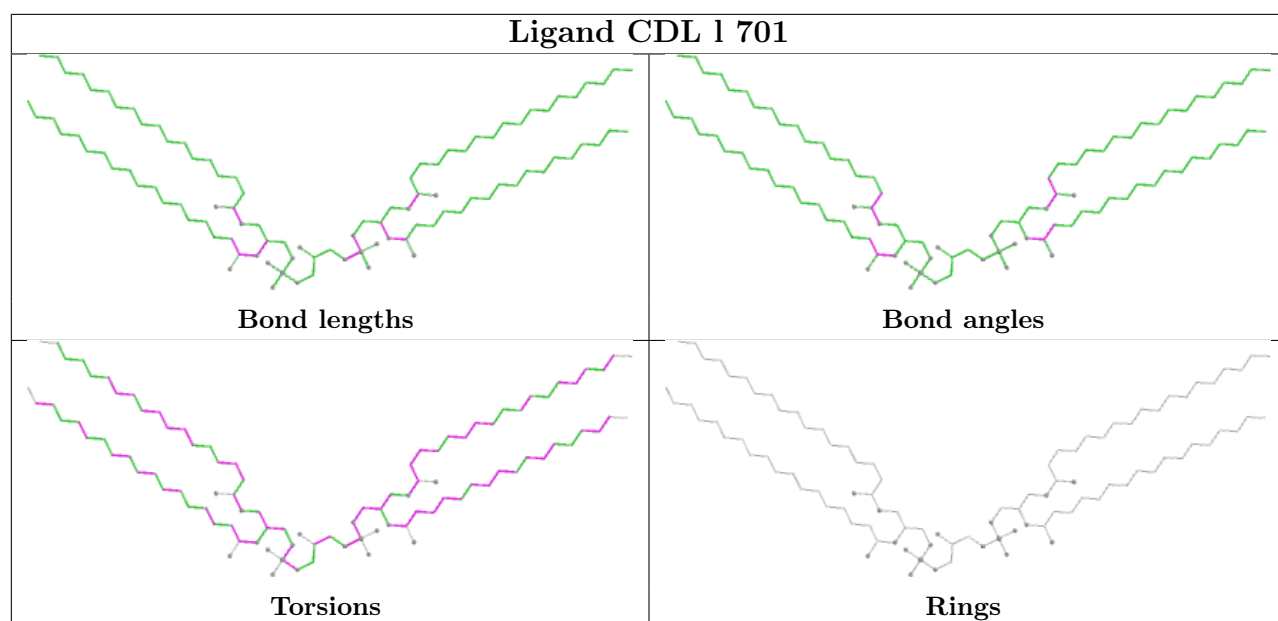
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 48  | V     | 204 | PEE  | 5       | 0            |
| 48  | V     | 202 | PEE  | 6       | 0            |
| 52  | a     | 201 | CDL  | 4       | 0            |
| 45  | C     | 301 | SF4  | 1       | 0            |
| 48  | Q     | 503 | PEE  | 11      | 0            |
| 48  | l     | 703 | PEE  | 9       | 0            |
| 50  | J     | 402 | UQ   | 11      | 0            |
| 46  | A     | 502 | FMN  | 4       | 0            |
| 52  | V     | 201 | CDL  | 4       | 0            |
| 48  | s     | 401 | PEE  | 4       | 0            |
| 49  | e     | 201 | PLX  | 7       | 0            |
| 53  | J     | 401 | NDP  | 1       | 0            |
| 49  | J     | 403 | PLX  | 6       | 0            |
| 49  | j     | 203 | PLX  | 3       | 0            |
| 51  | G     | 201 | 8Q1  | 4       | 0            |
| 58  | w     | 401 | ADP  | 3       | 0            |
| 48  | j     | 202 | PEE  | 9       | 0            |
| 48  | j     | 201 | PEE  | 11      | 0            |
| 52  | r     | 502 | CDL  | 7       | 0            |
| 49  | r     | 501 | PLX  | 3       | 0            |

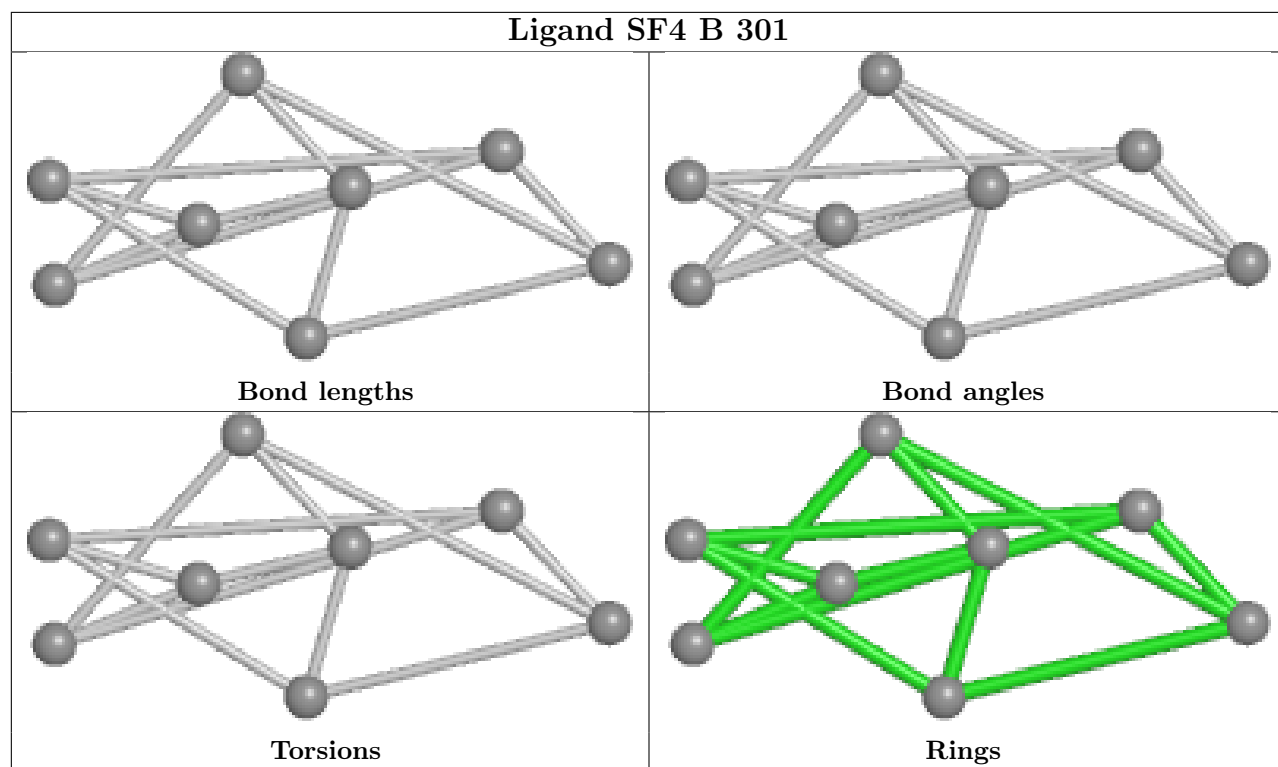
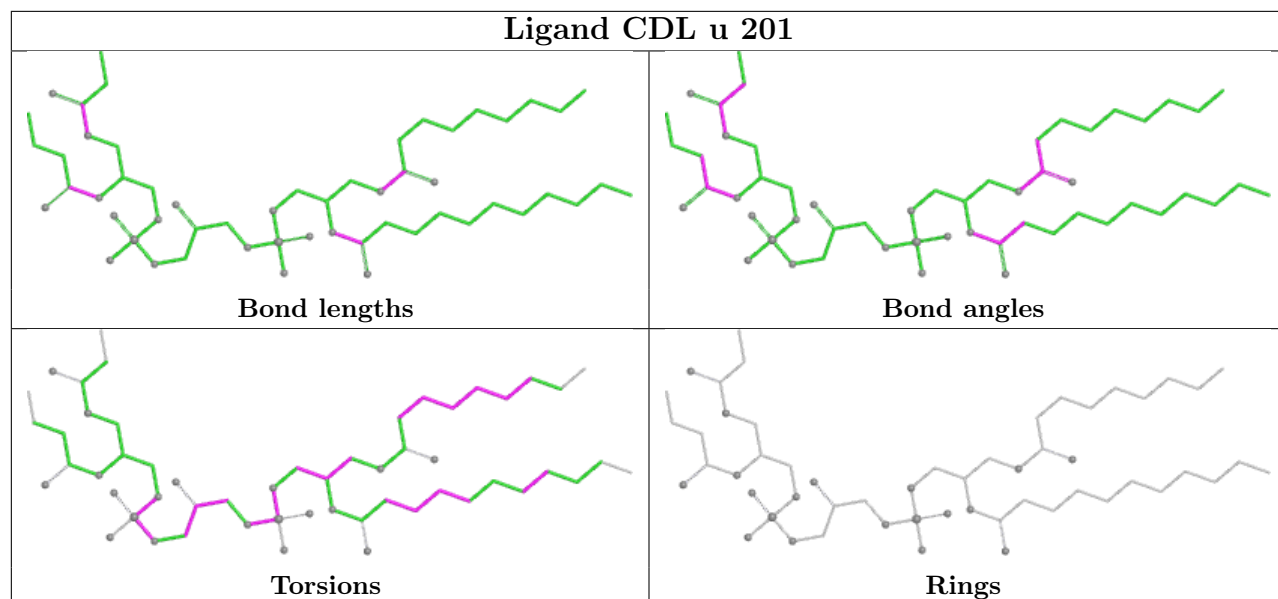
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

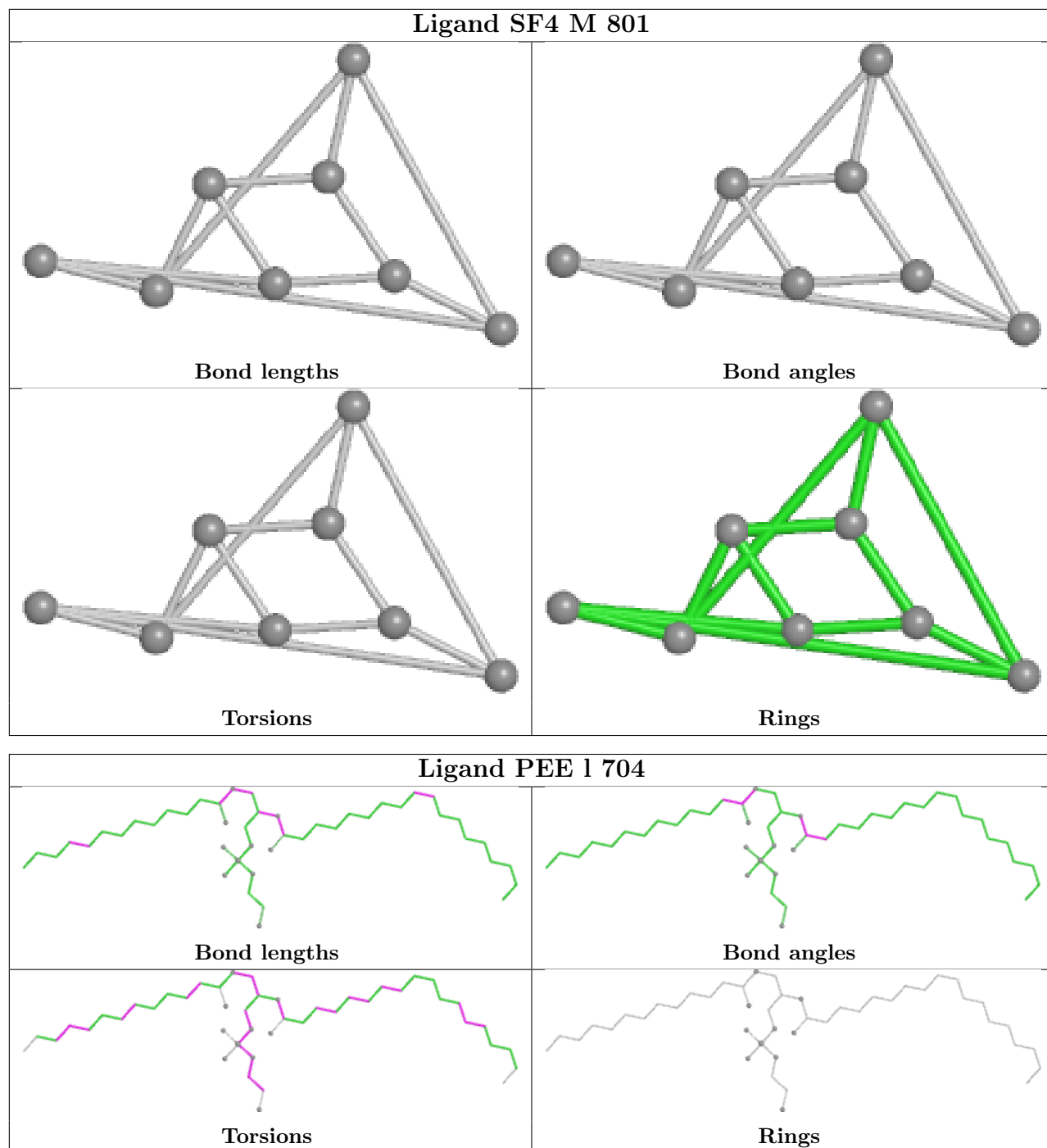


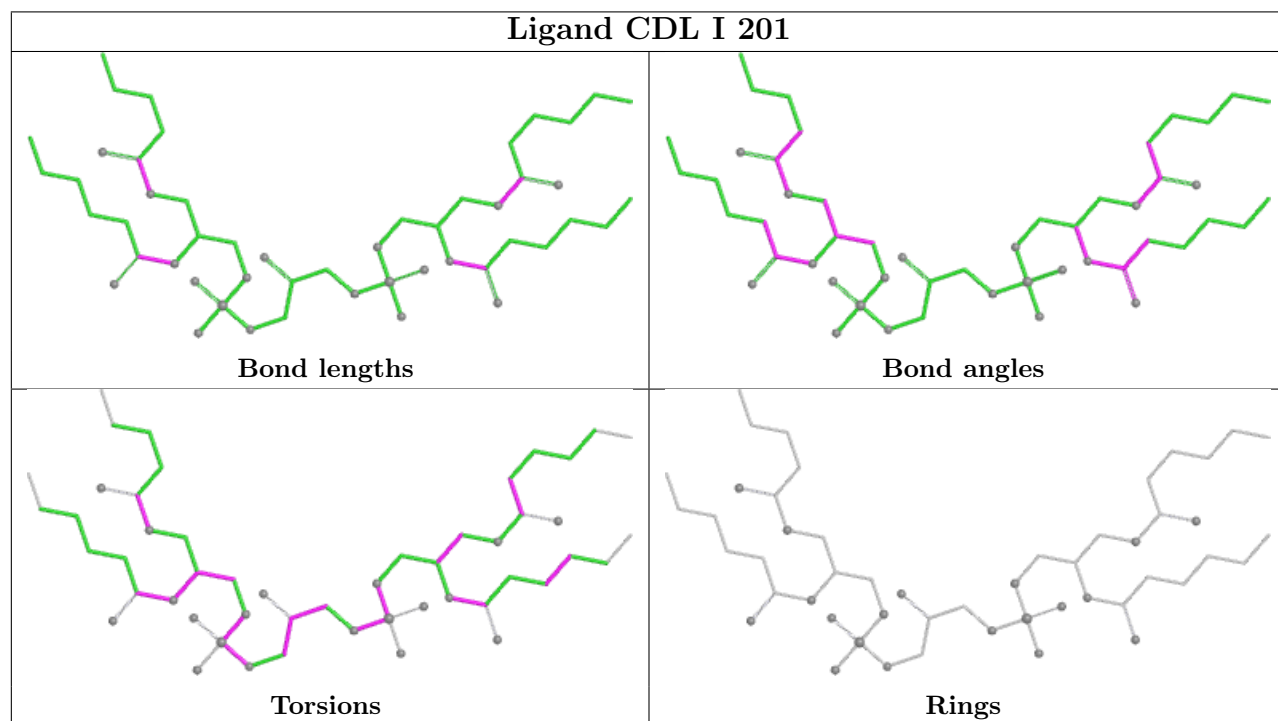
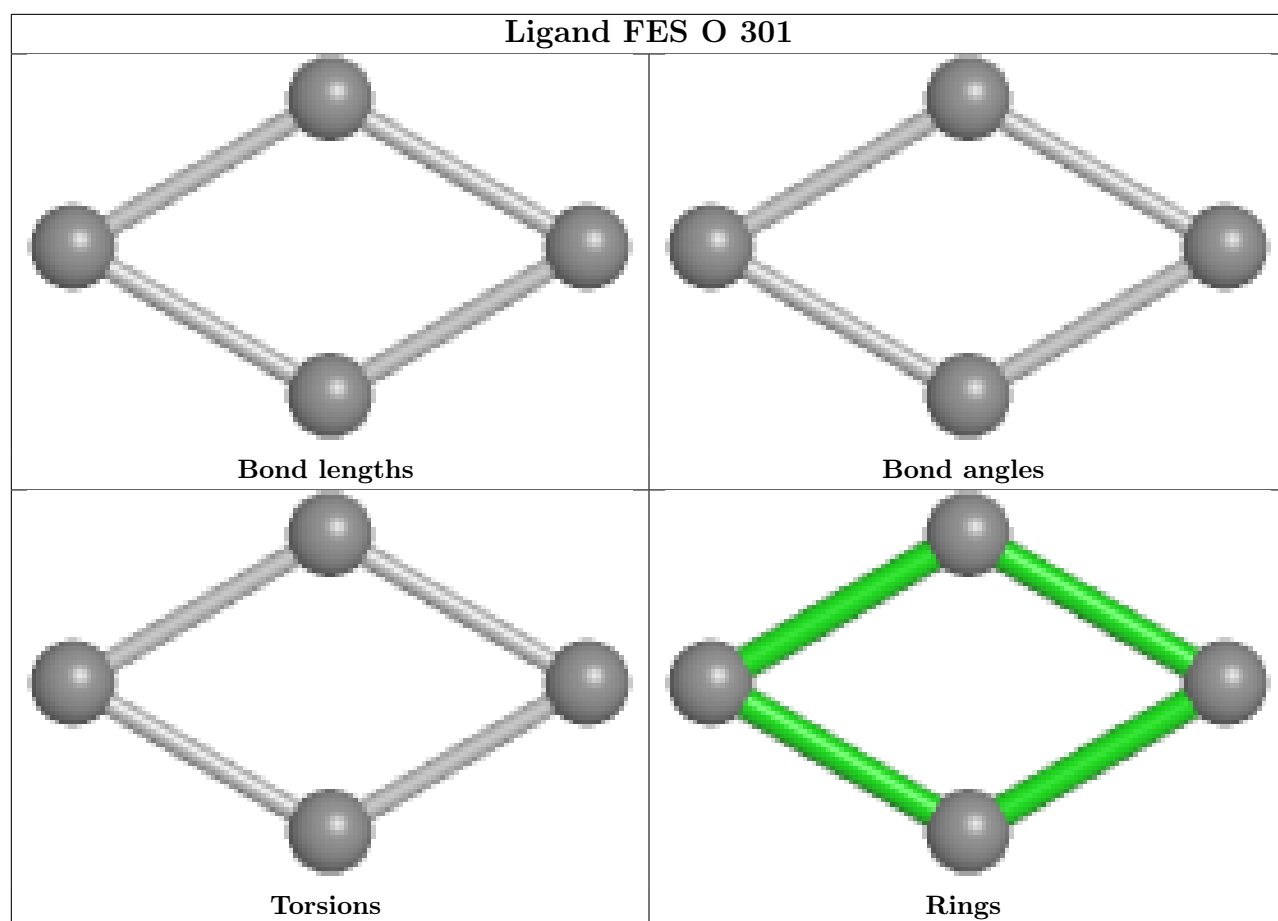






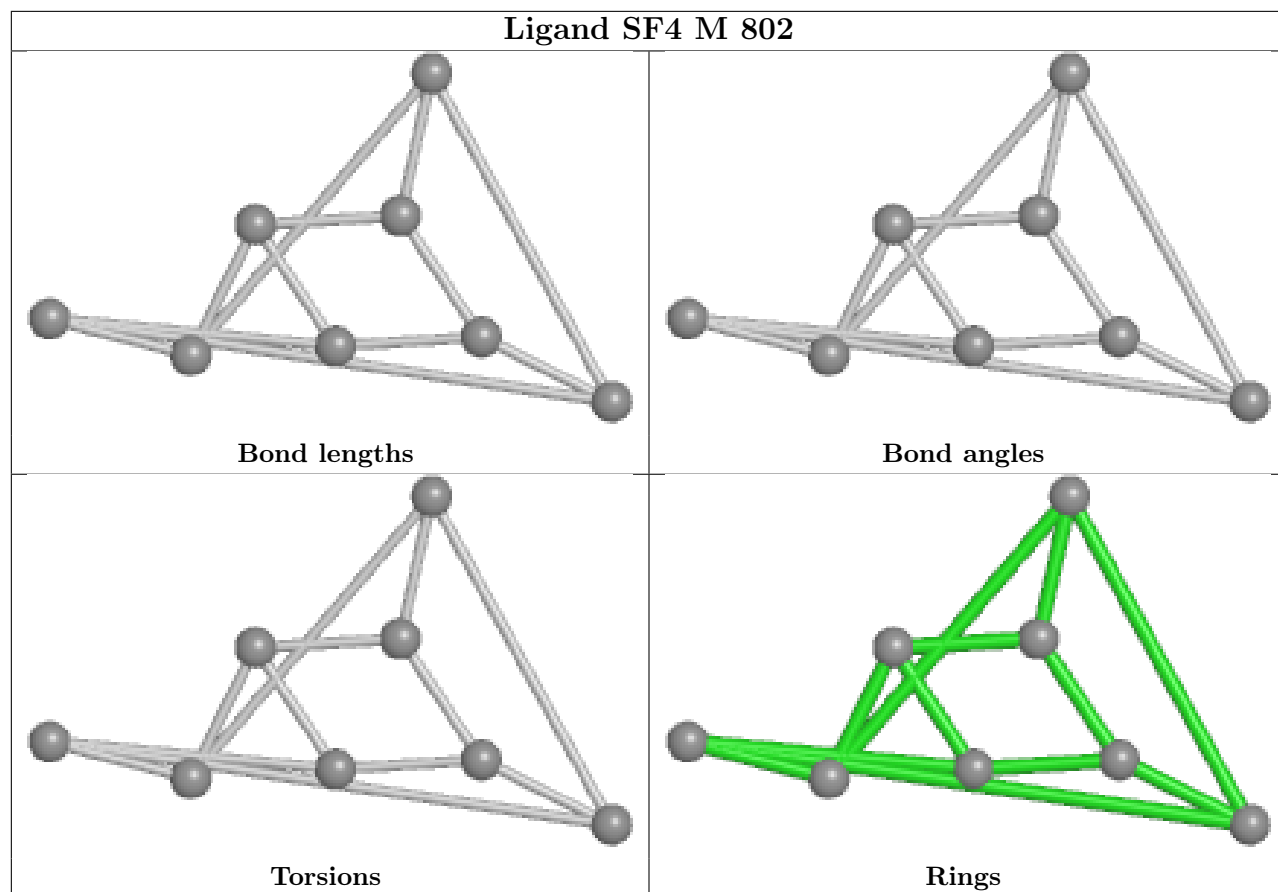




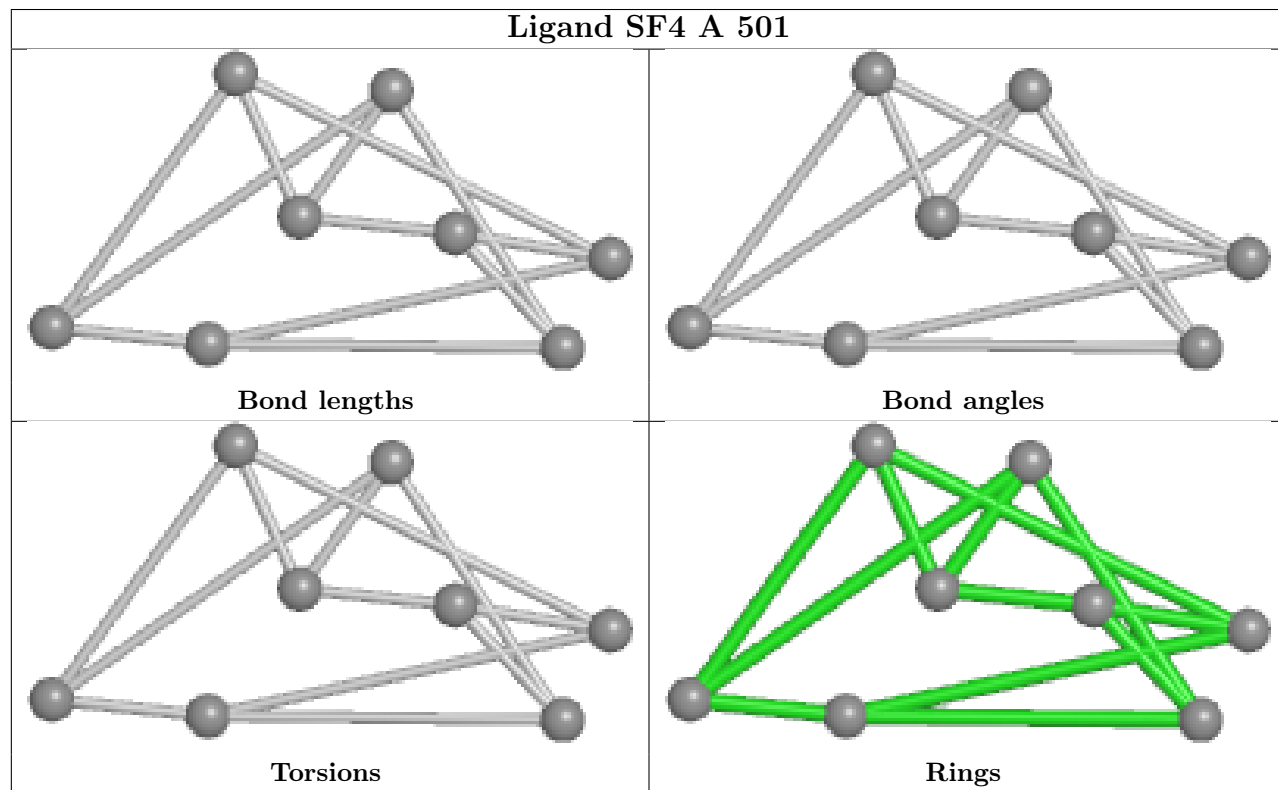




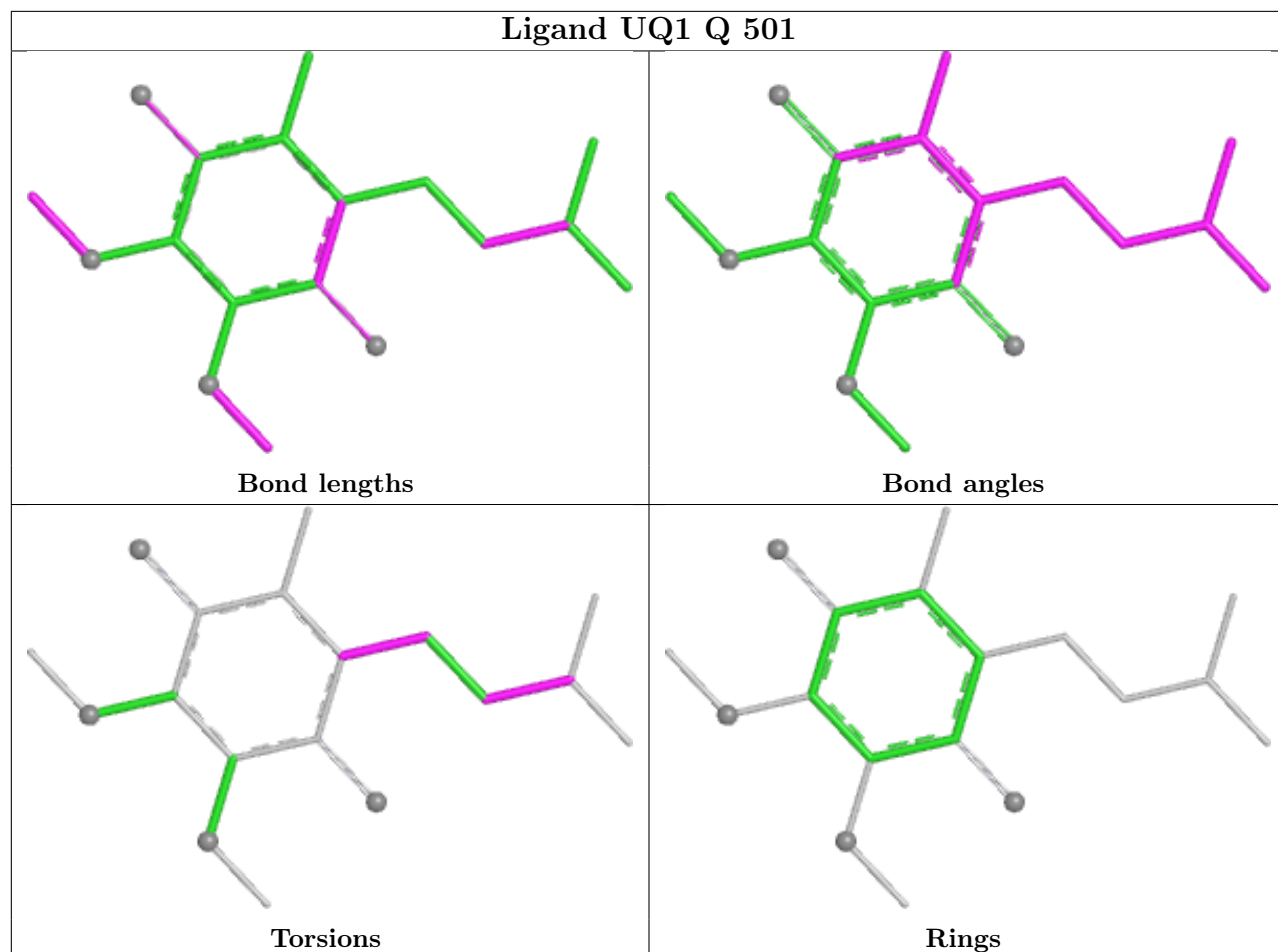
## Ligand SF4 M 802



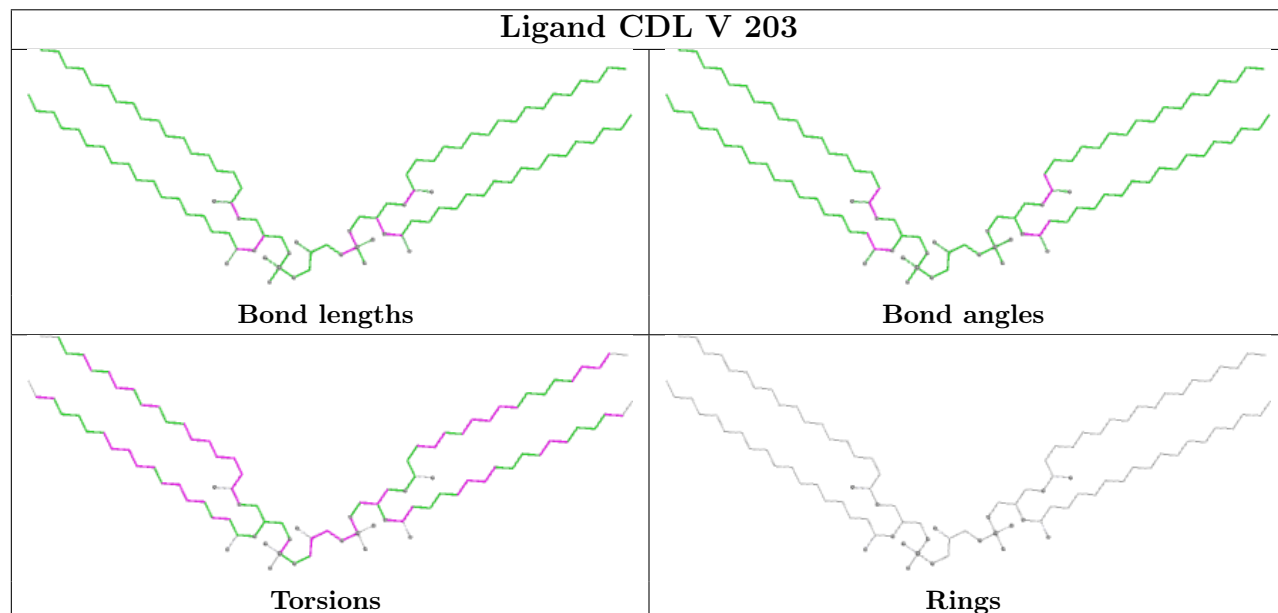
## Ligand SF4 A 501

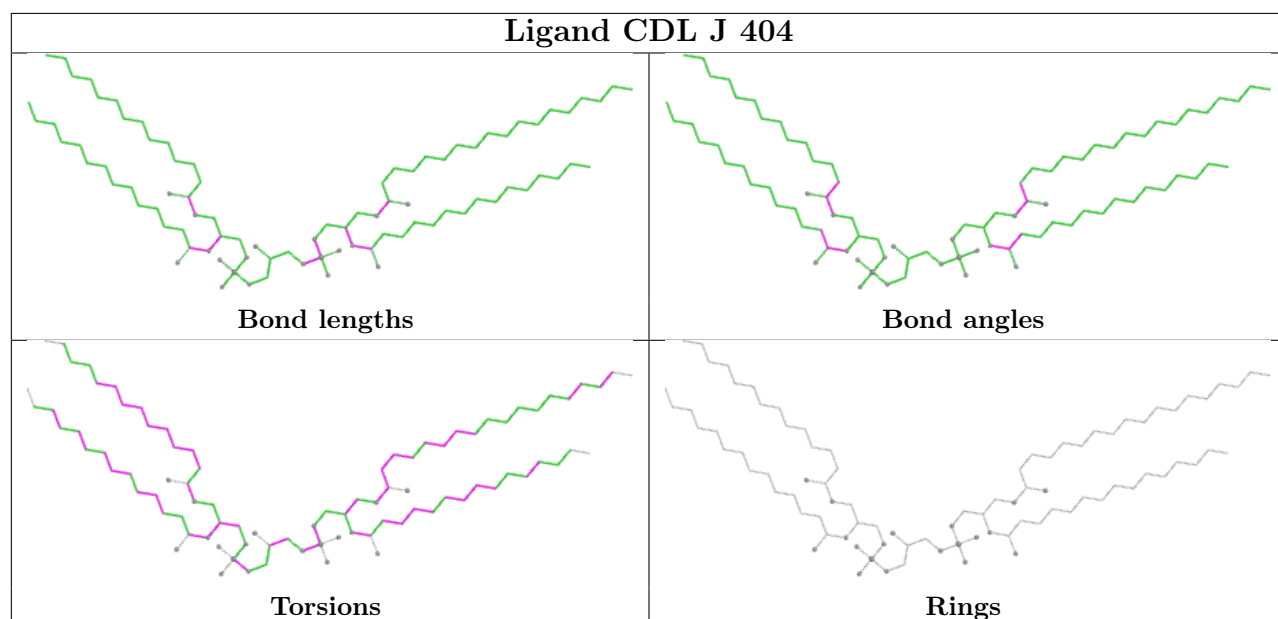
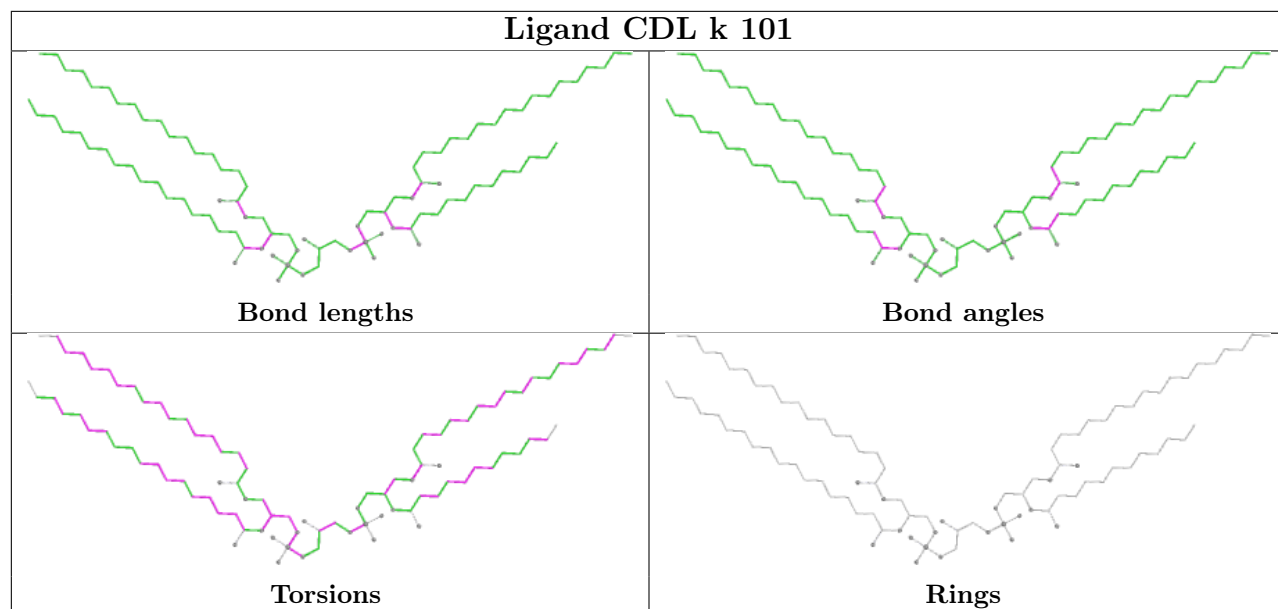


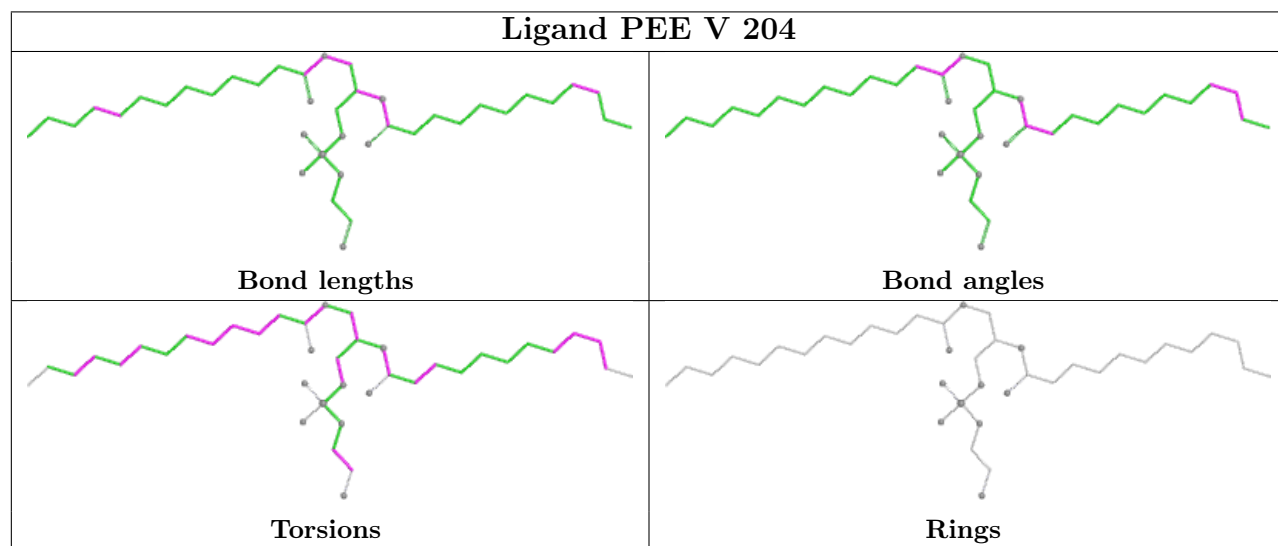
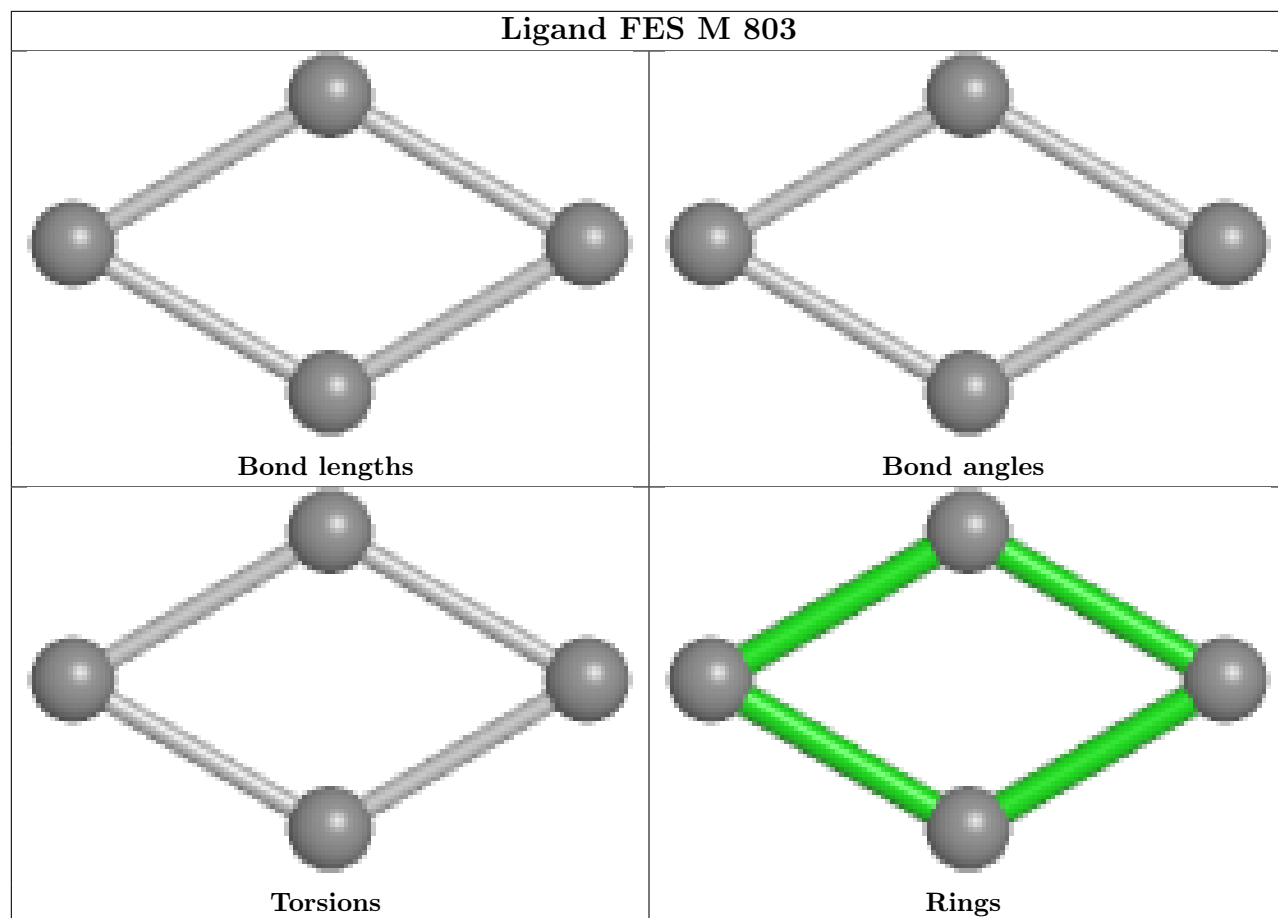
## Ligand UQ1 Q 501

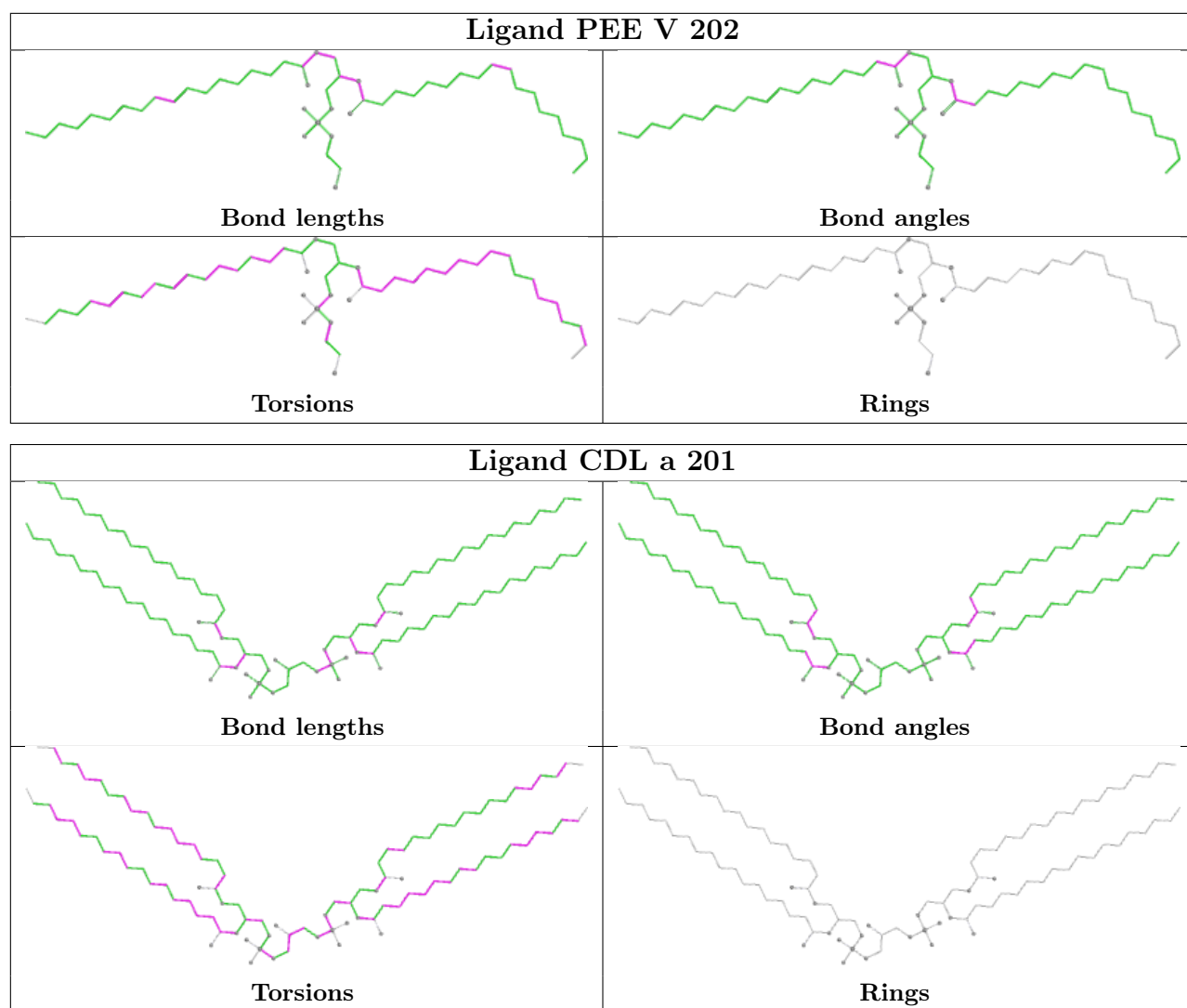


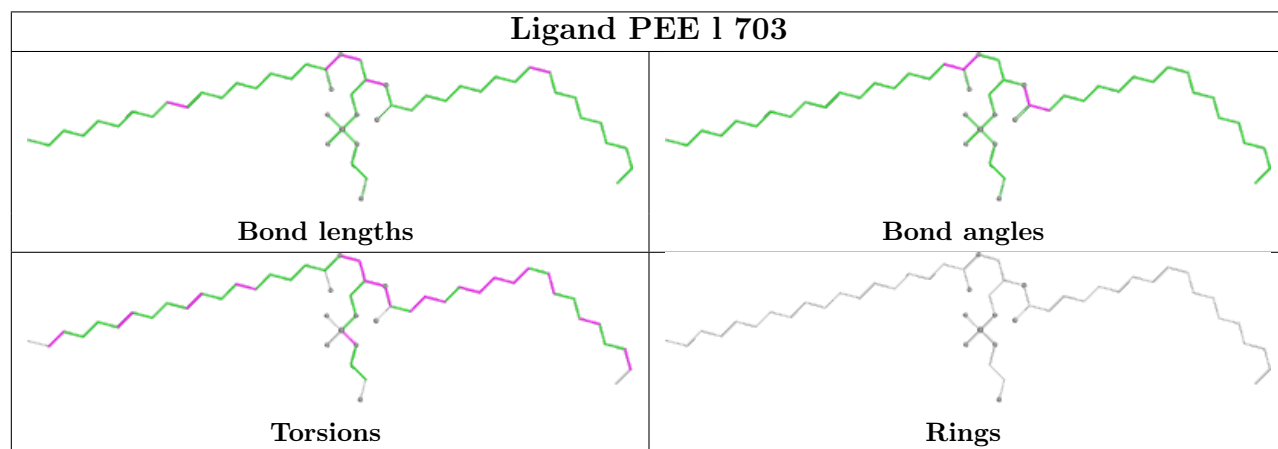
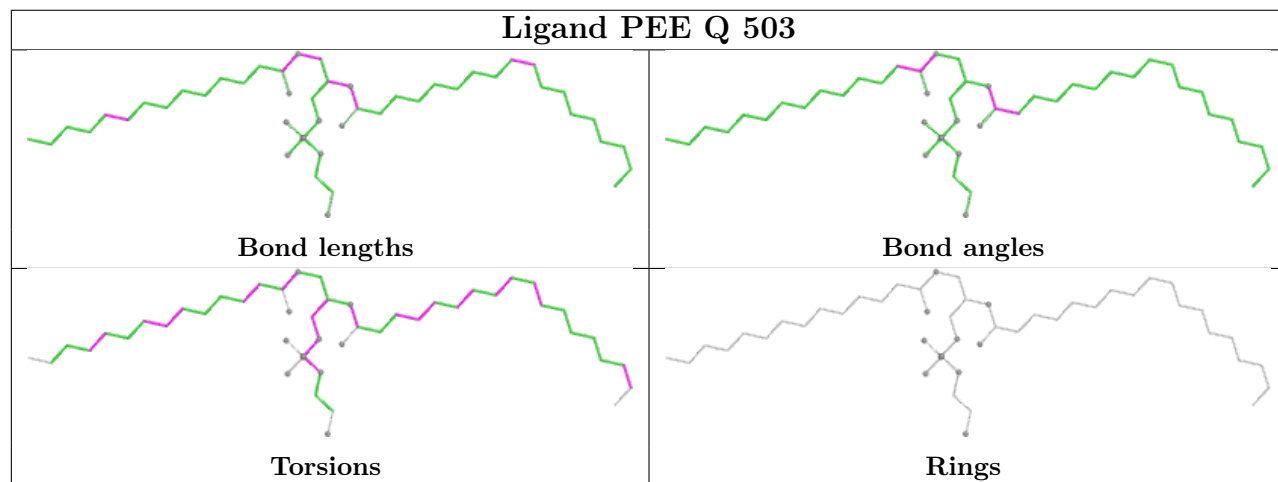
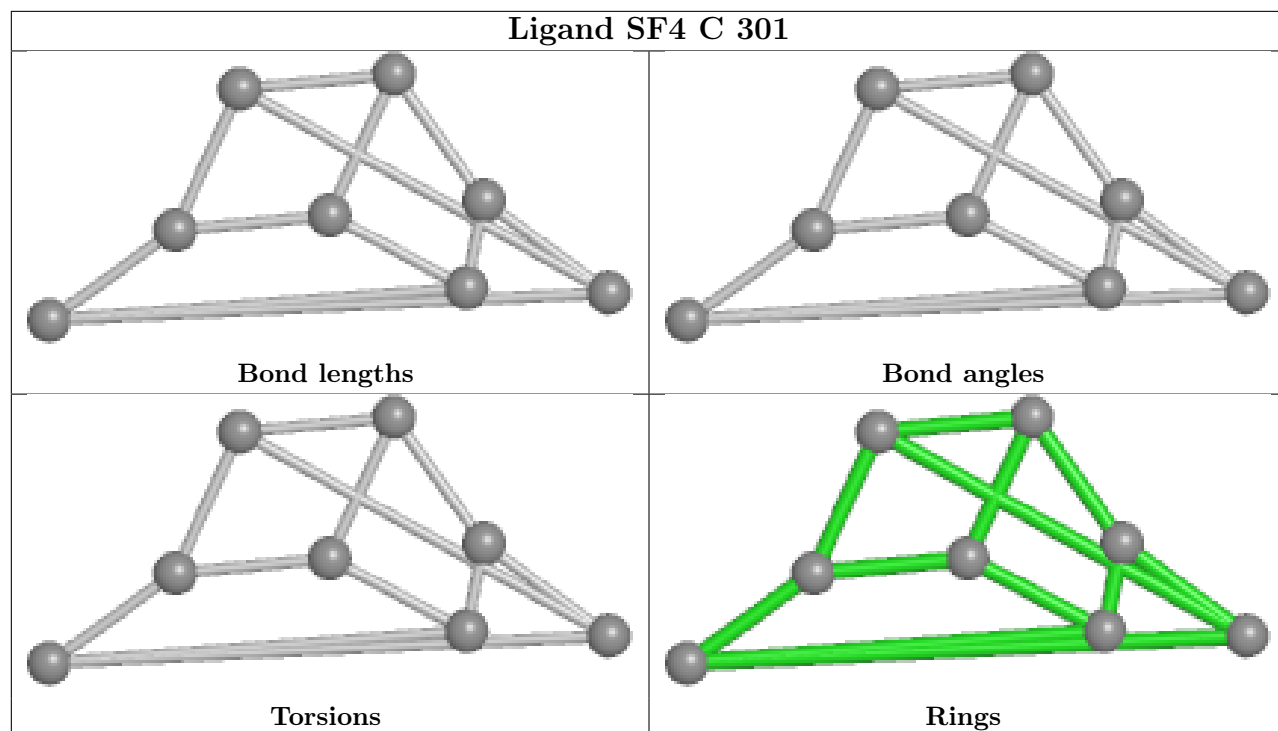
## Ligand CDL V 203

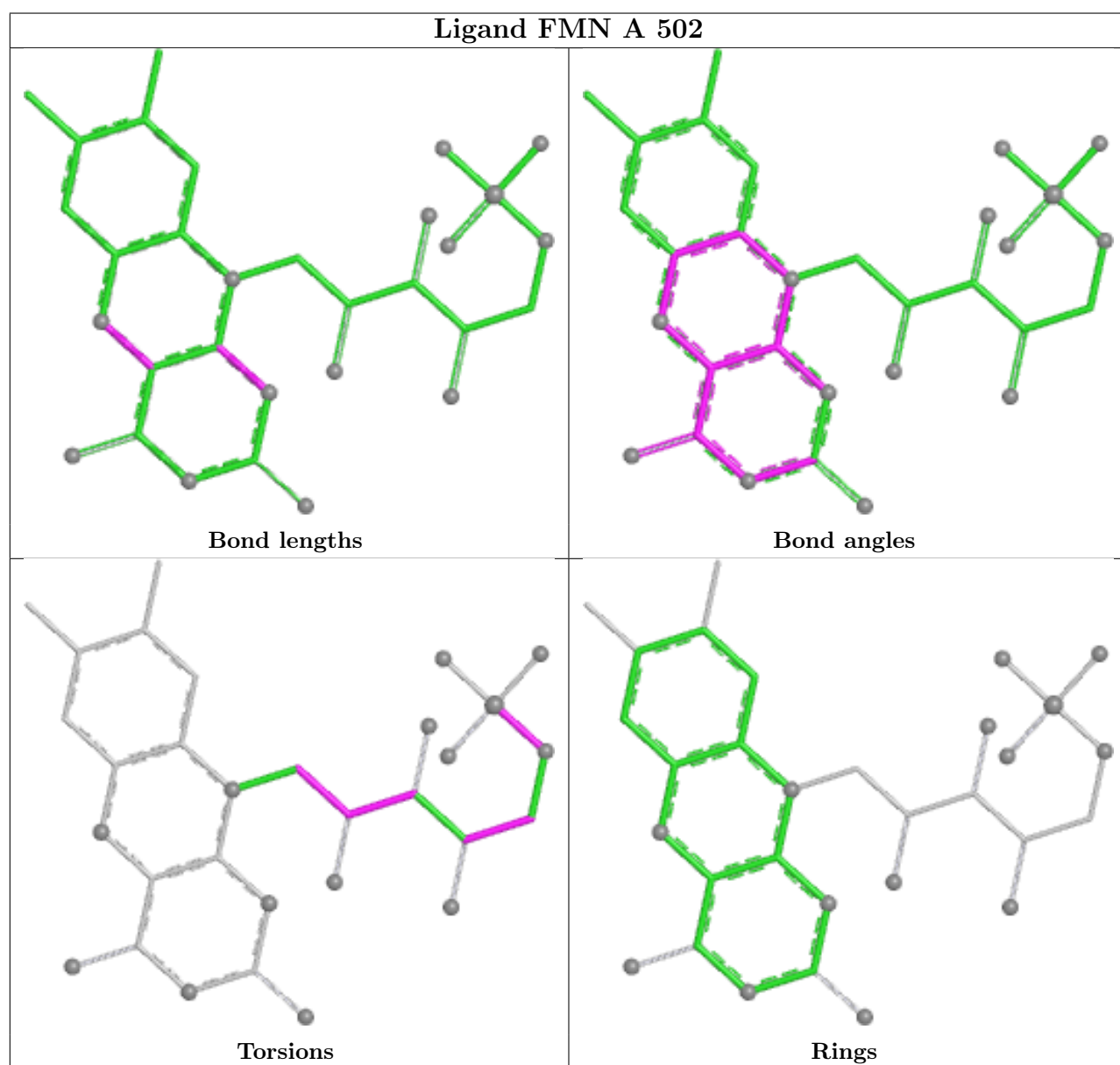
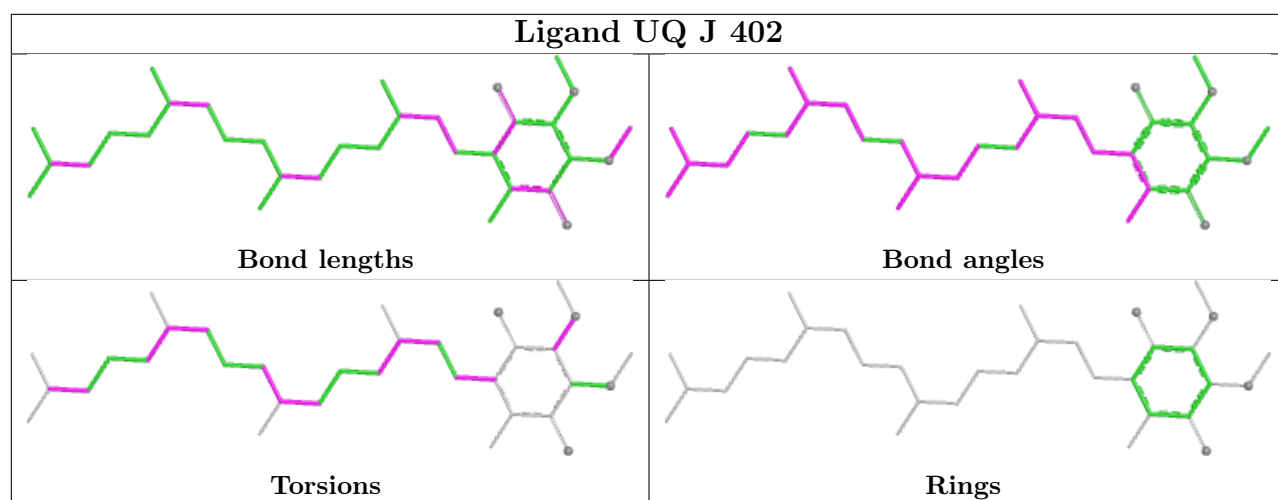


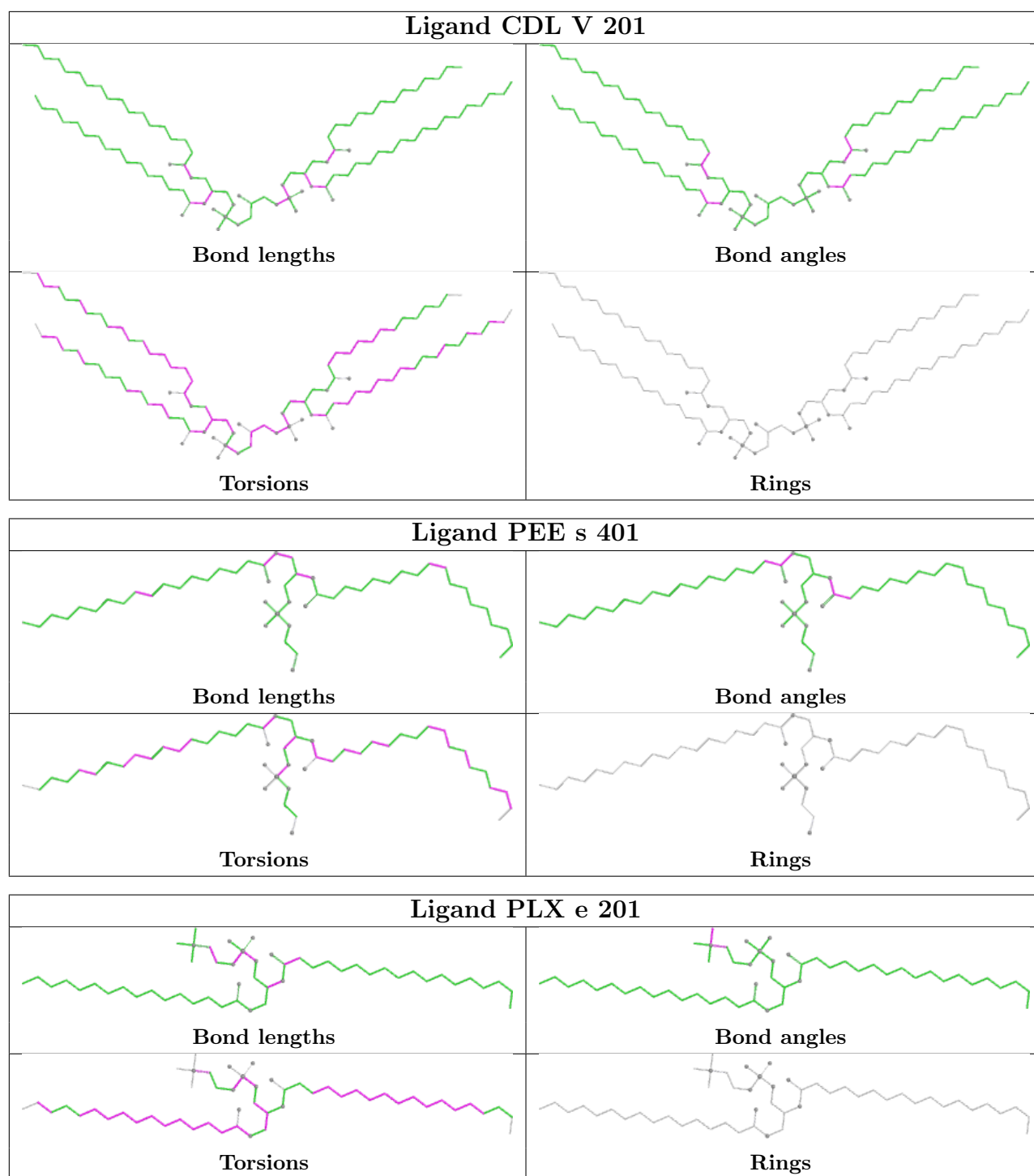




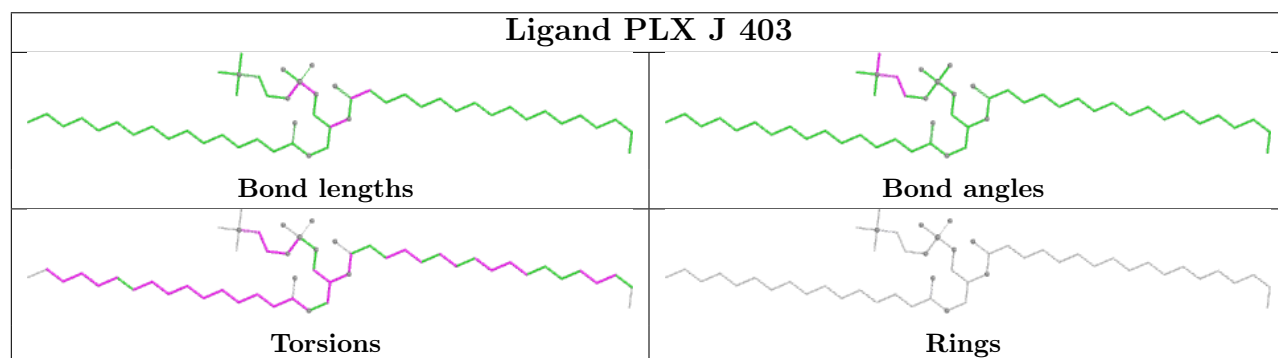
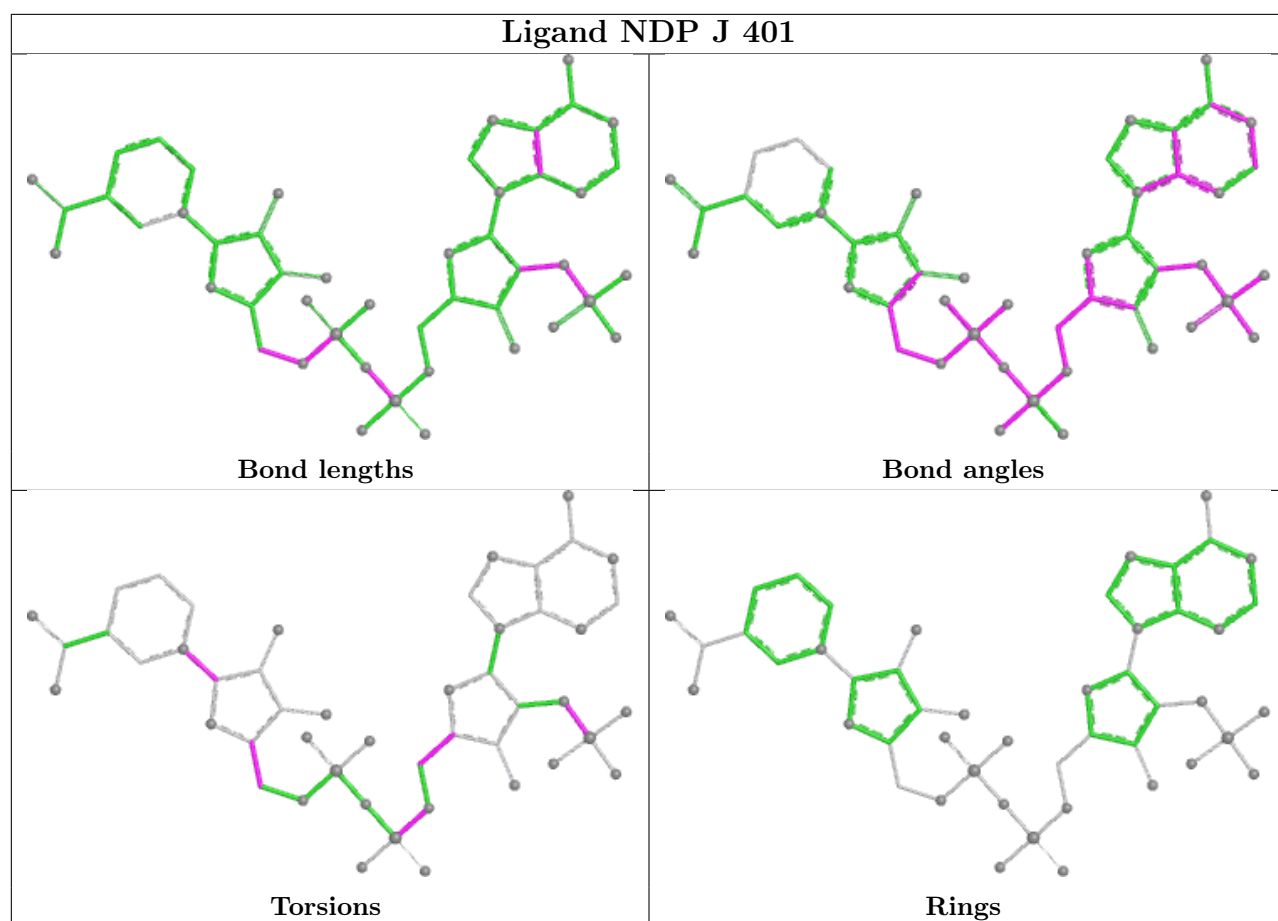


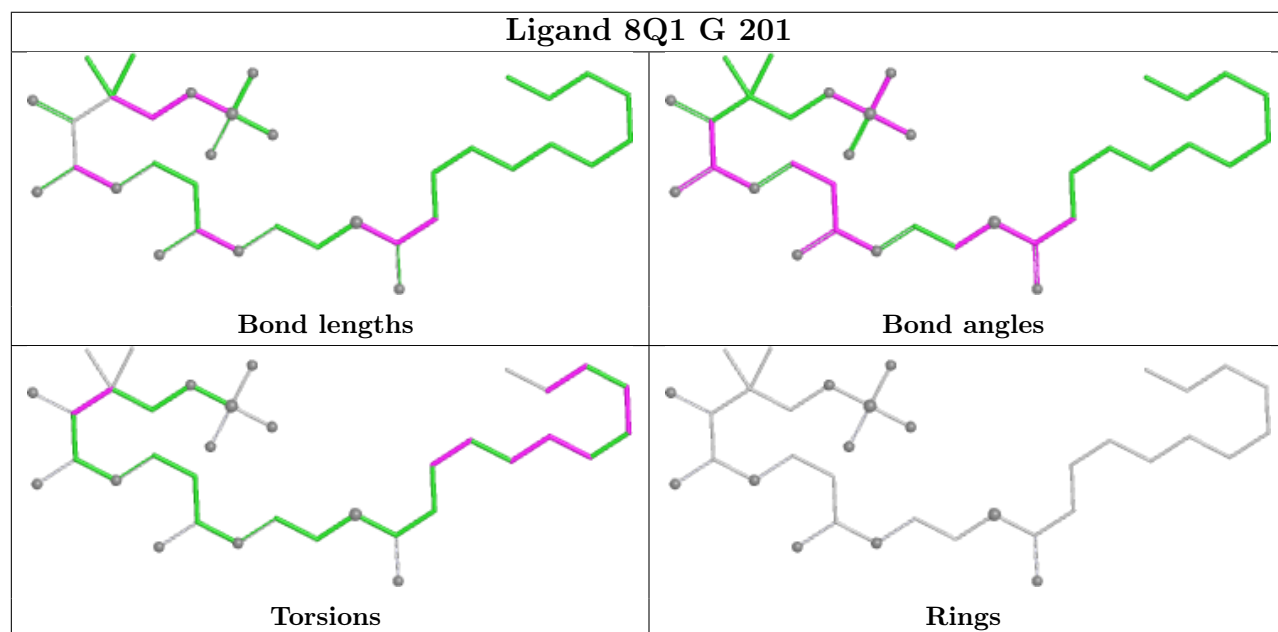
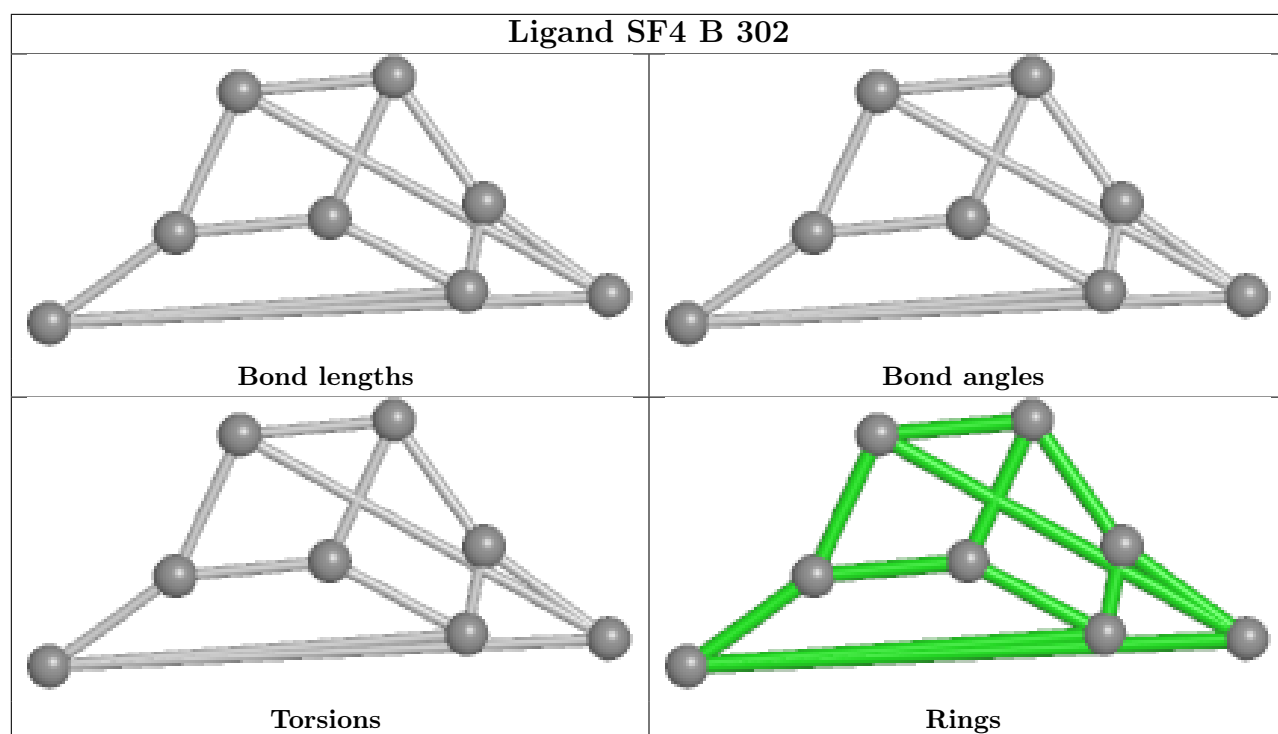


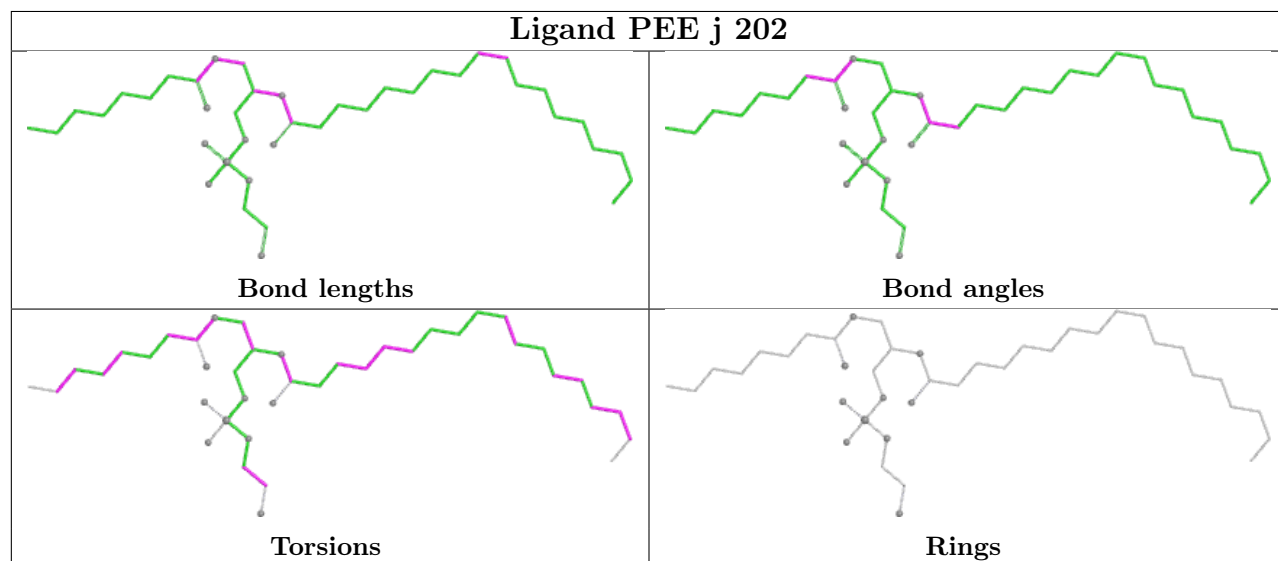
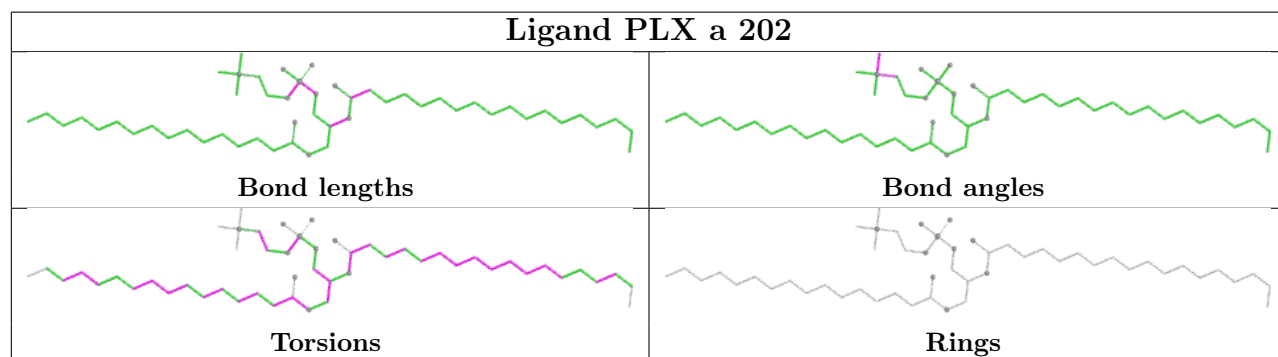
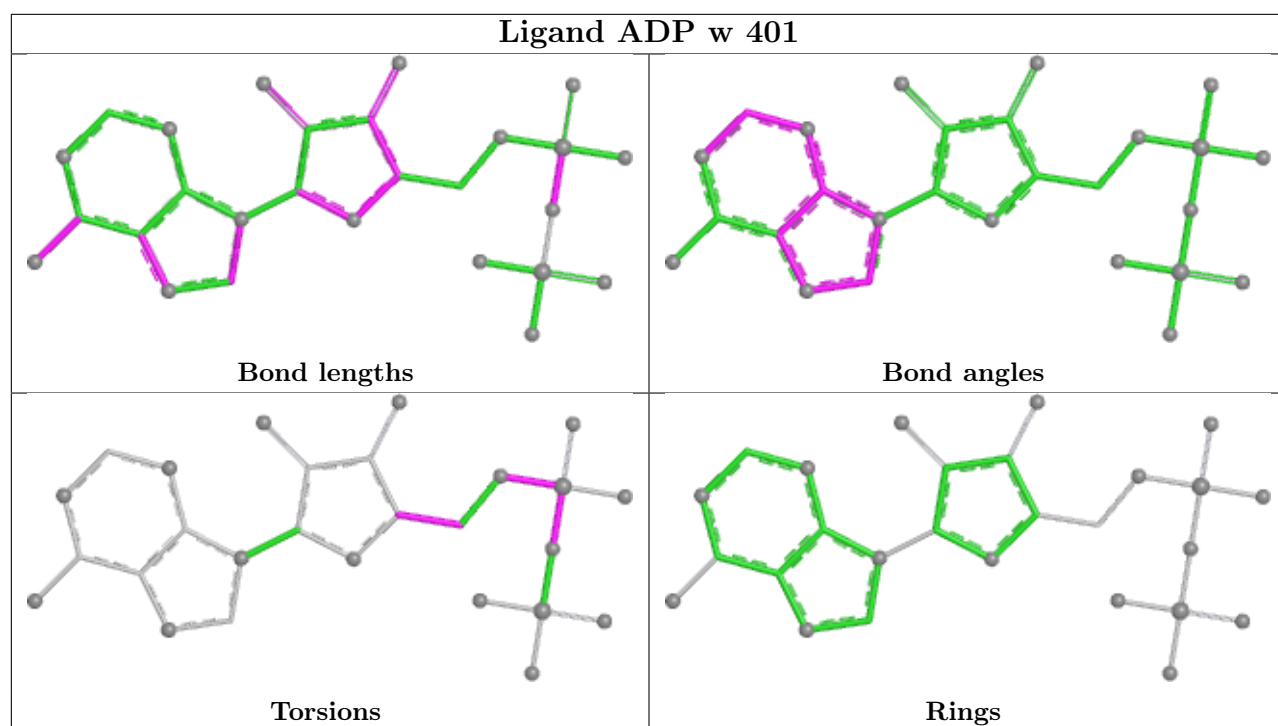


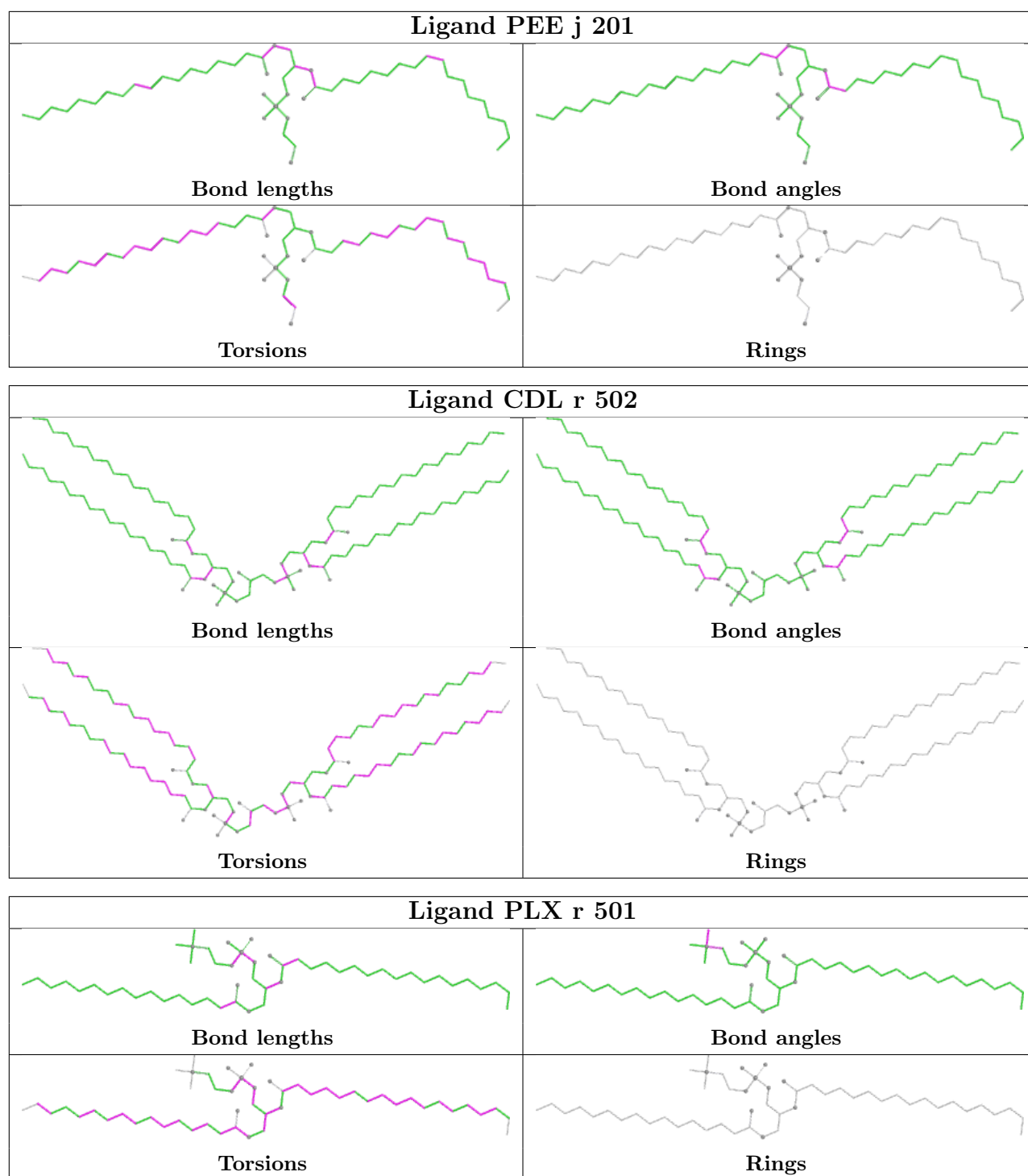












## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

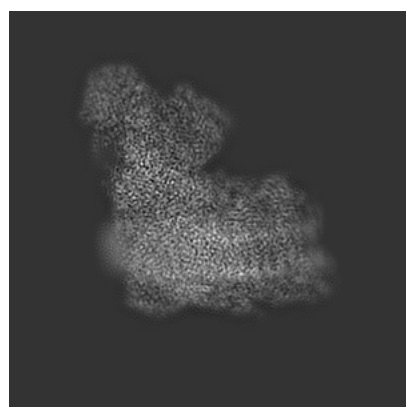
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31647. These allow visual inspection of the internal detail of the map and identification of artifacts.

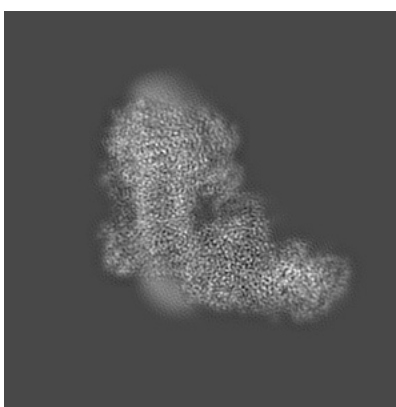
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

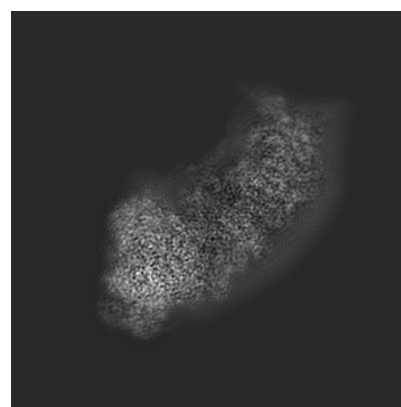
#### 6.1.1 Primary map



X



Y

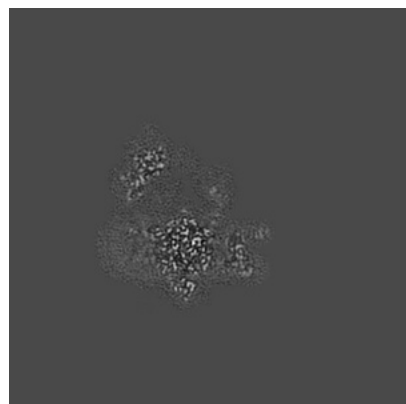


Z

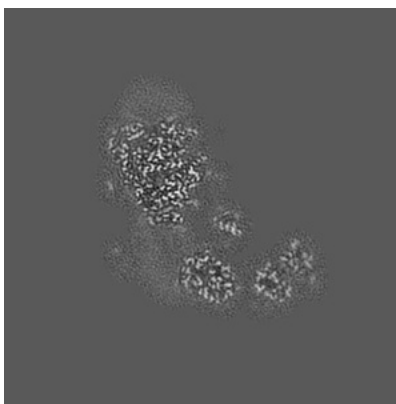
The images above show the map projected in three orthogonal directions.

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

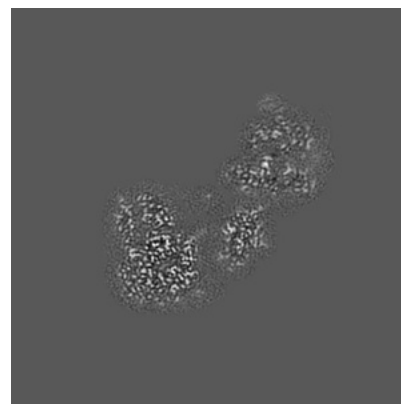
#### 6.2.1 Primary map



X Index: 152



Y Index: 152

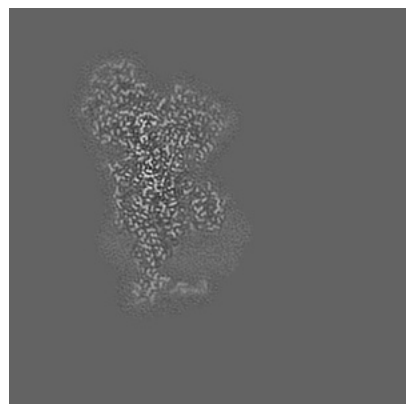


Z Index: 152

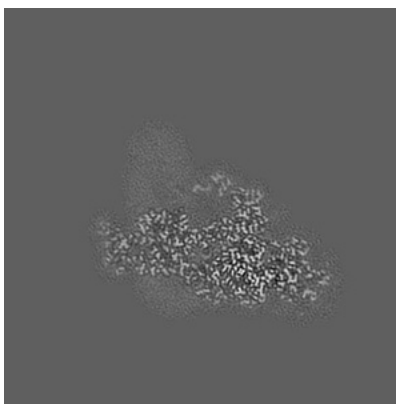
The images above show central slices of the map in three orthogonal directions.

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

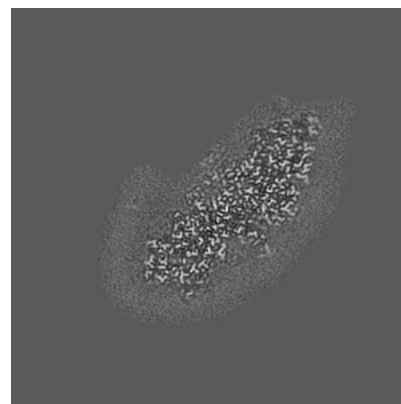
### 6.3.1 Primary map



X Index: 105



Y Index: 106

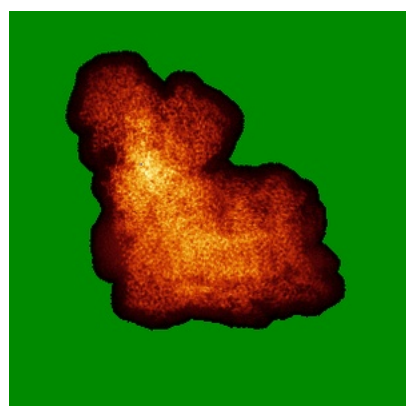


Z Index: 130

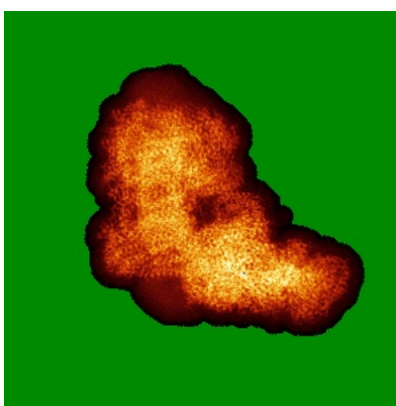
The images above show the largest variance slices of the map in three orthogonal directions.

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

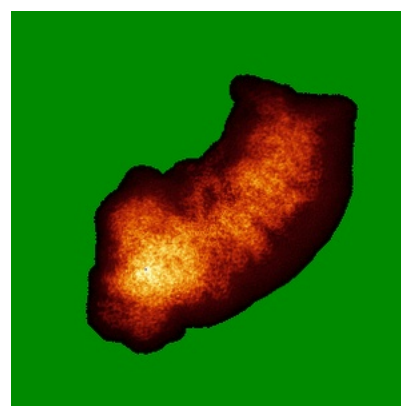
### 6.4.1 Primary map



X



Y

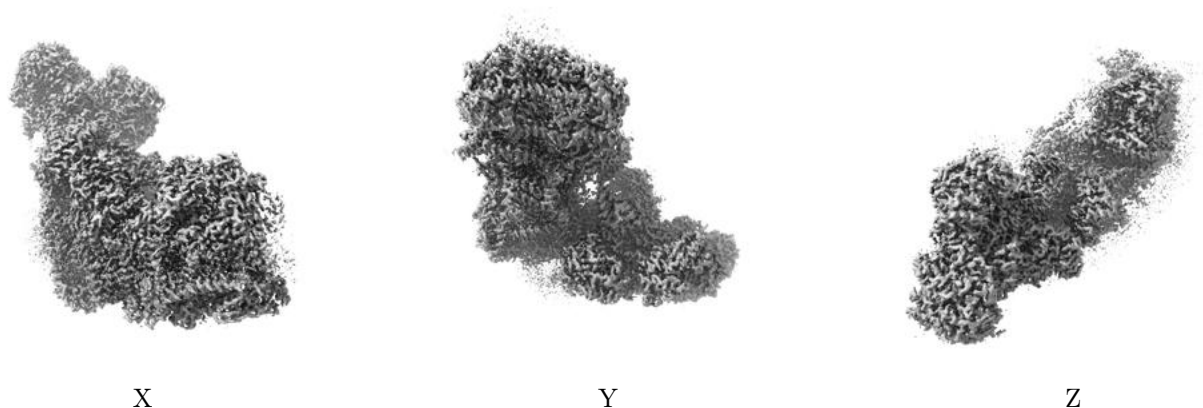


Z

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 0.027. 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](#)

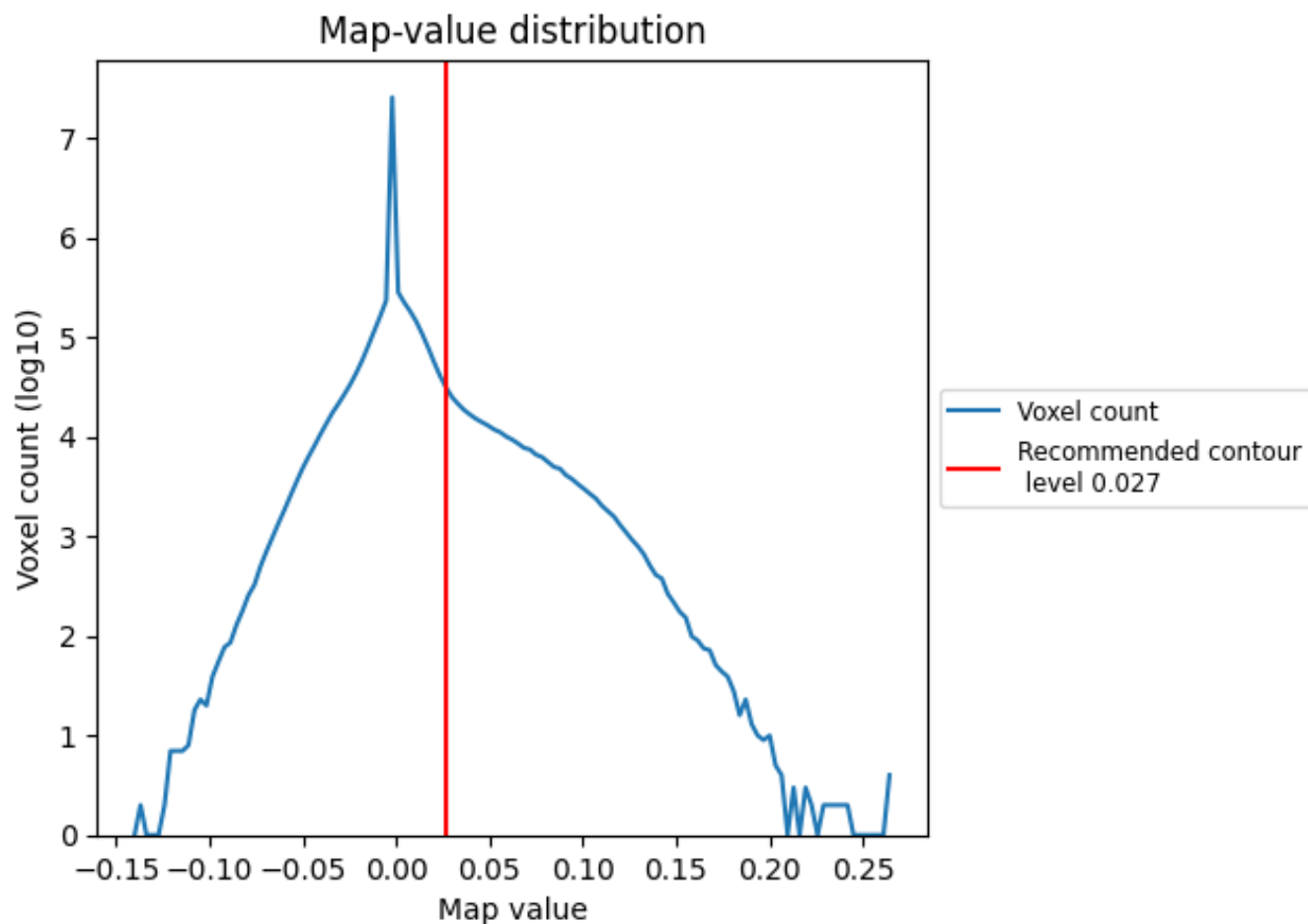
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

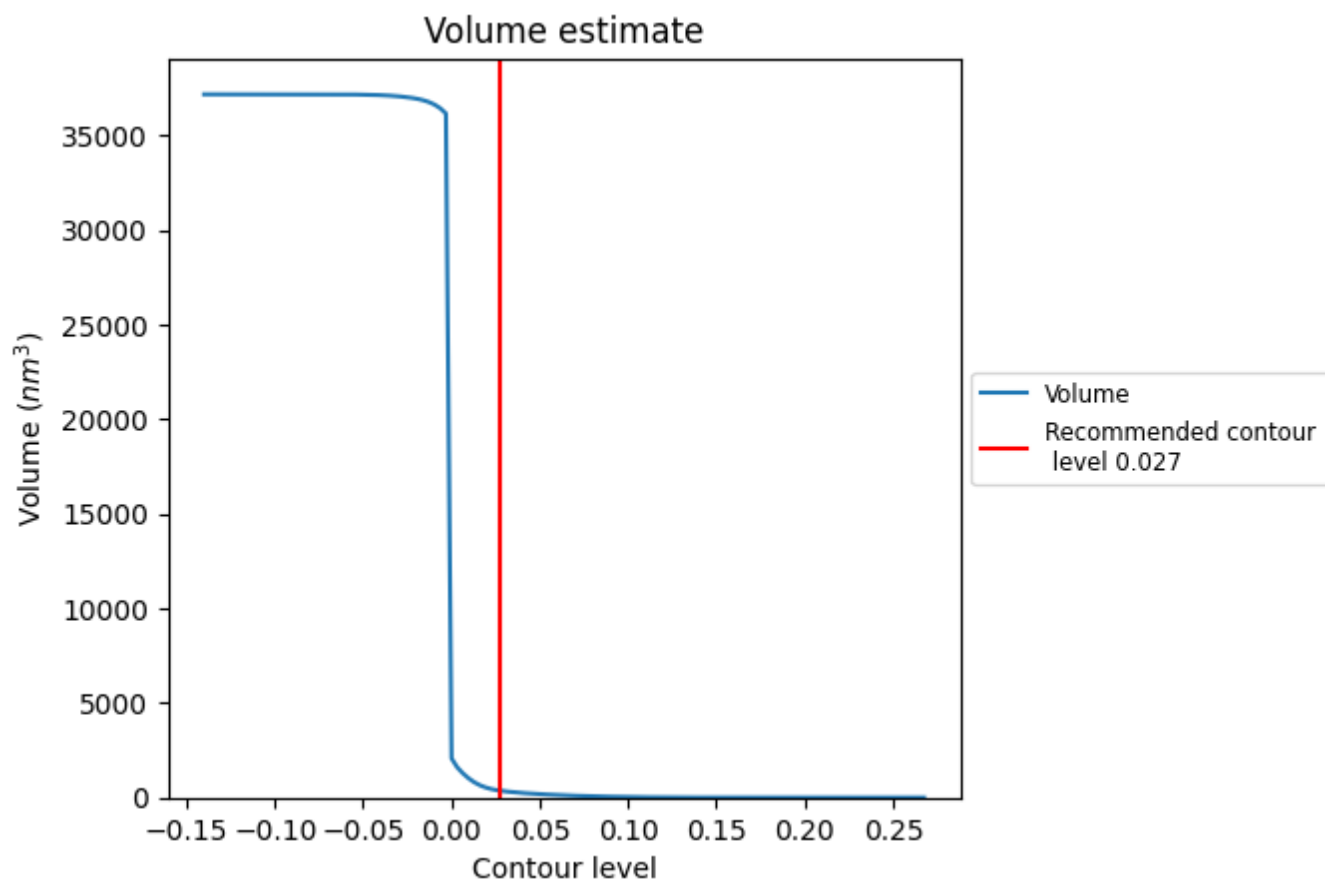
This section contains the results of statistical analysis of the map.

### 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.

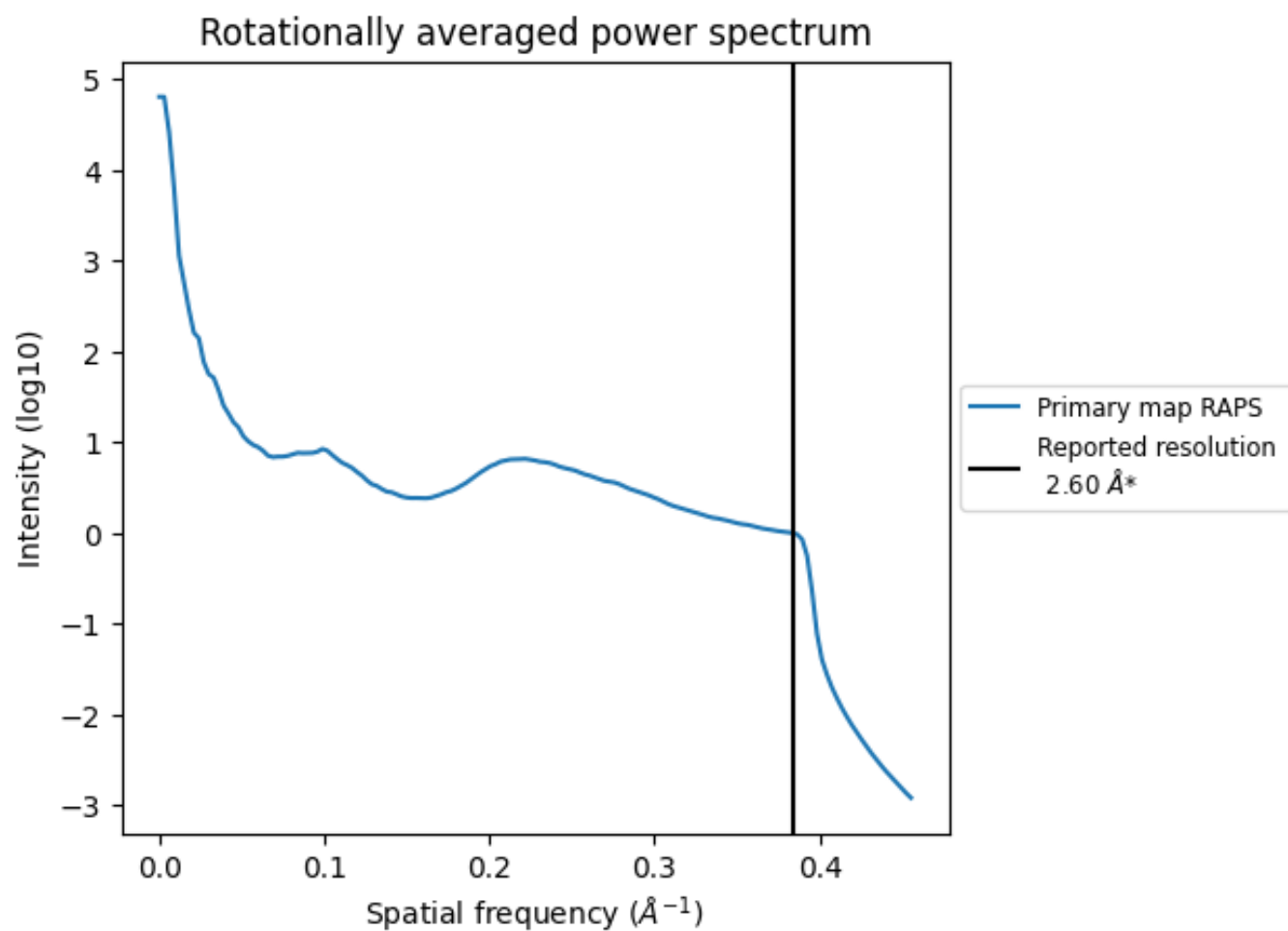
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 373 nm<sup>3</sup>; this corresponds to an approximate mass of 337 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 0.385 Å<sup>-1</sup>

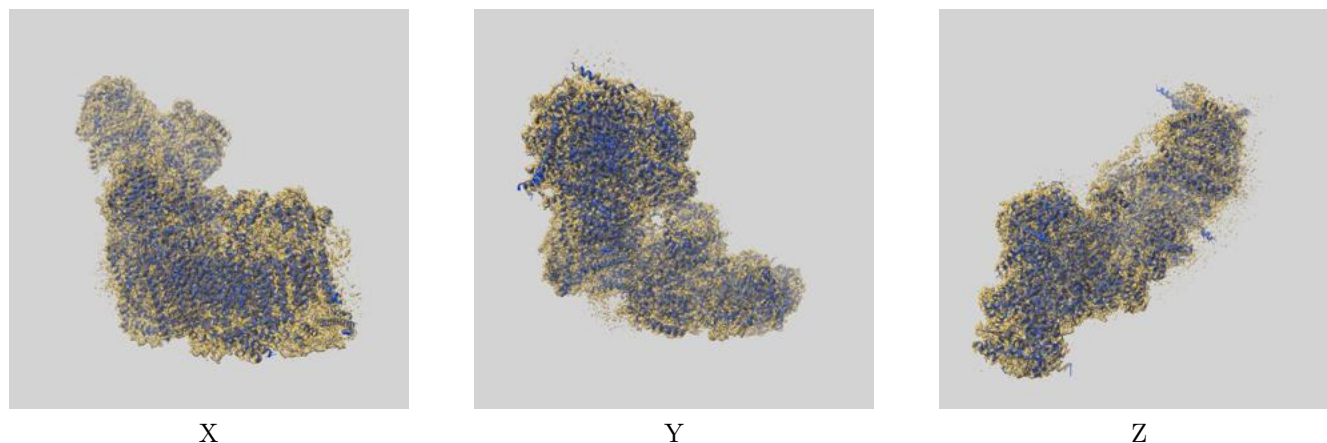
## 8 Fourier-Shell correlation ⓘ

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

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

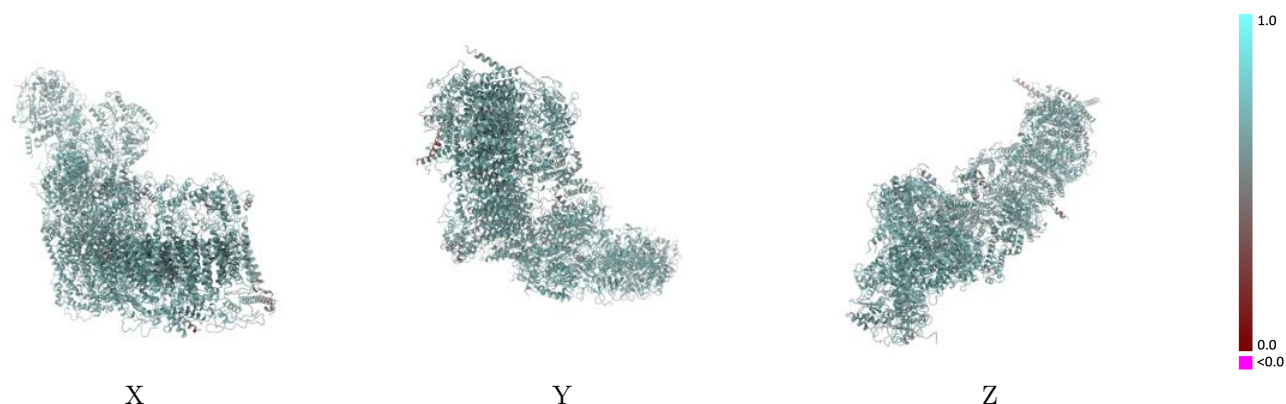
This section contains information regarding the fit between EMDB map EMD-31647 and PDB model 7V2R. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



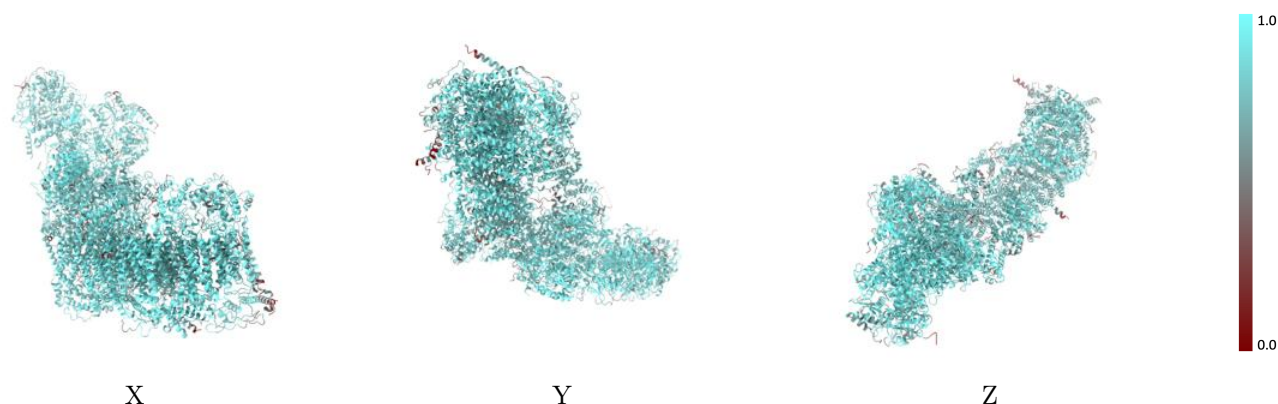
The images above show the 3D surface view of the map at the recommended contour level 0.027 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



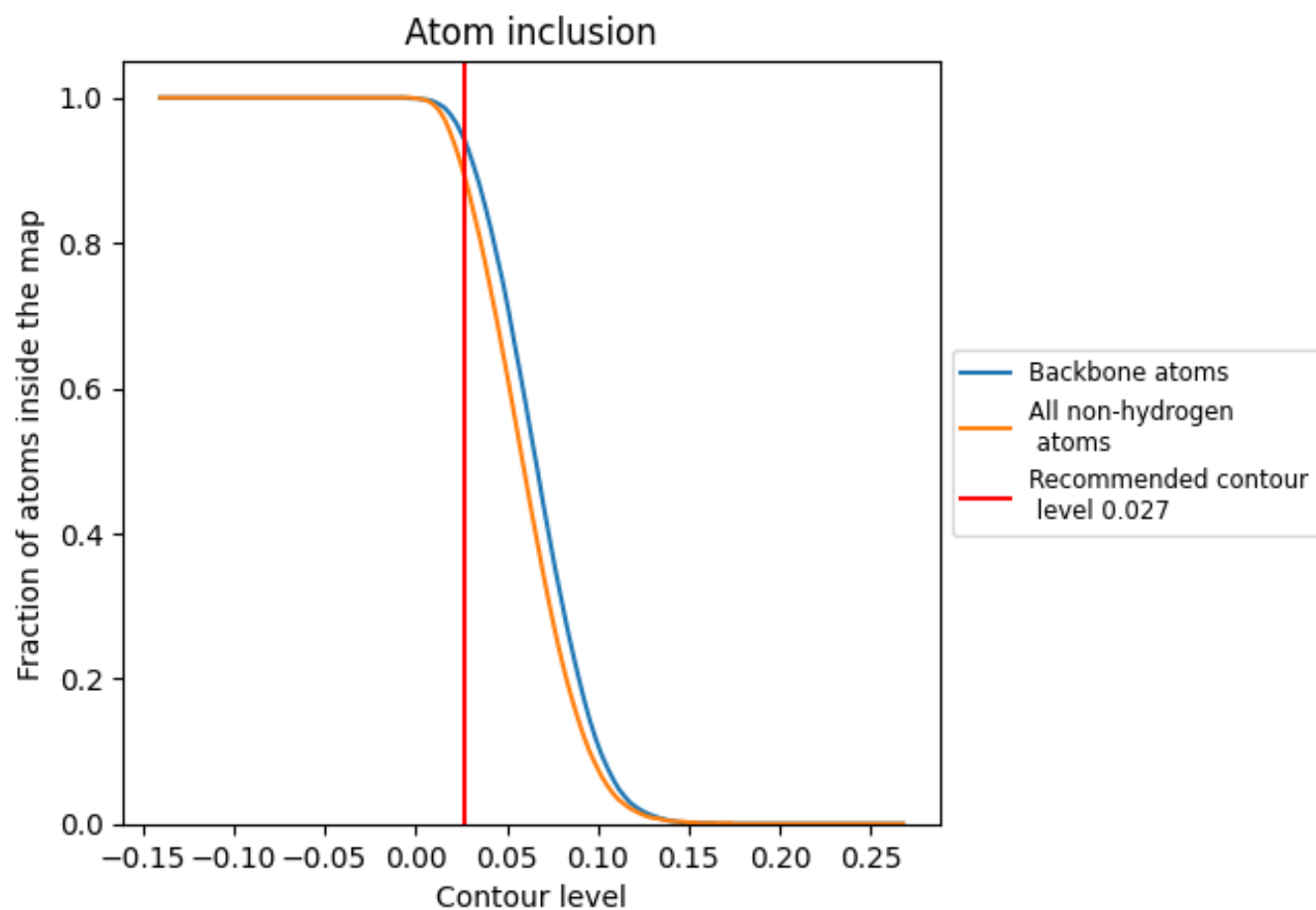
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.027) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8910   |  0.6460   |
| A     |  0.8620   |  0.6190   |
| B     |  0.9710   |  0.6880   |
| C     |  0.9430   |  0.6830   |
| E     |  0.9110   |  0.6600   |
| F     |  0.7770   |  0.5920   |
| G     |  0.6810   |  0.5480   |
| H     |  0.8820   |  0.6310   |
| I     |  0.8670   |  0.6370   |
| J     |  0.8920   |  0.6530   |
| K     |  0.8030   |  0.6010   |
| L     |  0.9070   |  0.6690   |
| M     |  0.9180   |  0.6510   |
| N     |  0.9150   |  0.6660   |
| O     |  0.8270  |  0.6090  |
| P     |  0.9700 |  0.6870 |
| Q     |  0.9600 |  0.6830 |
| S     |  0.9370 |  0.6600 |
| T     |  0.9170 |  0.6600 |
| U     |  0.8790 |  0.6390 |
| V     |  0.8070 |  0.6320 |
| W     |  0.8860 |  0.6290 |
| X     |  0.7850 |  0.6030 |
| Y     |  0.7360 |  0.5760 |
| Z     |  0.6740 |  0.5620 |
| a     |  0.8820 |  0.6560 |
| b     |  0.8090 |  0.6090 |
| c     |  0.8690 |  0.6370 |
| d     |  0.8540 |  0.6290 |
| e     |  0.8140 |  0.6180 |
| f     |  0.7380 |  0.5740 |
| g     |  0.9110 |  0.6560 |
| h     |  0.8690 |  0.6360 |
| i     |  0.9750 |  0.6830 |
| j     |  0.9050 |  0.6700 |



*Continued on next page...*



*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| k     |  0.9340 |  0.6740 |
| l     |  0.9000 |  0.6500 |
| m     |  0.8490 |  0.6280 |
| n     |  0.7760 |  0.5930 |
| o     |  0.8810 |  0.6450 |
| p     |  0.8710 |  0.6330 |
| r     |  0.9640 |  0.6740 |
| s     |  0.9750 |  0.6800 |
| u     |  0.8750 |  0.6300 |
| v     |  0.7230 |  0.5700 |
| w     |  0.8610 |  0.6290 |