



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 09:20 AM UTC

PDB ID : 7V2F / pdb\_00007v2f  
EMDB ID : EMD-31644  
Title : Deactive state complex I from Q10-NADH dataset  
Authors : Gu, J.K.; Yang, M.J.  
Deposited on : 2021-08-09  
Resolution : 3.10 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>.

---

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

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

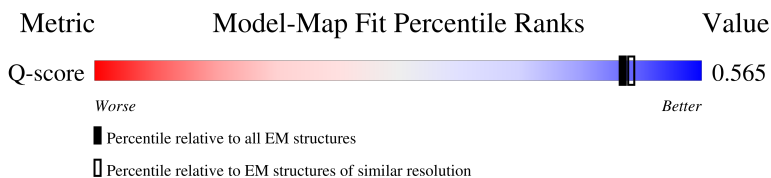
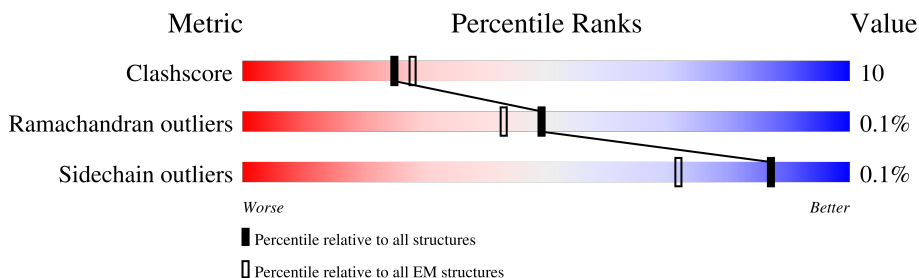
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

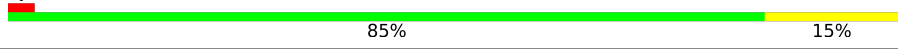
The reported resolution of this entry is 3.10 Å.

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                       | 14724 ( 2.60 - 3.60 )                                    |

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     | 431    |  73%27% |
| 2   | B     | 176    |  78%22% |
| 3   | C     | 156    |  83%17% |
| 4   | E     | 115    |  85%15% |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | F     | 86     |                  |
| 6   | G     | 88     |                  |
| 6   | X     | 88     |                  |
| 7   | H     | 112    |                  |
| 8   | I     | 112    |                  |
| 9   | J     | 341    |                  |
| 10  | K     | 42     |                  |
| 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     | 70     |                  |
| 23  | Z     | 84     |                  |
| 24  | a     | 140    |                  |
| 25  | b     | 126    |                  |
| 26  | c     | 156    |                  |
| 27  | d     | 175    |                  |
| 28  | e     | 107    |                  |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | f     | 42     |                  |
| 30  | g     | 121    |                  |
| 31  | h     | 105    |                  |
| 32  | i     | 347    |                  |
| 33  | j     | 113    |                  |
| 34  | k     | 98     |                  |
| 35  | l     | 603    |                  |
| 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       | -                |
| 48  | PEE  | C     | 311 | -         | -        | X       | -                |
| 48  | PEE  | V     | 202 | -         | -        | X       | -                |
| 54  | CDL  | l     | 712 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66939 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     | 431      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3318  | 2095 | 591 | 612 | 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     |
|     |       |          | 691   | 434 | 129 | 126 | 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     |
|     |       |          | 699   | 449 | 103 | 142 | 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     | 297      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2359  | 1514 | 421 | 416 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | K     | 42       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 355   | 219 | 67 | 68 | 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     | 419      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3377  | 2162 | 578 | 613 | 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     |
|     |       |          | 567   | 364 | 104 | 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     | 70       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 600   | 393 | 98 | 108 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Z     | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 674   | 437 | 116 | 120 | 1 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | a     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1165  | 762 | 199 | 201 | 3 |         |       |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | b     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 879   | 573 | 158 | 147 | 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     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 568 | 145 | 173 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 29  | f     | 42       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 342   | 225 | 58 | 59 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | g     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1000  | 650 | 173 | 171 | 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     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 800   | 545 | 118 | 132 | 5 |         |       |

- 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     | 603      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4785  | 3173 | 741 | 820 | 51 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | m     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 951   | 637 | 138 | 168 | 8 |         |       |

- 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     | 303      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2394  | 1607 | 369 | 397 | 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     |
|     |       |          | 1012  | 633 | 188 | 182 | 9 |         |       |

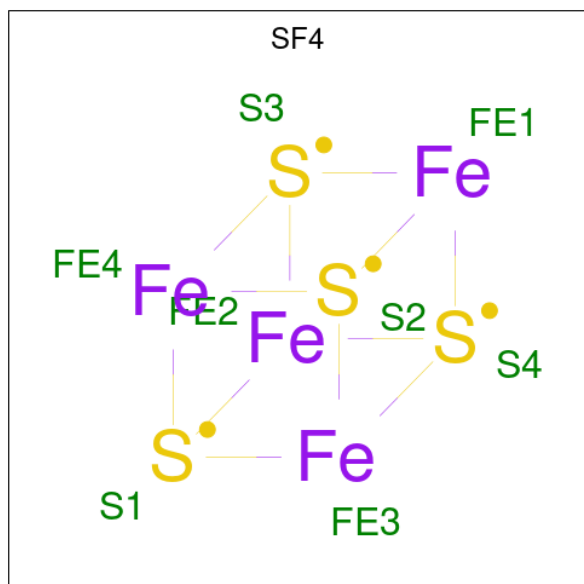
There is a discrepancy between the modelled and reference sequences:

| 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     |
|     |       |          | 2583  | 1646 | 437 | 491 | 9 |         |       |

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



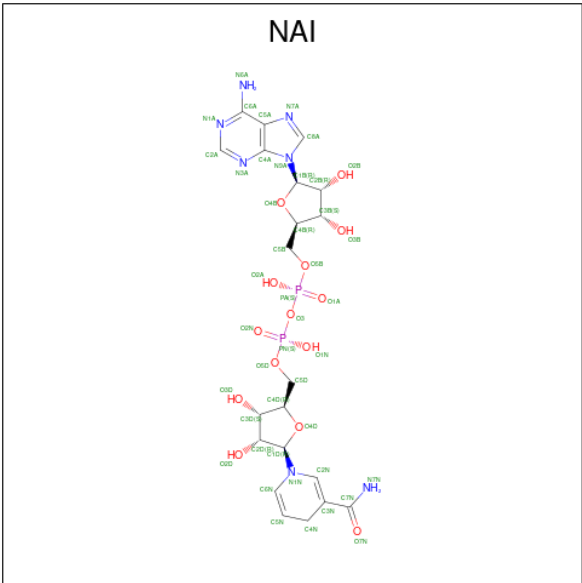
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8  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



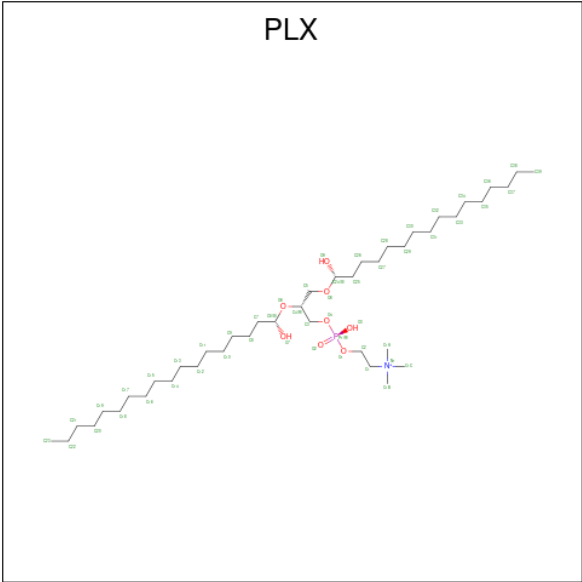
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 47  | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |

- 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).



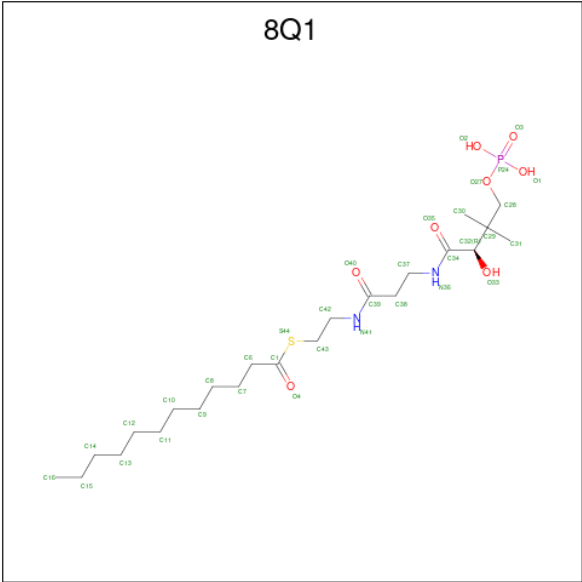
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | U     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 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  | l     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | l     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 48  | l     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 48  | m     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 41    | 31 | 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).



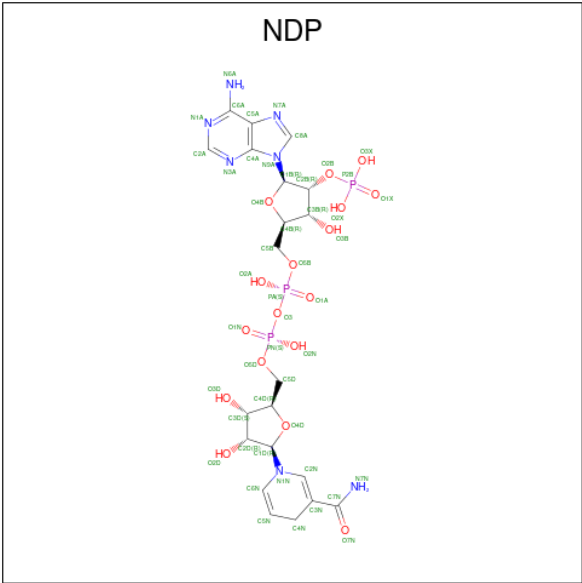
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 49  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | V     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | e     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | i     | 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  | n     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

- Molecule 50 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).



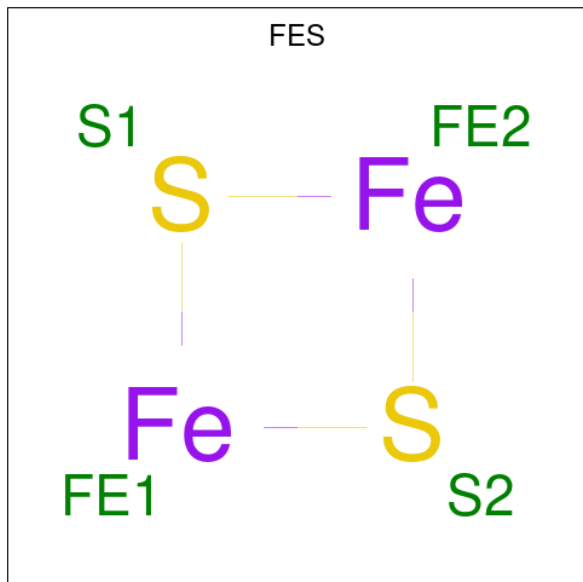
| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 50  | G     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 35    | 23 | 2 | 8 | 1 | 1 |         |
| 50  | X     | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 35    | 23 | 2 | 8 | 1 | 1 |         |

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 51  | J     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

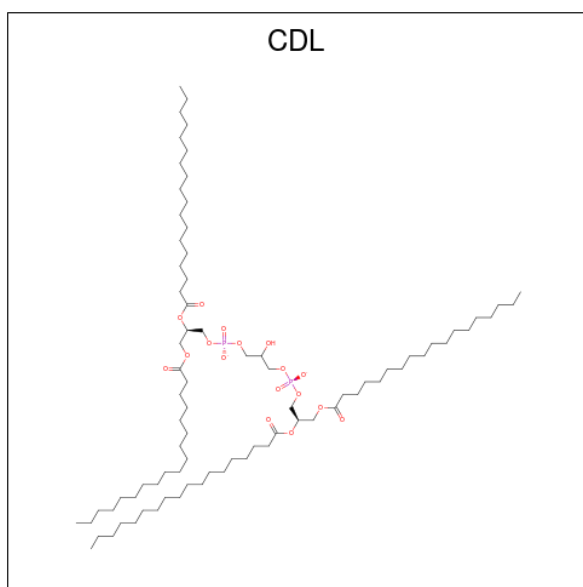


| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 52  | M     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 52  | O     | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 53  | M     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula:  $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).

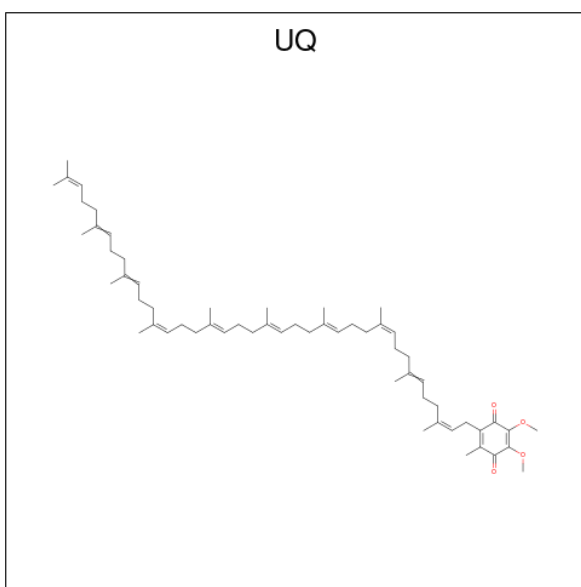


| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 54  | N     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 32 | 17 | 2 |         |
| 54  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 94    | 75 | 17 | 2 |         |
| 54  | V     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 68    | 49 | 17 | 2 |         |
| 54  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 91    | 72 | 17 | 2 |         |
| 54  | i     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 66    | 47 | 17 | 2 |         |
| 54  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 99    | 80 | 17 | 2 |         |
| 54  | l     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 54  | n     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 78    | 59 | 17 | 2 |         |
| 54  | r     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 97    | 78 | 17 | 2 |         |

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

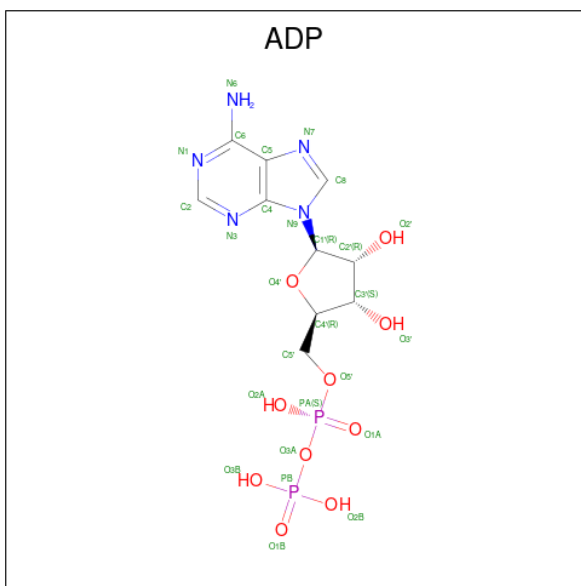
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | T     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 56 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 |
|-----|-------|----------|-------|----|---|---------|
| 56  | s     | 1        | Total | C  | O | 0       |
|     |       |          | 28    | 24 | 4 |         |

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

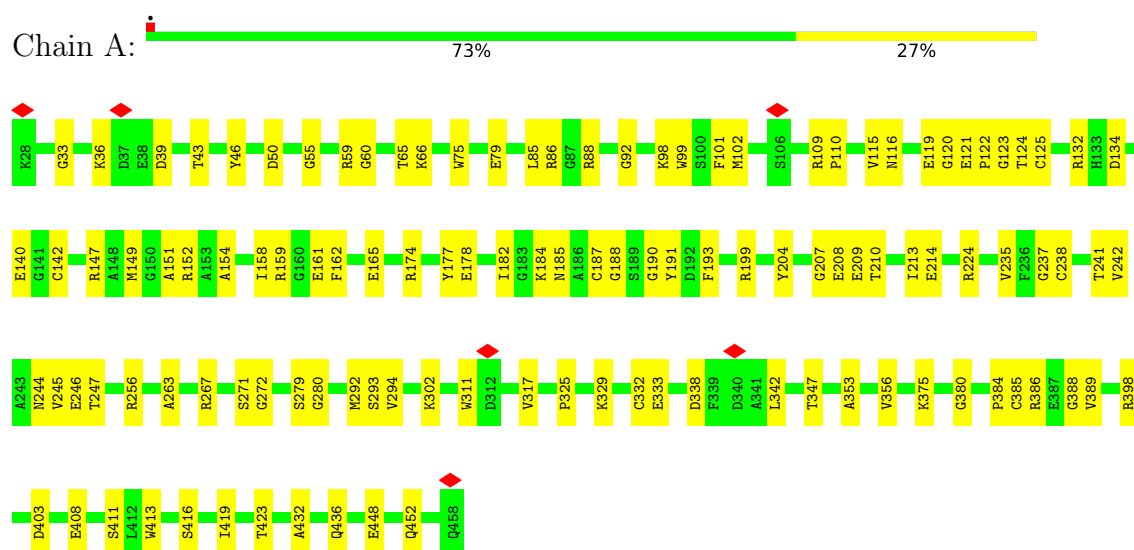


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 57  | w     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

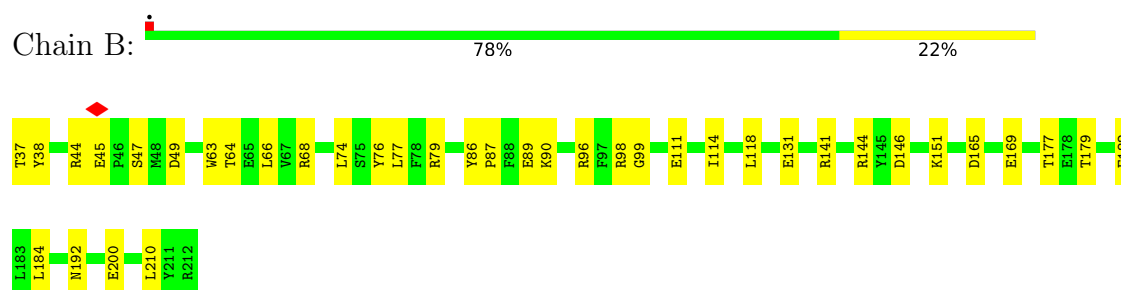
### 3 Residue-property plots

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

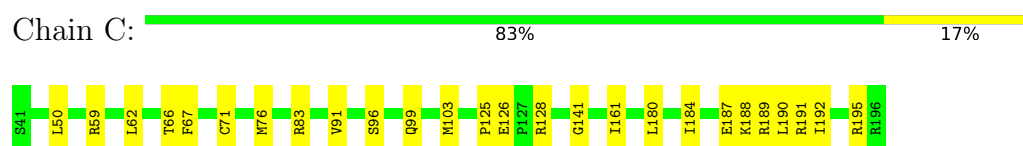
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



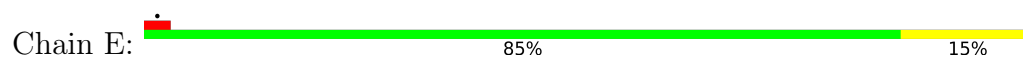
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



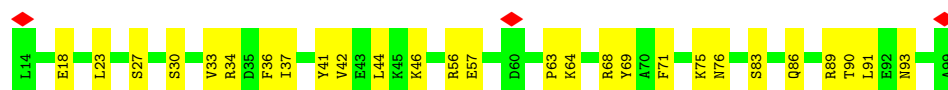
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



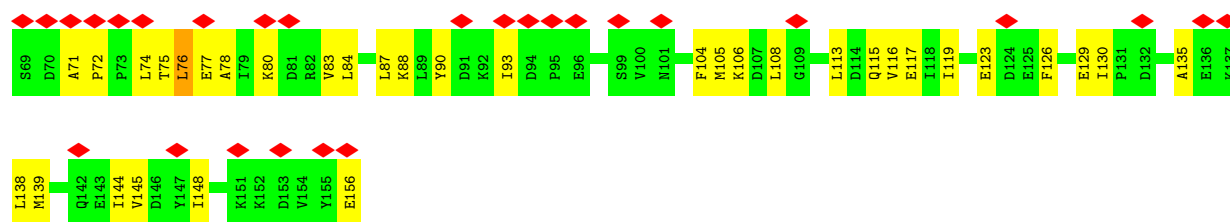
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



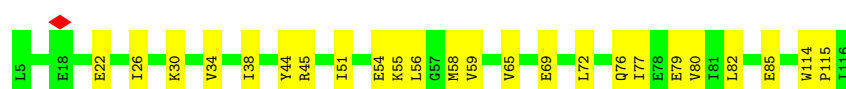
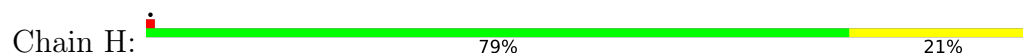
- Molecule 6: Acyl carrier protein, mitochondrial



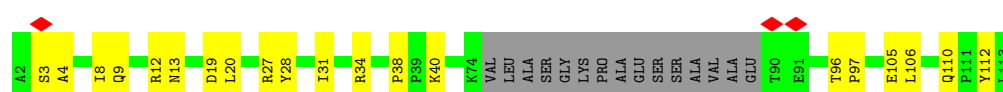
- Molecule 6: Acyl carrier protein, mitochondrial



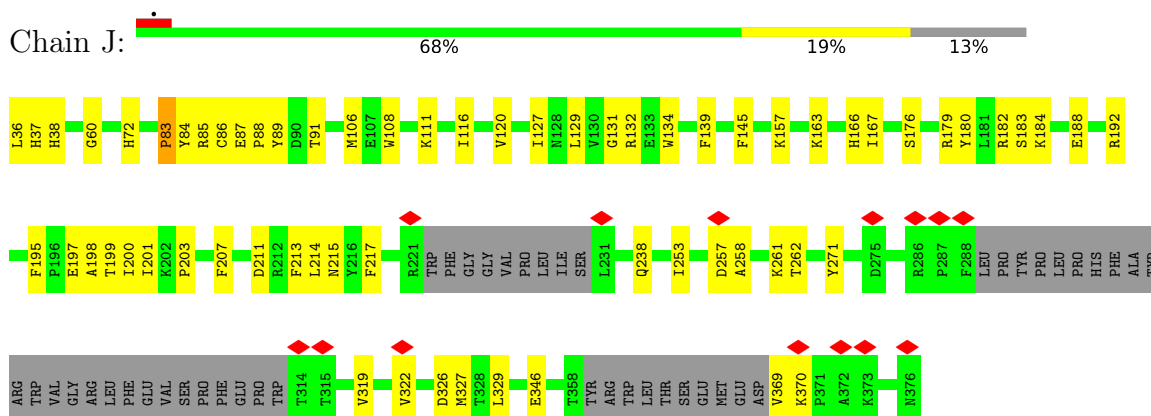
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



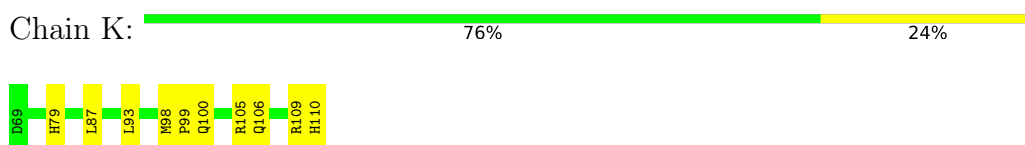
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



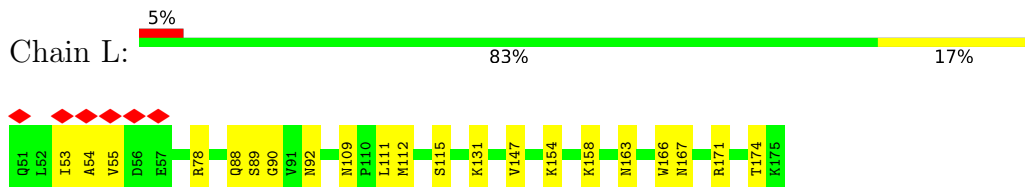
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



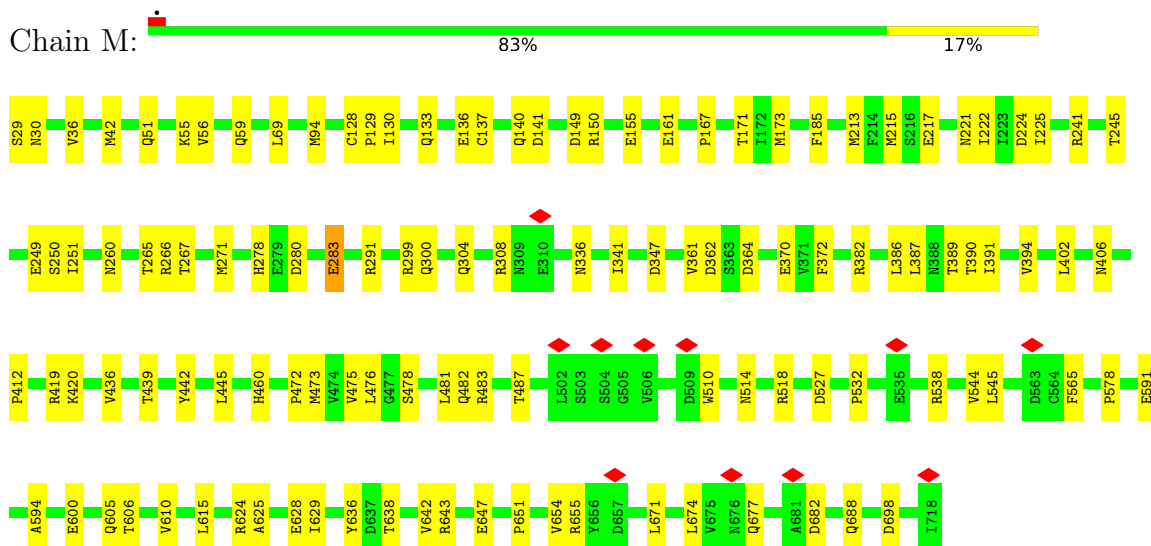
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



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



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

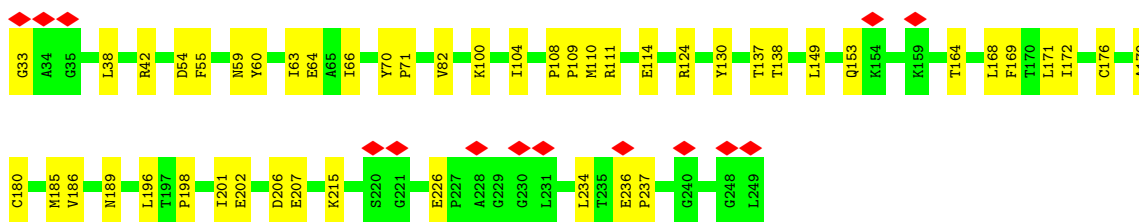
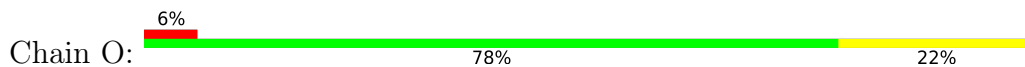


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

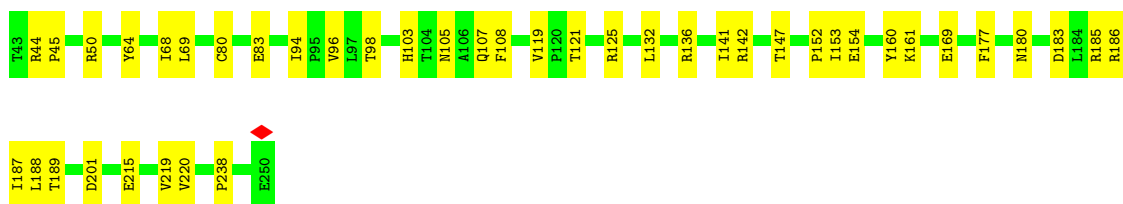
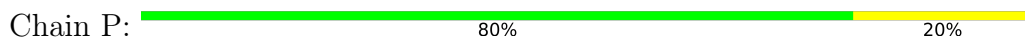




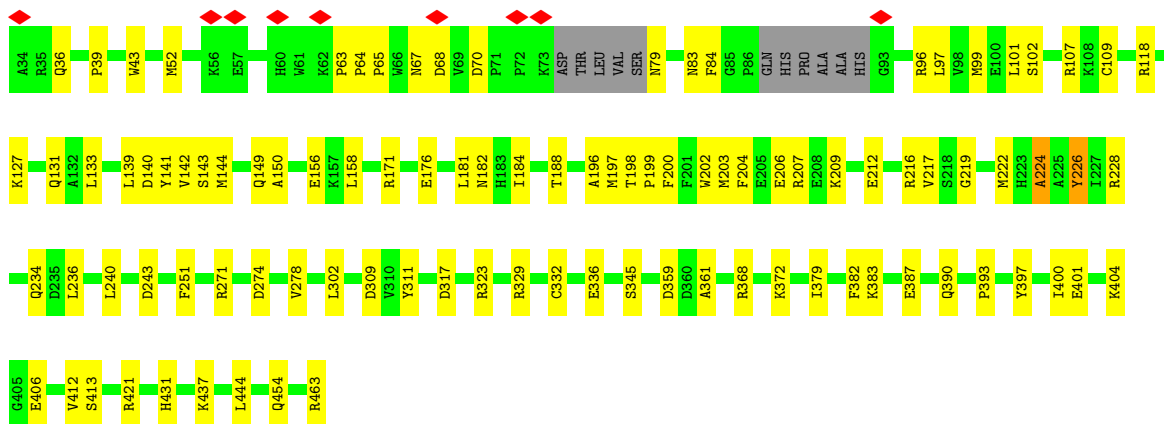
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- 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

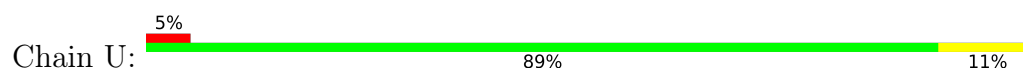




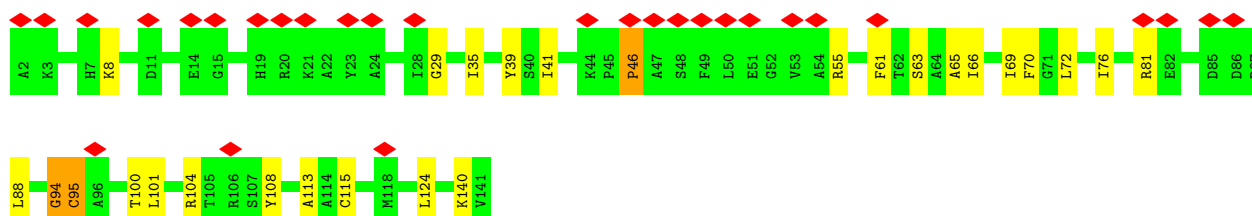
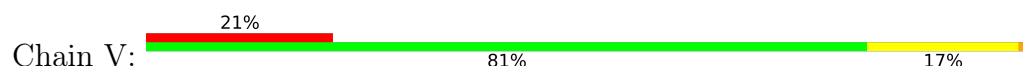
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



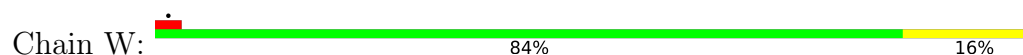
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



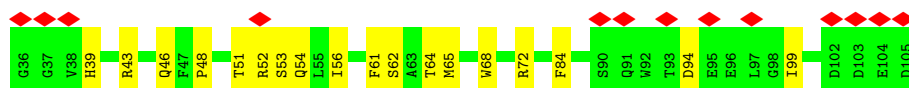
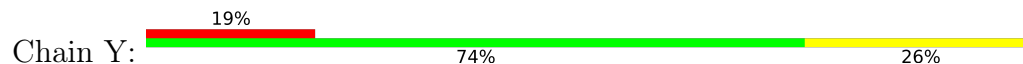
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



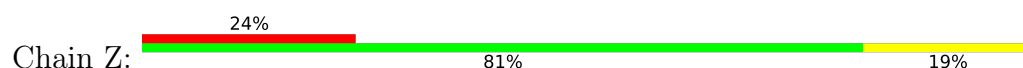
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

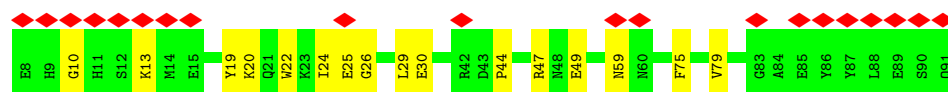


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

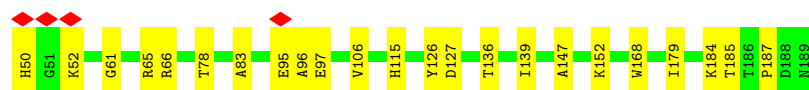
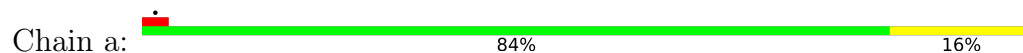


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

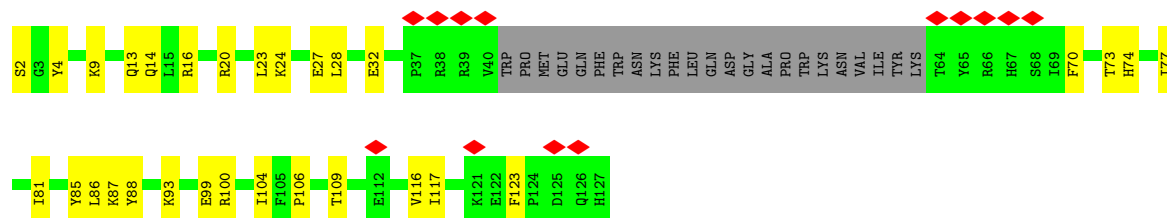




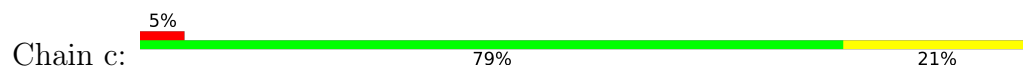
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



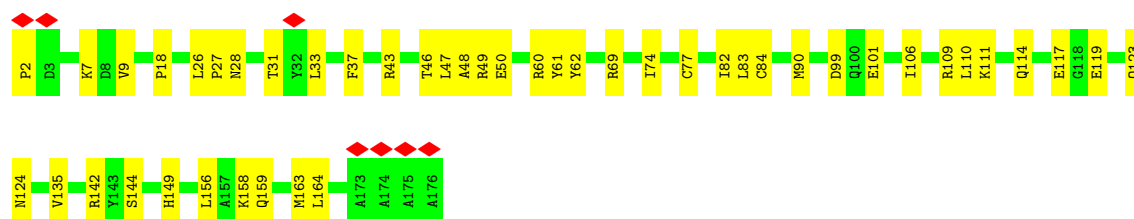
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



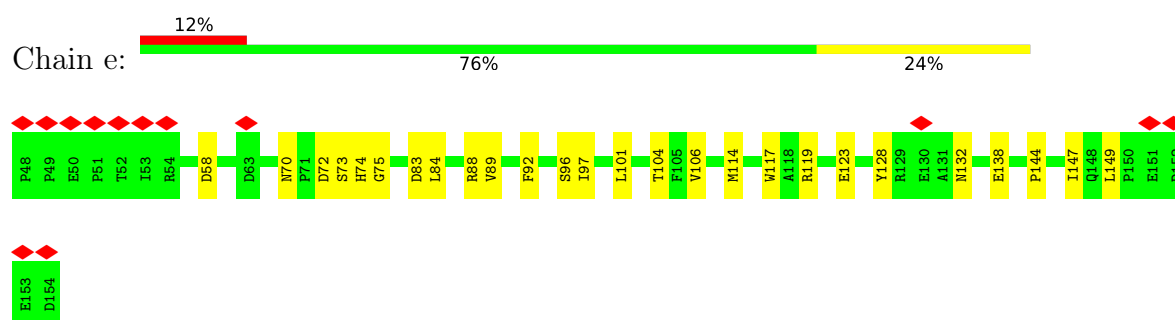
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



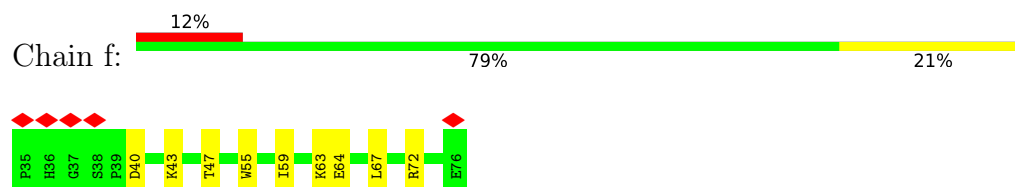
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



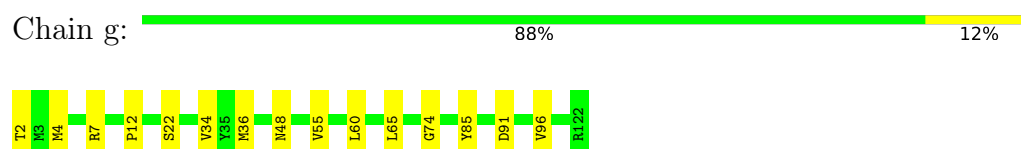
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



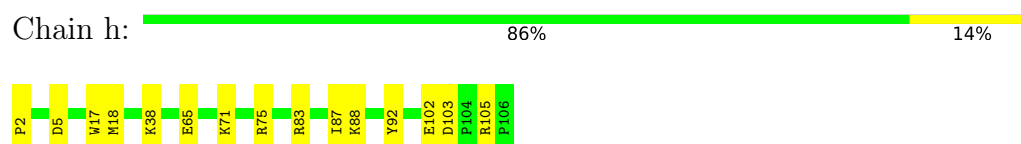
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



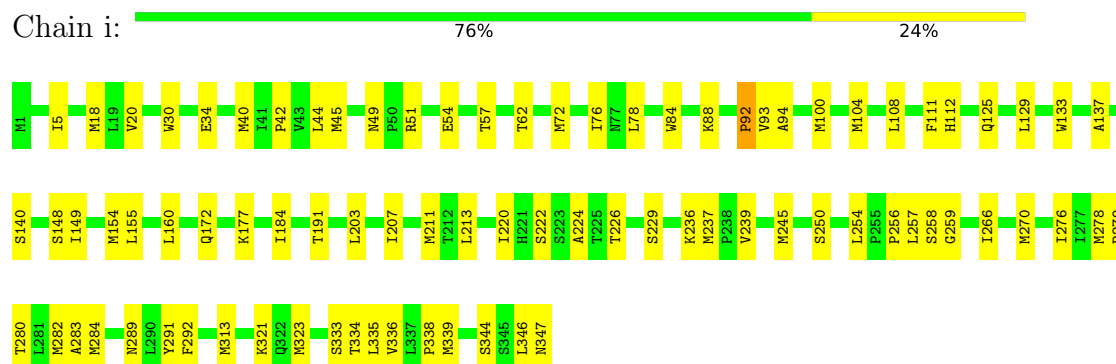
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

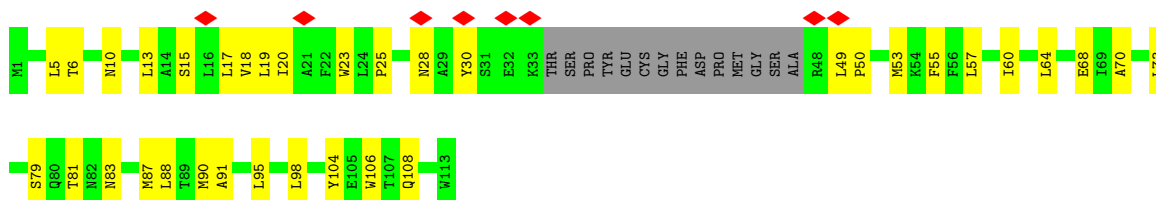


- Molecule 32: NADH-ubiquinone oxidoreductase chain 2

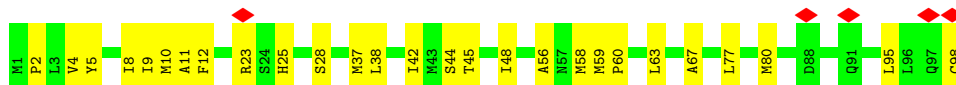


- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

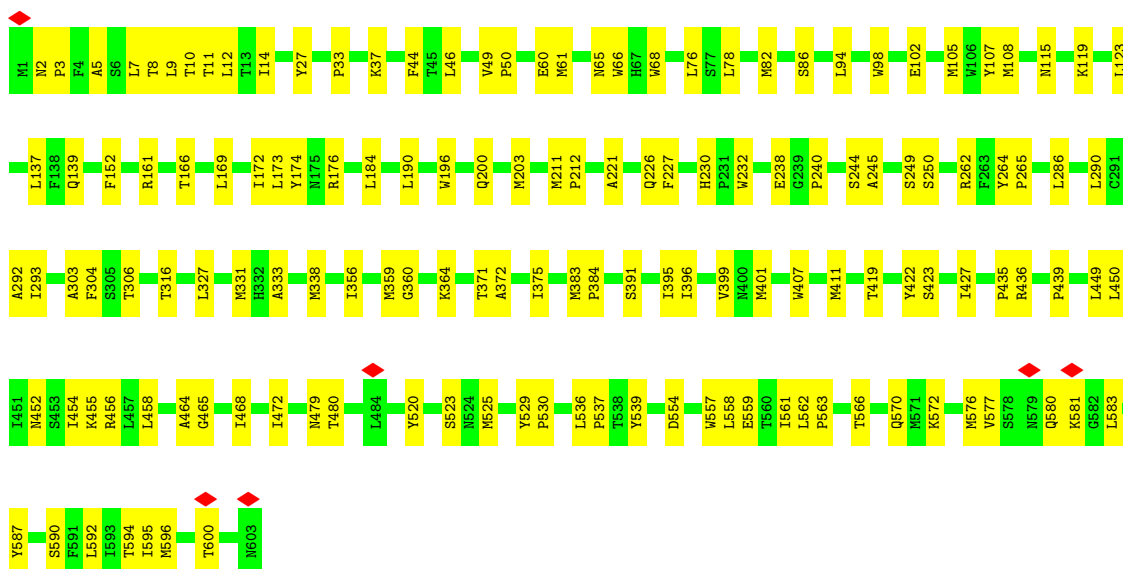
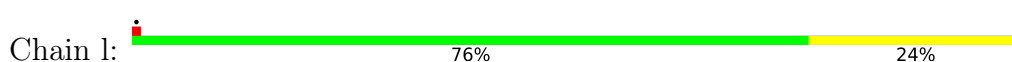




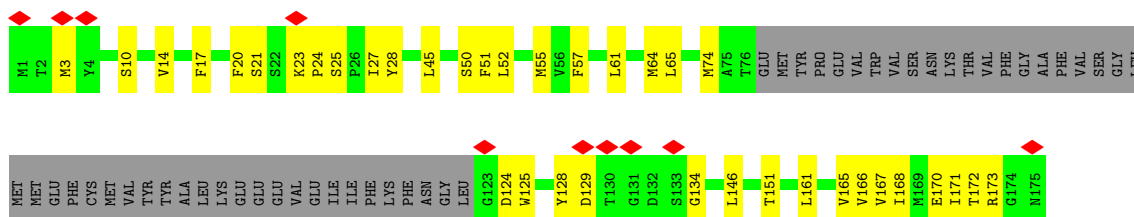
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



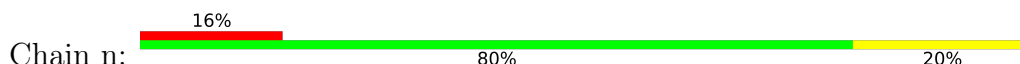
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

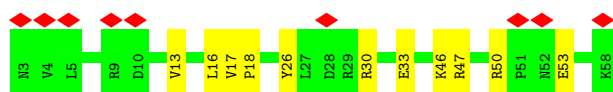


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

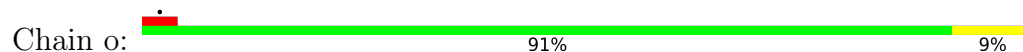


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

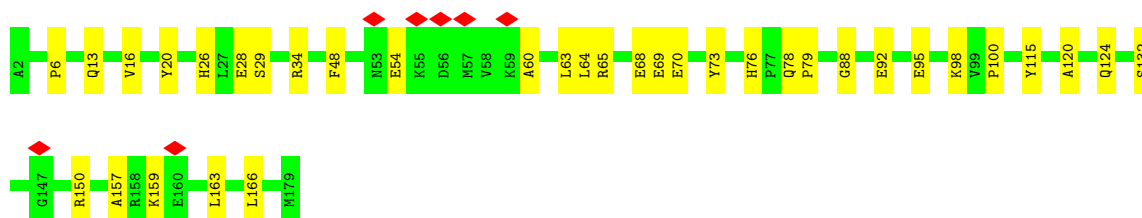
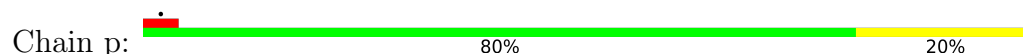




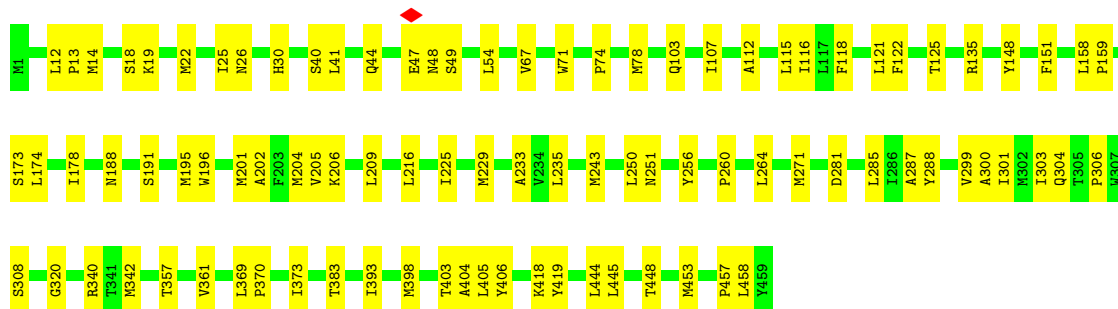
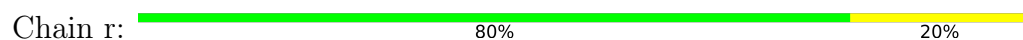
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



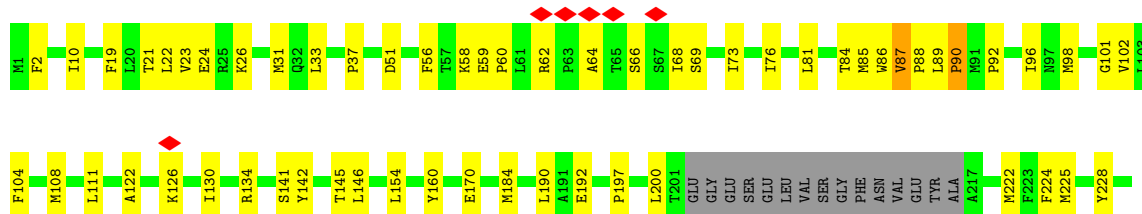
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

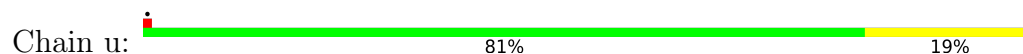


- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

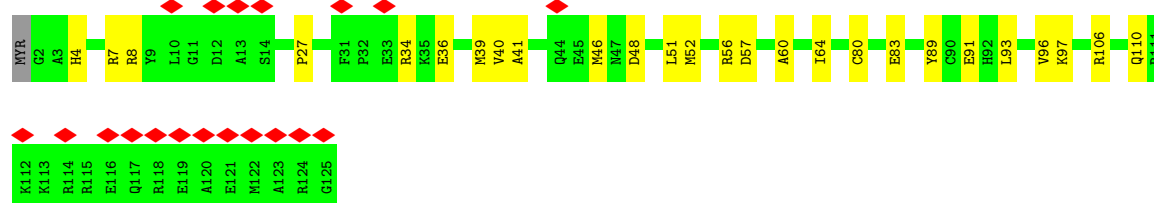




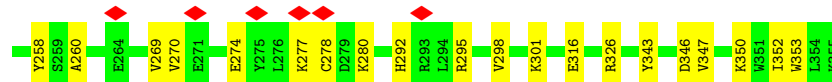
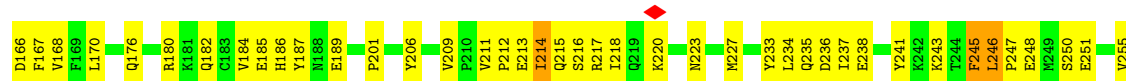
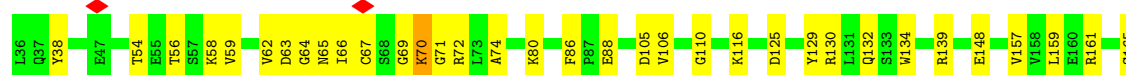
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



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



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 104881                                  | 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                    | 0.207                                   | Depositor |
| Minimum map value                    | -0.109                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.0232                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 333.002, 333.002, 333.002               | wwPDB     |
| Map dimensions                       | 310, 310, 310                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0742, 1.0742, 1.0742                  | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | A     | 0.19         | 0/3393      | 0.41        | 1/4584 (0.0%) |
| 2   | B     | 0.24         | 0/1443      | 0.36        | 0/1952        |
| 3   | C     | 0.22         | 0/1279      | 0.35        | 0/1730        |
| 4   | E     | 0.16         | 0/995       | 0.33        | 0/1340        |
| 5   | F     | 0.16         | 0/702       | 0.37        | 0/945         |
| 6   | G     | 0.19         | 0/705       | 0.51        | 0/956         |
| 6   | X     | 0.15         | 0/711       | 0.33        | 0/963         |
| 7   | H     | 0.18         | 0/929       | 0.40        | 0/1258        |
| 8   | I     | 0.21         | 0/798       | 0.47        | 0/1079        |
| 9   | J     | 0.18         | 0/2411      | 0.40        | 0/3254        |
| 10  | K     | 0.13         | 0/365       | 0.27        | 0/493         |
| 11  | L     | 0.20         | 0/1039      | 0.35        | 0/1403        |
| 12  | M     | 0.19         | 0/5384      | 0.34        | 0/7295        |
| 13  | N     | 0.18         | 0/1245      | 0.39        | 0/1694        |
| 14  | O     | 0.17         | 0/1711      | 0.42        | 0/2328        |
| 15  | P     | 0.22         | 0/1789      | 0.38        | 0/2436        |
| 16  | Q     | 0.24         | 0/3451      | 0.43        | 4/4672 (0.1%) |
| 17  | S     | 0.21         | 0/582       | 0.42        | 0/783         |
| 18  | T     | 0.16         | 0/755       | 0.30        | 0/1018        |
| 19  | U     | 0.16         | 0/664       | 0.31        | 0/912         |
| 20  | V     | 0.20         | 0/1042      | 0.42        | 3/1411 (0.2%) |
| 21  | W     | 0.19         | 0/1198      | 0.28        | 0/1617        |
| 22  | Y     | 0.15         | 0/626       | 0.34        | 0/857         |
| 23  | Z     | 0.16         | 0/695       | 0.35        | 0/939         |
| 24  | a     | 0.19         | 0/1199      | 0.37        | 0/1623        |
| 25  | b     | 0.15         | 0/906       | 0.35        | 0/1232        |
| 26  | c     | 0.18         | 0/1371      | 0.35        | 0/1875        |
| 27  | d     | 0.16         | 0/1494      | 0.29        | 0/2015        |
| 28  | e     | 0.16         | 0/916       | 0.35        | 0/1246        |
| 29  | f     | 0.15         | 0/350       | 0.30        | 0/473         |
| 30  | g     | 0.18         | 0/1031      | 0.32        | 0/1394        |
| 31  | h     | 0.19         | 0/889       | 0.36        | 0/1190        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 32  | i     | 0.21         | 0/2773  | 0.39        | 0/3768          |
| 33  | j     | 0.23         | 0/819   | 0.42        | 0/1117          |
| 34  | k     | 0.22         | 0/759   | 0.39        | 0/1029          |
| 35  | l     | 0.20         | 0/4914  | 0.39        | 0/6683          |
| 36  | m     | 0.21         | 0/973   | 0.41        | 0/1320          |
| 37  | n     | 0.22         | 0/491   | 0.59        | 1/663 (0.2%)    |
| 38  | o     | 0.17         | 0/1092  | 0.33        | 0/1481          |
| 39  | p     | 0.17         | 0/1590  | 0.33        | 0/2155          |
| 40  | r     | 0.22         | 0/3723  | 0.39        | 0/5078          |
| 41  | s     | 0.24         | 0/2464  | 0.51        | 2/3369 (0.1%)   |
| 42  | u     | 0.19         | 0/1436  | 0.40        | 0/1938          |
| 43  | v     | 0.17         | 0/1036  | 0.48        | 0/1393          |
| 44  | w     | 0.19         | 0/2643  | 0.45        | 1/3580 (0.0%)   |
| All | All   | 0.20         | 0/66781 | 0.39        | 12/90541 (0.0%) |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 120 | GLY  | N-CA-C   | 8.10  | 122.45      | 112.73   |
| 41  | s     | 87  | VAL  | CA-C-N   | 8.07  | 127.65      | 118.85   |
| 41  | s     | 87  | VAL  | C-N-CA   | 8.07  | 127.65      | 118.85   |
| 16  | Q     | 217 | VAL  | N-CA-C   | 6.04  | 116.82      | 110.72   |
| 16  | Q     | 142 | VAL  | N-CA-C   | -6.00 | 107.65      | 113.53   |
| 20  | V     | 95  | CYS  | CA-CB-SG | 5.99  | 128.18      | 114.40   |
| 20  | V     | 94  | GLY  | CA-C-N   | -5.88 | 112.83      | 122.54   |
| 20  | V     | 94  | GLY  | C-N-CA   | -5.88 | 112.83      | 122.54   |
| 37  | n     | 16  | LEU  | N-CA-C   | 5.85  | 117.66      | 111.28   |
| 44  | w     | 245 | PHE  | N-CA-C   | 5.73  | 117.20      | 111.07   |
| 16  | Q     | 224 | ALA  | N-CA-C   | 5.42  | 117.19      | 111.28   |
| 16  | Q     | 226 | TYR  | N-CA-C   | 5.24  | 117.07      | 111.36   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3318  | 0        | 3280     | 87      | 0            |
| 2   | B     | 1412  | 0        | 1363     | 41      | 0            |
| 3   | C     | 1248  | 0        | 1254     | 32      | 0            |
| 4   | E     | 971   | 0        | 975      | 13      | 0            |
| 5   | F     | 691   | 0        | 704      | 19      | 0            |
| 6   | G     | 693   | 0        | 671      | 24      | 0            |
| 6   | X     | 699   | 0        | 674      | 18      | 0            |
| 7   | H     | 910   | 0        | 950      | 16      | 0            |
| 8   | I     | 780   | 0        | 808      | 22      | 0            |
| 9   | J     | 2359  | 0        | 2402     | 47      | 0            |
| 10  | K     | 355   | 0        | 329      | 14      | 0            |
| 11  | L     | 1016  | 0        | 1016     | 22      | 0            |
| 12  | M     | 5296  | 0        | 5326     | 89      | 0            |
| 13  | N     | 1204  | 0        | 1162     | 33      | 0            |
| 14  | O     | 1671  | 0        | 1673     | 36      | 0            |
| 15  | P     | 1738  | 0        | 1693     | 28      | 0            |
| 16  | Q     | 3377  | 0        | 3319     | 63      | 0            |
| 17  | S     | 567   | 0        | 565      | 5       | 0            |
| 18  | T     | 741   | 0        | 702      | 8       | 0            |
| 19  | U     | 643   | 0        | 642      | 9       | 0            |
| 20  | V     | 1021  | 0        | 1027     | 22      | 0            |
| 21  | W     | 1167  | 0        | 1155     | 22      | 0            |
| 22  | Y     | 600   | 0        | 539      | 12      | 0            |
| 23  | Z     | 674   | 0        | 643      | 12      | 0            |
| 24  | a     | 1165  | 0        | 1174     | 25      | 0            |
| 25  | b     | 879   | 0        | 899      | 32      | 0            |
| 26  | c     | 1315  | 0        | 1208     | 25      | 0            |
| 27  | d     | 1461  | 0        | 1429     | 35      | 0            |
| 28  | e     | 890   | 0        | 837      | 20      | 0            |
| 29  | f     | 342   | 0        | 341      | 6       | 0            |
| 30  | g     | 1000  | 0        | 994      | 14      | 0            |
| 31  | h     | 867   | 0        | 871      | 13      | 0            |
| 32  | i     | 2710  | 0        | 2874     | 78      | 0            |
| 33  | j     | 800   | 0        | 855      | 29      | 0            |
| 34  | k     | 748   | 0        | 799      | 23      | 0            |
| 35  | l     | 4785  | 0        | 4933     | 114     | 0            |
| 36  | m     | 951   | 0        | 962      | 37      | 0            |
| 37  | n     | 479   | 0        | 486      | 14      | 0            |
| 38  | o     | 1062  | 0        | 1072     | 9       | 0            |
| 39  | p     | 1534  | 0        | 1470     | 29      | 0            |
| 40  | r     | 3631  | 0        | 3839     | 88      | 0            |
| 41  | s     | 2394  | 0        | 2508     | 83      | 0            |
| 42  | u     | 1398  | 0        | 1378     | 24      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 43  | v     | 1012  | 0        | 947      | 21      | 0            |
| 44  | w     | 2583  | 0        | 2539     | 78      | 0            |
| 45  | A     | 8     | 0        | 0        | 2       | 0            |
| 45  | B     | 16    | 0        | 0        | 0       | 0            |
| 45  | C     | 8     | 0        | 0        | 0       | 0            |
| 45  | M     | 16    | 0        | 0        | 1       | 0            |
| 46  | A     | 31    | 0        | 19       | 4       | 0            |
| 47  | A     | 44    | 0        | 27       | 4       | 0            |
| 48  | C     | 47    | 0        | 71       | 21      | 0            |
| 48  | U     | 51    | 0        | 82       | 6       | 0            |
| 48  | V     | 91    | 0        | 136      | 28      | 0            |
| 48  | l     | 139   | 0        | 209      | 38      | 0            |
| 48  | m     | 41    | 0        | 59       | 8       | 0            |
| 48  | s     | 51    | 0        | 82       | 2       | 0            |
| 49  | C     | 52    | 0        | 88       | 2       | 0            |
| 49  | V     | 52    | 0        | 88       | 4       | 0            |
| 49  | e     | 52    | 0        | 88       | 7       | 0            |
| 49  | i     | 52    | 0        | 88       | 1       | 0            |
| 49  | j     | 52    | 0        | 88       | 2       | 0            |
| 49  | n     | 52    | 0        | 88       | 9       | 0            |
| 50  | G     | 35    | 0        | 0        | 0       | 0            |
| 50  | X     | 35    | 0        | 0        | 1       | 0            |
| 51  | J     | 48    | 0        | 25       | 6       | 0            |
| 52  | M     | 4     | 0        | 0        | 0       | 0            |
| 52  | O     | 4     | 0        | 0        | 0       | 0            |
| 53  | M     | 1     | 0        | 0        | 0       | 0            |
| 54  | N     | 51    | 0        | 46       | 12      | 0            |
| 54  | V     | 162   | 0        | 221      | 34      | 0            |
| 54  | a     | 91    | 0        | 132      | 18      | 0            |
| 54  | i     | 66    | 0        | 76       | 16      | 0            |
| 54  | l     | 199   | 0        | 307      | 46      | 0            |
| 54  | n     | 78    | 0        | 103      | 13      | 0            |
| 54  | r     | 97    | 0        | 147      | 8       | 0            |
| 55  | T     | 1     | 0        | 0        | 0       | 0            |
| 56  | s     | 28    | 0        | 31       | 4       | 0            |
| 57  | w     | 27    | 0        | 11       | 4       | 0            |
| All | All   | 66939 | 0        | 67599    | 1406    | 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 10.

All (1406) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:50:LEU:CD2    | 48:C:311:PEE:H25  | 1.53                     | 1.39              |
| 44:w:67:CYS:CB    | 44:w:218:ILE:HD11 | 1.65                     | 1.27              |
| 51:J:401:NDP:O4D  | 51:J:401:NDP:C4D  | 1.68                     | 1.21              |
| 54:V:201:CDL:H601 | 54:V:201:CDL:H732 | 1.24                     | 1.18              |
| 3:C:50:LEU:CD2    | 48:C:311:PEE:C17  | 2.20                     | 1.18              |
| 48:l:718:PEE:H36  | 48:l:718:PEE:H28  | 1.25                     | 1.17              |
| 44:w:69:GLY:O     | 44:w:71:GLY:N     | 1.77                     | 1.17              |
| 48:V:202:PEE:H78  | 40:r:201:MET:CE   | 1.75                     | 1.15              |
| 54:V:203:CDL:H342 | 54:V:203:CDL:H112 | 1.26                     | 1.13              |
| 54:l:712:CDL:H842 | 54:l:712:CDL:H631 | 1.14                     | 1.13              |
| 48:V:202:PEE:H77  | 40:r:201:MET:HE2  | 1.14                     | 1.12              |
| 3:C:50:LEU:HD21   | 48:C:311:PEE:C17  | 1.79                     | 1.11              |
| 54:l:712:CDL:H791 | 54:l:712:CDL:H611 | 1.33                     | 1.11              |
| 48:V:202:PEE:C45  | 40:r:201:MET:HE2  | 1.82                     | 1.09              |
| 54:l:712:CDL:H601 | 54:l:712:CDL:H772 | 1.26                     | 1.09              |
| 37:n:13:VAL:CG1   | 40:r:14:MET:HG2   | 1.82                     | 1.09              |
| 41:s:87:VAL:HG23  | 41:s:88:PRO:HD3   | 1.21                     | 1.09              |
| 48:V:207:PEE:H2   | 48:V:207:PEE:H9   | 1.25                     | 1.07              |
| 3:C:50:LEU:HD22   | 48:C:311:PEE:H25  | 1.30                     | 1.07              |
| 54:l:712:CDL:H541 | 54:l:712:CDL:HA62 | 1.35                     | 1.06              |
| 54:l:712:CDL:H422 | 40:r:448:THR:HG21 | 1.36                     | 1.06              |
| 37:n:13:VAL:HG12  | 40:r:14:MET:HG2   | 1.08                     | 1.03              |
| 1:A:121:GLU:HB2   | 47:A:503:NAI:H42N | 1.36                     | 1.02              |
| 20:V:95:CYS:HB2   | 20:V:115:CYS:HA   | 1.40                     | 1.02              |
| 24:a:95:GLU:OE2   | 54:a:201:CDL:O1   | 1.80                     | 1.00              |
| 48:V:202:PEE:H77  | 40:r:201:MET:CE   | 1.91                     | 0.99              |
| 44:w:67:CYS:CB    | 44:w:218:ILE:CD1  | 2.39                     | 0.99              |
| 54:V:203:CDL:H832 | 54:V:203:CDL:H791 | 1.42                     | 0.98              |
| 54:l:712:CDL:H312 | 54:l:712:CDL:H742 | 1.01                     | 0.98              |
| 54:N:202:CDL:H312 | 54:N:202:CDL:H522 | 1.44                     | 0.98              |
| 54:l:712:CDL:H742 | 54:l:712:CDL:C31  | 1.93                     | 0.97              |
| 54:N:202:CDL:H541 | 54:N:202:CDL:H321 | 1.47                     | 0.96              |
| 54:a:201:CDL:H521 | 48:l:720:PEE:H13  | 1.47                     | 0.96              |
| 54:l:712:CDL:H842 | 54:l:712:CDL:C63  | 1.96                     | 0.96              |
| 32:i:133:TRP:HE3  | 54:i:401:CDL:H392 | 1.31                     | 0.96              |
| 48:V:202:PEE:C46  | 40:r:201:MET:CE   | 2.45                     | 0.95              |
| 41:s:87:VAL:CG2   | 41:s:88:PRO:HD3   | 1.97                     | 0.94              |
| 44:w:235:GLN:OE1  | 44:w:238:GLU:OE2  | 1.87                     | 0.93              |
| 41:s:84:THR:O     | 41:s:87:VAL:HG22  | 1.69                     | 0.92              |
| 54:a:201:CDL:H521 | 48:l:720:PEE:C11  | 1.99                     | 0.91              |
| 32:i:133:TRP:CE3  | 54:i:401:CDL:H392 | 2.06                     | 0.90              |
| 48:V:207:PEE:H2   | 48:V:207:PEE:C4   | 2.00                     | 0.90              |

Continued on next page...

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:l:712:CDL:H791 | 54:l:712:CDL:C61  | 2.02                     | 0.89              |
| 48:l:718:PEE:H28  | 48:l:718:PEE:C22  | 2.03                     | 0.89              |
| 41:s:87:VAL:HG23  | 41:s:88:PRO:CD    | 2.04                     | 0.88              |
| 48:V:202:PEE:H78  | 40:r:201:MET:HE3  | 1.55                     | 0.88              |
| 54:l:712:CDL:H312 | 54:l:712:CDL:C74  | 1.97                     | 0.87              |
| 48:l:719:PEE:C11  | 48:l:719:PEE:H7   | 2.04                     | 0.87              |
| 48:V:202:PEE:C45  | 40:r:201:MET:CE   | 2.52                     | 0.87              |
| 54:a:201:CDL:H251 | 54:a:201:CDL:H211 | 1.57                     | 0.87              |
| 54:a:201:CDL:H532 | 48:l:720:PEE:H56  | 1.55                     | 0.86              |
| 54:V:203:CDL:H112 | 54:V:203:CDL:C34  | 2.05                     | 0.86              |
| 34:k:37:MET:HE1   | 36:m:64:MET:HE1   | 1.56                     | 0.86              |
| 32:i:321:LYS:HE3  | 54:i:401:CDL:OA4  | 1.77                     | 0.85              |
| 44:w:214:ILE:HG21 | 44:w:234:LEU:HD13 | 1.59                     | 0.85              |
| 9:J:176:SER:O     | 9:J:182:ARG:NH2   | 2.11                     | 0.84              |
| 54:l:712:CDL:HA62 | 54:l:712:CDL:C54  | 2.07                     | 0.84              |
| 41:s:24:GLU:OE2   | 41:s:228:TYR:OH   | 1.95                     | 0.83              |
| 54:N:202:CDL:H541 | 54:N:202:CDL:C32  | 2.08                     | 0.83              |
| 54:V:203:CDL:H342 | 54:V:203:CDL:C11  | 2.07                     | 0.83              |
| 9:J:83:PRO:HA     | 9:J:106:MET:O     | 1.79                     | 0.82              |
| 48:m:202:PEE:H25  | 48:m:202:PEE:H54  | 1.58                     | 0.82              |
| 37:n:13:VAL:HG12  | 40:r:14:MET:CG    | 2.02                     | 0.82              |
| 54:V:201:CDL:H452 | 54:V:201:CDL:H211 | 1.61                     | 0.81              |
| 54:n:102:CDL:H581 | 54:n:102:CDL:H542 | 1.61                     | 0.81              |
| 48:C:311:PEE:H72  | 41:s:56:PHE:CD2   | 2.16                     | 0.81              |
| 48:V:202:PEE:C46  | 40:r:201:MET:HE2  | 2.09                     | 0.81              |
| 20:V:66:ILE:HD11  | 20:V:101:LEU:HD13 | 1.61                     | 0.81              |
| 3:C:50:LEU:HD11   | 48:C:311:PEE:H59  | 1.62                     | 0.81              |
| 24:a:127:ASP:OD1  | 49:n:101:PLX:H1C2 | 1.81                     | 0.80              |
| 1:A:86:ARG:NE     | 1:A:92:GLY:O      | 2.15                     | 0.80              |
| 6:X:91:ASP:HB3    | 23:Z:47:ARG:HH12  | 1.46                     | 0.79              |
| 48:C:311:PEE:H72  | 41:s:56:PHE:HD2   | 1.47                     | 0.79              |
| 33:j:68:GLU:HG2   | 36:m:161:LEU:HD13 | 1.64                     | 0.79              |
| 32:i:133:TRP:HE3  | 54:i:401:CDL:C39  | 1.96                     | 0.78              |
| 2:B:111:GLU:O     | 2:B:141:ARG:NH1   | 2.17                     | 0.78              |
| 1:A:398:ARG:NH1   | 12:M:155:GLU:OE2  | 2.17                     | 0.78              |
| 1:A:398:ARG:NH2   | 1:A:408:GLU:OE1   | 2.17                     | 0.78              |
| 54:V:201:CDL:C74  | 54:V:201:CDL:H611 | 2.13                     | 0.78              |
| 8:I:8:ILE:HG13    | 54:N:202:CDL:HA32 | 1.66                     | 0.78              |
| 21:W:10:MET:HE3   | 21:W:11:PRO:HD2   | 1.64                     | 0.78              |
| 6:G:74:LEU:H      | 6:G:74:LEU:HD23   | 1.49                     | 0.78              |
| 1:A:204:TYR:OH    | 47:A:503:NAI:H5N  | 1.84                     | 0.77              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:P:83:GLU:OE1   | 15:P:142:ARG:NH2  | 2.18                     | 0.77              |
| 33:j:18:VAL:HG22  | 41:s:222:MET:HG3  | 1.66                     | 0.77              |
| 54:l:712:CDL:H541 | 54:l:712:CDL:CA6  | 2.13                     | 0.77              |
| 54:n:102:CDL:H542 | 54:n:102:CDL:C58  | 2.15                     | 0.77              |
| 35:l:286:LEU:HD22 | 35:l:411:MET:HE3  | 1.68                     | 0.76              |
| 1:A:388:GLY:HA3   | 1:A:419:ILE:HD11  | 1.67                     | 0.76              |
| 24:a:126:TYR:O    | 49:n:101:PLX:H1B3 | 1.85                     | 0.76              |
| 54:l:712:CDL:H772 | 54:l:712:CDL:C60  | 2.12                     | 0.76              |
| 12:M:213:MET:HG3  | 12:M:215:MET:HG2  | 1.68                     | 0.76              |
| 44:w:235:GLN:CD   | 44:w:238:GLU:OE2  | 2.29                     | 0.75              |
| 41:s:87:VAL:N     | 41:s:88:PRO:HD2   | 2.02                     | 0.75              |
| 12:M:387:LEU:HD12 | 12:M:514:ASN:HB3  | 1.69                     | 0.74              |
| 44:w:65:ASN:ND2   | 44:w:238:GLU:HB3  | 2.03                     | 0.74              |
| 3:C:126:GLU:O     | 9:J:89:TYR:OH     | 2.06                     | 0.74              |
| 2:B:165:ASP:OD1   | 16:Q:368:ARG:NH2  | 2.21                     | 0.73              |
| 1:A:60:GLY:O      | 1:A:256:ARG:NH1   | 2.22                     | 0.73              |
| 35:l:356:ILE:HA   | 35:l:359:MET:HE3  | 1.71                     | 0.73              |
| 54:l:712:CDL:H642 | 54:l:712:CDL:H871 | 1.70                     | 0.73              |
| 26:c:116:ARG:HG2  | 48:l:719:PEE:H49  | 1.68                     | 0.73              |
| 24:a:179:ILE:HG21 | 31:h:38:LYS:HG3   | 1.70                     | 0.73              |
| 16:Q:149:GLN:NE2  | 16:Q:309:ASP:OD2  | 2.21                     | 0.73              |
| 9:J:83:PRO:HB2    | 9:J:108:TRP:CD1   | 2.24                     | 0.72              |
| 44:w:69:GLY:O     | 44:w:70:LYS:C     | 2.32                     | 0.72              |
| 11:L:112:MET:HE3  | 13:N:126:PRO:HB2  | 1.71                     | 0.72              |
| 3:C:50:LEU:CD2    | 48:C:311:PEE:H26  | 2.15                     | 0.72              |
| 48:V:202:PEE:O4   | 40:r:195:MET:HB2  | 1.90                     | 0.72              |
| 48:C:311:PEE:H27  | 48:C:311:PEE:H58  | 1.71                     | 0.72              |
| 48:V:202:PEE:H3   | 40:r:191:SER:HB3  | 1.73                     | 0.71              |
| 54:V:201:CDL:H601 | 54:V:201:CDL:C73  | 2.14                     | 0.71              |
| 1:A:121:GLU:HB2   | 47:A:503:NAI:C4N  | 2.20                     | 0.71              |
| 10:K:105:ARG:NH1  | 11:L:167:ASN:O    | 2.23                     | 0.70              |
| 32:i:129:LEU:CD1  | 54:i:401:CDL:H341 | 2.21                     | 0.70              |
| 3:C:59:ARG:NH1    | 49:C:312:PLX:O3   | 2.23                     | 0.70              |
| 35:l:359:MET:O    | 35:l:436:ARG:NH2  | 2.25                     | 0.70              |
| 44:w:165:SER:HB3  | 44:w:245:PHE:CE1  | 2.26                     | 0.70              |
| 32:i:125:GLN:HG2  | 54:i:401:CDL:OA3  | 1.90                     | 0.70              |
| 24:a:97:GLU:OE2   | 27:d:60:ARG:NH1   | 2.24                     | 0.70              |
| 25:b:16:ARG:HD3   | 25:b:20:ARG:NH1   | 2.07                     | 0.70              |
| 44:w:250:SER:O    | 44:w:280:LYS:NZ   | 2.22                     | 0.70              |
| 21:W:85:GLN:OE1   | 31:h:105:ARG:NH1  | 2.23                     | 0.70              |
| 25:b:16:ARG:HD3   | 25:b:20:ARG:HH12  | 1.57                     | 0.70              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:88:GLU:OE2   | 44:w:161:ARG:NH1  | 2.25                     | 0.70              |
| 32:i:129:LEU:HD12 | 54:i:401:CDL:H341 | 1.74                     | 0.70              |
| 48:l:719:PEE:H7   | 48:l:719:PEE:H14  | 1.74                     | 0.70              |
| 1:A:33:GLY:O      | 1:A:302:LYS:NZ    | 2.25                     | 0.69              |
| 12:M:472:PRO:O    | 12:M:510:TRP:NE1  | 2.22                     | 0.69              |
| 35:l:227:PHE:O    | 35:l:230:HIS:ND1  | 2.24                     | 0.69              |
| 40:r:188:ASN:OD1  | 40:r:256:TYR:OH   | 2.10                     | 0.69              |
| 3:C:125:PRO:HB2   | 41:s:58:LYS:HE3   | 1.74                     | 0.69              |
| 44:w:246:LEU:HD12 | 44:w:255:VAL:HG11 | 1.73                     | 0.69              |
| 3:C:50:LEU:HD21   | 48:C:311:PEE:C18  | 2.23                     | 0.69              |
| 9:J:85:ARG:NH2    | 51:J:401:NDP:O2X  | 2.23                     | 0.69              |
| 54:n:102:CDL:H581 | 54:n:102:CDL:C54  | 2.20                     | 0.69              |
| 48:C:311:PEE:C43  | 41:s:56:PHE:HD2   | 2.05                     | 0.69              |
| 11:L:88:GLN:NE2   | 12:M:141:ASP:OD2  | 2.23                     | 0.69              |
| 20:V:95:CYS:CB    | 20:V:115:CYS:HA   | 2.21                     | 0.69              |
| 35:l:596:MET:O    | 35:l:600:THR:HG23 | 1.92                     | 0.69              |
| 32:i:92:PRO:O     | 32:i:94:ALA:N     | 2.26                     | 0.69              |
| 54:l:712:CDL:H622 | 54:l:712:CDL:H581 | 1.73                     | 0.69              |
| 54:V:203:CDL:H852 | 35:l:558:LEU:HD21 | 1.74                     | 0.69              |
| 26:c:161:TYR:HB3  | 26:c:166:LEU:HG   | 1.74                     | 0.68              |
| 54:l:712:CDL:H631 | 54:l:712:CDL:C84  | 2.08                     | 0.68              |
| 32:i:125:GLN:CG   | 54:i:401:CDL:OA3  | 2.42                     | 0.68              |
| 35:l:250:SER:HB2  | 35:l:333:ALA:HA   | 1.75                     | 0.68              |
| 54:l:712:CDL:H552 | 54:l:712:CDL:H792 | 1.75                     | 0.68              |
| 41:s:87:VAL:CG2   | 41:s:88:PRO:CD    | 2.68                     | 0.68              |
| 25:b:14:GLN:HE22  | 39:p:157:ALA:HB3  | 1.56                     | 0.67              |
| 44:w:139:ARG:NH1  | 44:w:166:ASP:OD1  | 2.27                     | 0.67              |
| 6:X:155:TYR:CE1   | 25:b:23:LEU:HB3   | 2.29                     | 0.67              |
| 16:Q:79:ASN:HA    | 16:Q:101:LEU:O    | 1.94                     | 0.67              |
| 54:V:201:CDL:H611 | 54:V:201:CDL:H741 | 1.75                     | 0.67              |
| 54:V:201:CDL:HA62 | 54:V:201:CDL:OA7  | 1.92                     | 0.67              |
| 41:s:184:MET:HE1  | 41:s:296:LEU:HB2  | 1.75                     | 0.67              |
| 26:c:165:ASP:OD2  | 26:c:170:ARG:NH2  | 2.27                     | 0.67              |
| 2:B:89:GLU:OE2    | 13:N:34:ARG:NH2   | 2.28                     | 0.67              |
| 11:L:109:ASN:ND2  | 11:L:111:LEU:O    | 2.27                     | 0.67              |
| 43:v:39:MET:HE3   | 43:v:41:ALA:H     | 1.58                     | 0.67              |
| 29:f:40:ASP:OD2   | 29:f:43:LYS:NZ    | 2.27                     | 0.67              |
| 22:Y:43:ARG:HB3   | 22:Y:46:GLN:HG2   | 1.77                     | 0.67              |
| 32:i:321:LYS:CE   | 54:i:401:CDL:OA4  | 2.43                     | 0.67              |
| 20:V:72:LEU:O     | 20:V:76:ILE:HG12  | 1.95                     | 0.66              |
| 6:X:76:LEU:HD21   | 25:b:20:ARG:HH21  | 1.60                     | 0.66              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:d:69:ARG:HH22  | 37:n:46:LYS:HB3   | 1.59                     | 0.66              |
| 6:G:119:ILE:HG21  | 6:G:135:ALA:HB1   | 1.77                     | 0.66              |
| 25:b:104:ILE:HB   | 43:v:48:ASP:HB3   | 1.76                     | 0.66              |
| 33:j:25:PRO:HB2   | 41:s:60:PRO:HD3   | 1.76                     | 0.66              |
| 35:l:401:MET:SD   | 35:l:479:ASN:ND2  | 2.66                     | 0.66              |
| 1:A:121:GLU:HG3   | 1:A:122:PRO:HD2   | 1.77                     | 0.66              |
| 25:b:28:LEU:HG    | 25:b:32:GLU:HG2   | 1.78                     | 0.66              |
| 33:j:60:ILE:HG21  | 36:m:168:ILE:HG21 | 1.78                     | 0.66              |
| 2:B:192:ASN:ND2   | 18:T:61:GLU:OE2   | 2.26                     | 0.66              |
| 44:w:235:GLN:O    | 44:w:238:GLU:HG3  | 1.95                     | 0.66              |
| 12:M:483:ARG:HH22 | 12:M:682:ASP:HB3  | 1.60                     | 0.66              |
| 41:s:51:ASP:HB3   | 56:s:403:UQ:H8    | 1.77                     | 0.66              |
| 1:A:159:ARG:NH2   | 14:O:176:CYS:O    | 2.28                     | 0.66              |
| 1:A:185:ASN:OD1   | 1:A:190:GLY:N     | 2.21                     | 0.66              |
| 1:A:311:TRP:NE1   | 1:A:333:GLU:OE2   | 2.28                     | 0.66              |
| 44:w:125:ASP:O    | 44:w:130:ARG:NH2  | 2.29                     | 0.66              |
| 1:A:152:ARG:NH2   | 10:K:99:PRO:O     | 2.29                     | 0.65              |
| 48:V:202:PEE:H3   | 40:r:191:SER:CB   | 2.26                     | 0.65              |
| 42:u:44:MET:HB3   | 42:u:48:TRP:HZ3   | 1.62                     | 0.65              |
| 48:l:719:PEE:H22  | 48:l:719:PEE:H64  | 1.79                     | 0.65              |
| 25:b:109:THR:HG22 | 25:b:116:VAL:HG22 | 1.78                     | 0.65              |
| 32:i:100:MET:HE1  | 35:l:595:ILE:HG23 | 1.78                     | 0.65              |
| 48:l:720:PEE:O2P  | 48:l:720:PEE:N    | 2.21                     | 0.65              |
| 9:J:369:VAL:HG12  | 9:J:370:LYS:HG2   | 1.78                     | 0.65              |
| 15:P:50:ARG:HH12  | 15:P:80:CYS:HB2   | 1.62                     | 0.65              |
| 5:F:57:GLU:O      | 12:M:655:ARG:NH2  | 2.30                     | 0.65              |
| 32:i:108:LEU:HD11 | 32:i:191:THR:HG21 | 1.79                     | 0.65              |
| 54:l:712:CDL:C84  | 54:l:712:CDL:H651 | 2.27                     | 0.64              |
| 7:H:44:TYR:HB2    | 15:P:68:ILE:HG23  | 1.78                     | 0.64              |
| 38:o:23:TYR:OH    | 39:p:68:GLU:OE1   | 2.15                     | 0.64              |
| 41:s:235:ASN:HD21 | 41:s:270:PHE:HE2  | 1.45                     | 0.64              |
| 3:C:83:ARG:NH1    | 16:Q:212:GLU:OE2  | 2.24                     | 0.64              |
| 10:K:100:GLN:HB3  | 14:O:71:PRO:HA    | 1.78                     | 0.64              |
| 54:l:712:CDL:H601 | 54:l:712:CDL:C77  | 2.16                     | 0.64              |
| 20:V:69:ILE:HG13  | 20:V:100:THR:HG21 | 1.78                     | 0.64              |
| 3:C:50:LEU:HD23   | 48:C:311:PEE:C17  | 2.24                     | 0.63              |
| 6:G:105:MET:HE2   | 6:G:139:MET:HE1   | 1.79                     | 0.63              |
| 6:G:138:LEU:HD23  | 6:G:144:ILE:HG12  | 1.80                     | 0.63              |
| 27:d:119:GLU:HG2  | 43:v:52:MET:HA    | 1.81                     | 0.63              |
| 49:V:205:PLX:H132 | 40:r:260:PRO:HG2  | 1.78                     | 0.63              |
| 28:e:89:VAL:HG21  | 40:r:25:ILE:HG23  | 1.79                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:s:235:ASN:ND2  | 41:s:270:PHE:HE2  | 1.96                     | 0.63              |
| 22:Y:62:SER:HG    | 35:l:371:THR:HG1  | 1.46                     | 0.63              |
| 27:d:111:LYS:NZ   | 35:l:200:GLN:OE1  | 2.32                     | 0.63              |
| 3:C:50:LEU:HD21   | 48:C:311:PEE:H26  | 1.73                     | 0.63              |
| 44:w:246:LEU:N    | 44:w:247:PRO:HD2  | 2.13                     | 0.63              |
| 9:J:213:PHE:HD1   | 9:J:214:LEU:HD12  | 1.62                     | 0.63              |
| 54:V:201:CDL:H732 | 54:V:201:CDL:C60  | 2.16                     | 0.63              |
| 49:e:201:PLX:O2   | 48:l:720:PEE:H3   | 1.98                     | 0.63              |
| 44:w:233:TYR:CZ   | 44:w:237:ILE:HD11 | 2.34                     | 0.62              |
| 35:l:391:SER:O    | 35:l:395:ILE:HG12 | 1.99                     | 0.62              |
| 35:l:407:TRP:O    | 35:l:411:MET:HG2  | 1.99                     | 0.62              |
| 9:J:157:LYS:NZ    | 9:J:197:GLU:OE2   | 2.33                     | 0.62              |
| 12:M:149:ASP:HB2  | 16:Q:361:ALA:HB3  | 1.81                     | 0.62              |
| 40:r:48:ASN:OD1   | 40:r:49:SER:N     | 2.30                     | 0.62              |
| 44:w:38:TYR:HH    | 44:w:292:HIS:HD1  | 1.48                     | 0.62              |
| 41:s:62:ARG:HD3   | 41:s:64:ALA:H     | 1.63                     | 0.62              |
| 2:B:131:GLU:HB2   | 2:B:144:ARG:HB3   | 1.82                     | 0.62              |
| 9:J:132:ARG:NH2   | 51:J:401:NDP:O2X  | 2.33                     | 0.62              |
| 9:J:327:MET:HE2   | 9:J:329:LEU:HD11  | 1.79                     | 0.62              |
| 11:L:131:LYS:HE3  | 11:L:147:VAL:HG11 | 1.82                     | 0.62              |
| 1:A:398:ARG:HG2   | 1:A:403:ASP:HB3   | 1.82                     | 0.61              |
| 12:M:394:VAL:HG22 | 12:M:473:MET:HE1  | 1.82                     | 0.61              |
| 50:X:201:8Q1:O3   | 39:p:13:GLN:NE2   | 2.33                     | 0.61              |
| 15:P:169:GLU:OE2  | 16:Q:463:ARG:NH2  | 2.33                     | 0.61              |
| 49:e:201:PLX:H122 | 54:l:712:CDL:H652 | 1.81                     | 0.61              |
| 41:s:184:MET:HE2  | 41:s:293:PHE:HA   | 1.83                     | 0.61              |
| 14:O:149:LEU:O    | 14:O:153:GLN:HG2  | 2.01                     | 0.61              |
| 49:e:201:PLX:H102 | 48:l:720:PEE:H23  | 1.83                     | 0.61              |
| 33:j:79:SER:HA    | 33:j:87:MET:HE2   | 1.81                     | 0.61              |
| 2:B:177:THR:HG22  | 2:B:179:THR:H     | 1.65                     | 0.61              |
| 9:J:145:PHE:CE1   | 9:J:184:LYS:HE3   | 2.36                     | 0.61              |
| 16:Q:387:GLU:OE2  | 16:Q:390:GLN:NE2  | 2.34                     | 0.61              |
| 30:g:34:VAL:HG21  | 54:n:102:CDL:OA7  | 1.99                     | 0.61              |
| 14:O:60:TYR:O     | 14:O:64:GLU:HG3   | 2.01                     | 0.61              |
| 16:Q:216:ARG:NH1  | 16:Q:243:ASP:OD2  | 2.27                     | 0.61              |
| 27:d:2:PRO:O      | 27:d:7:LYS:NZ     | 2.33                     | 0.61              |
| 28:e:104:THR:HG21 | 49:n:101:PLX:H212 | 1.81                     | 0.61              |
| 11:L:78:ARG:NH2   | 12:M:249:GLU:OE1  | 2.25                     | 0.61              |
| 12:M:636:TYR:CD1  | 12:M:642:VAL:HG22 | 2.36                     | 0.61              |
| 25:b:73:THR:HA    | 25:b:77:ILE:HD12  | 1.83                     | 0.61              |
| 35:l:119:LYS:NZ   | 54:l:712:CDL:H512 | 2.16                     | 0.61              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:l:590:SER:O    | 35:l:594:THR:HG23 | 2.01                     | 0.61              |
| 48:m:202:PEE:H25  | 48:m:202:PEE:C34  | 2.27                     | 0.61              |
| 41:s:235:ASN:HD22 | 41:s:266:LEU:HB3  | 1.66                     | 0.61              |
| 2:B:184:LEU:HD23  | 11:L:112:MET:HG3  | 1.83                     | 0.61              |
| 28:e:92:PHE:O     | 28:e:96:SER:OG    | 2.17                     | 0.61              |
| 54:l:712:CDL:H651 | 54:l:712:CDL:H841 | 1.83                     | 0.61              |
| 39:p:29:SER:HB3   | 39:p:76:HIS:HD2   | 1.66                     | 0.61              |
| 41:s:69:SER:O     | 41:s:73:ILE:HG12  | 2.00                     | 0.61              |
| 8:I:27:ARG:NH1    | 16:Q:212:GLU:OE1  | 2.34                     | 0.60              |
| 15:P:154:GLU:OE2  | 15:P:180:ASN:ND2  | 2.30                     | 0.60              |
| 41:s:146:LEU:HD11 | 41:s:192:GLU:HG3  | 1.83                     | 0.60              |
| 1:A:214:GLU:OE2   | 1:A:224:ARG:NE    | 2.29                     | 0.60              |
| 2:B:177:THR:HG21  | 2:B:182:GLU:HB2   | 1.82                     | 0.60              |
| 48:V:202:PEE:H14  | 48:V:202:PEE:H7   | 1.82                     | 0.60              |
| 6:X:85:TYR:OH     | 23:Z:22:TRP:NE1   | 2.28                     | 0.60              |
| 2:B:77:LEU:HD12   | 41:s:31:MET:HG3   | 1.83                     | 0.60              |
| 48:V:202:PEE:H14  | 32:i:276:ILE:HG21 | 1.84                     | 0.60              |
| 31:h:18:MET:HE3   | 34:k:56:ALA:HA    | 1.83                     | 0.60              |
| 14:O:111:ARG:NH1  | 14:O:114:GLU:OE2  | 2.35                     | 0.60              |
| 32:i:149:ILE:HD13 | 32:i:154:MET:HE3  | 1.84                     | 0.60              |
| 36:m:21:SER:O     | 36:m:23:LYS:NZ    | 2.34                     | 0.60              |
| 36:m:25:SER:O     | 36:m:28:TYR:N     | 2.34                     | 0.60              |
| 13:N:5:GLN:OE1    | 13:N:9:ARG:NH1    | 2.34                     | 0.60              |
| 48:V:202:PEE:C1   | 40:r:191:SER:HB3  | 2.32                     | 0.60              |
| 26:c:62:TYR:OH    | 26:c:74:ASP:OD1   | 2.19                     | 0.60              |
| 32:i:239:VAL:HG23 | 54:r:714:CDL:H311 | 1.83                     | 0.60              |
| 1:A:177:TYR:HD2   | 10:K:93:LEU:HD22  | 1.66                     | 0.60              |
| 34:k:10:MET:HE3   | 36:m:14:VAL:HG11  | 1.82                     | 0.60              |
| 41:s:102:VAL:HG11 | 41:s:154:LEU:HD11 | 1.83                     | 0.60              |
| 14:O:70:TYR:HB3   | 14:O:71:PRO:HD2   | 1.83                     | 0.60              |
| 15:P:187:ILE:HG23 | 15:P:188:LEU:HG   | 1.83                     | 0.59              |
| 33:j:6:THR:HG21   | 41:s:87:VAL:HG11  | 1.84                     | 0.59              |
| 35:l:68:TRP:CE3   | 48:l:720:PEE:H47  | 2.37                     | 0.59              |
| 44:w:176:GLN:NE2  | 44:w:236:ASP:OD2  | 2.34                     | 0.59              |
| 6:G:115:GLN:O     | 6:G:119:ILE:HG12  | 2.01                     | 0.59              |
| 49:e:201:PLX:O2   | 48:l:720:PEE:H9   | 2.01                     | 0.59              |
| 1:A:384:PRO:HB2   | 1:A:423:THR:HG22  | 1.83                     | 0.59              |
| 54:r:714:CDL:H742 | 54:r:714:CDL:H271 | 1.83                     | 0.59              |
| 32:i:213:LEU:HD13 | 54:i:401:CDL:H141 | 1.84                     | 0.59              |
| 44:w:65:ASN:HD21  | 44:w:238:GLU:HB3  | 1.65                     | 0.59              |
| 6:X:100:VAL:HG22  | 6:X:142:GLN:HB2   | 1.84                     | 0.59              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:l:712:CDL:H422 | 40:r:448:THR:CG2  | 2.22                     | 0.59              |
| 28:e:106:VAL:HG13 | 40:r:453:MET:HE2  | 1.84                     | 0.59              |
| 2:B:144:ARG:NH1   | 2:B:146:ASP:OD2   | 2.34                     | 0.59              |
| 7:H:22:GLU:O      | 7:H:26:ILE:HG12   | 2.02                     | 0.59              |
| 54:l:712:CDL:H581 | 54:l:712:CDL:H872 | 1.85                     | 0.59              |
| 39:p:95:GLU:OE1   | 39:p:98:LYS:NZ    | 2.29                     | 0.59              |
| 41:s:62:ARG:HH21  | 41:s:68:ILE:HB    | 1.67                     | 0.59              |
| 54:V:201:CDL:H611 | 54:V:201:CDL:H742 | 1.85                     | 0.59              |
| 54:V:201:CDL:H741 | 54:V:201:CDL:C61  | 2.33                     | 0.59              |
| 12:M:299:ARG:HG2  | 12:M:300:GLN:HG2  | 1.84                     | 0.58              |
| 12:M:308:ARG:NH2  | 12:M:578:PRO:O    | 2.36                     | 0.58              |
| 34:k:98:CYS:HB2   | 35:l:580:GLN:HB2  | 1.85                     | 0.58              |
| 1:A:88:ARG:HG3    | 1:A:246:GLU:HG2   | 1.84                     | 0.58              |
| 5:F:69:TYR:HE2    | 5:F:75:LYS:HG3    | 1.68                     | 0.58              |
| 9:J:60:GLY:HA2    | 51:J:401:NDP:O3B  | 2.04                     | 0.58              |
| 12:M:390:THR:HA   | 12:M:600:GLU:HG2  | 1.84                     | 0.58              |
| 26:c:153:TYR:OH   | 43:v:8:ARG:NH1    | 2.32                     | 0.58              |
| 43:v:93:LEU:O     | 43:v:97:LYS:HG3   | 2.02                     | 0.58              |
| 16:Q:302:LEU:HB2  | 16:Q:401:GLU:HB2  | 1.86                     | 0.58              |
| 12:M:260:ASN:HD22 | 12:M:278:HIS:HB2  | 1.67                     | 0.58              |
| 1:A:132:ARG:HB3   | 1:A:165:GLU:HG3   | 1.85                     | 0.58              |
| 17:S:15:CYS:HA    | 17:S:18:ILE:HD12  | 1.85                     | 0.58              |
| 44:w:59:VAL:HG13  | 44:w:201:PRO:HA   | 1.86                     | 0.58              |
| 1:A:385:CYS:HB2   | 45:A:501:SF4:S4   | 2.42                     | 0.58              |
| 3:C:71:CYS:HB3    | 16:Q:141:TYR:CG   | 2.39                     | 0.58              |
| 12:M:222:ILE:HA   | 12:M:225:ILE:HG12 | 1.86                     | 0.58              |
| 32:i:278:MET:O    | 32:i:282:MET:HG3  | 2.04                     | 0.58              |
| 48:U:101:PEE:H20  | 33:j:106:TRP:CE3  | 2.39                     | 0.58              |
| 6:X:69:SER:OG     | 6:X:70:ASP:N      | 2.36                     | 0.58              |
| 54:a:201:CDL:H521 | 48:l:720:PEE:H14  | 1.83                     | 0.58              |
| 33:j:70:ALA:HA    | 33:j:73:LEU:HD12  | 1.85                     | 0.58              |
| 35:l:66:TRP:HZ3   | 48:l:720:PEE:H38  | 1.69                     | 0.58              |
| 12:M:336:ASN:O    | 12:M:336:ASN:ND2  | 2.37                     | 0.58              |
| 13:N:13:GLN:NE2   | 13:N:33:VAL:HG23  | 2.19                     | 0.58              |
| 16:Q:156:GLU:OE2  | 16:Q:171:ARG:NH2  | 2.36                     | 0.58              |
| 1:A:174:ARG:HA    | 10:K:93:LEU:HD21  | 1.86                     | 0.58              |
| 11:L:90:GLY:HA3   | 15:P:238:PRO:HB2  | 1.86                     | 0.58              |
| 12:M:304:GLN:HG2  | 12:M:615:LEU:HD12 | 1.86                     | 0.58              |
| 12:M:647:GLU:HB2  | 12:M:654:VAL:HG21 | 1.86                     | 0.58              |
| 23:Z:26:GLY:N     | 23:Z:30:GLU:OE2   | 2.34                     | 0.58              |
| 12:M:283:GLU:OE2  | 12:M:420:LYS:NZ   | 2.33                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:V:202:PEE:H78  | 40:r:201:MET:HE1  | 1.77                     | 0.57              |
| 6:X:125:GLU:HG2   | 35:l:439:PRO:HG2  | 1.84                     | 0.57              |
| 40:r:373:ILE:HD11 | 40:r:444:LEU:HD23 | 1.86                     | 0.57              |
| 19:U:9:LEU:HD11   | 48:U:101:PEE:H68  | 1.85                     | 0.57              |
| 30:g:12:PRO:HB3   | 31:h:5:ASP:HB3    | 1.86                     | 0.57              |
| 35:l:360:GLY:HA3  | 35:l:435:PRO:HA   | 1.86                     | 0.57              |
| 48:m:202:PEE:H52  | 41:s:104:PHE:HE1  | 1.70                     | 0.57              |
| 44:w:132:GLN:OE1  | 57:w:401:ADP:N6   | 2.37                     | 0.57              |
| 35:l:559:GLU:O    | 35:l:563:PRO:HD2  | 2.04                     | 0.57              |
| 48:C:311:PEE:C43  | 41:s:56:PHE:CD2   | 2.83                     | 0.57              |
| 34:k:5:TYR:O      | 34:k:9:ILE:HG12   | 2.04                     | 0.57              |
| 43:v:4:HIS:HA     | 43:v:7:ARG:HE     | 1.69                     | 0.57              |
| 12:M:370:GLU:OE2  | 12:M:518:ARG:NH2  | 2.38                     | 0.57              |
| 54:l:712:CDL:H351 | 40:r:361:VAL:HG13 | 1.85                     | 0.57              |
| 36:m:45:LEU:HD23  | 36:m:50:SER:HA    | 1.86                     | 0.57              |
| 44:w:69:GLY:C     | 44:w:71:GLY:N     | 2.55                     | 0.57              |
| 1:A:33:GLY:HA2    | 1:A:294:VAL:HG22  | 1.86                     | 0.57              |
| 8:I:3:SER:O       | 54:N:202:CDL:HA22 | 2.05                     | 0.57              |
| 12:M:150:ARG:NH2  | 16:Q:359:ASP:OD1  | 2.38                     | 0.57              |
| 6:X:155:TYR:HE1   | 25:b:23:LEU:HB3   | 1.70                     | 0.57              |
| 40:r:196:TRP:CD1  | 40:r:250:LEU:HB3  | 2.40                     | 0.57              |
| 6:G:104:PHE:HA    | 6:G:108:LEU:HD12  | 1.86                     | 0.57              |
| 32:i:133:TRP:CE3  | 54:i:401:CDL:C39  | 2.79                     | 0.57              |
| 16:Q:99:MET:HG2   | 16:Q:109:CYS:HA   | 1.86                     | 0.57              |
| 35:l:290:LEU:O    | 35:l:523:SER:OG   | 2.22                     | 0.57              |
| 15:P:94:ILE:O     | 15:P:98:THR:OG1   | 2.18                     | 0.56              |
| 33:j:88:LEU:HD13  | 41:s:309:ILE:HD12 | 1.86                     | 0.56              |
| 12:M:137:CYS:HB3  | 12:M:140:GLN:HB2  | 1.88                     | 0.56              |
| 21:W:74:LEU:O     | 21:W:78:GLU:HG3   | 2.05                     | 0.56              |
| 32:i:42:PRO:HG2   | 36:m:167:VAL:HG22 | 1.87                     | 0.56              |
| 54:n:102:CDL:H121 | 54:n:102:CDL:H762 | 1.87                     | 0.56              |
| 12:M:133:GLN:HG3  | 12:M:136:GLU:HG3  | 1.88                     | 0.56              |
| 15:P:147:THR:HB   | 15:P:153:ILE:HD11 | 1.86                     | 0.56              |
| 24:a:115:HIS:NE2  | 54:a:201:CDL:OB4  | 2.38                     | 0.56              |
| 12:M:591:GLU:HG2  | 12:M:610:VAL:HG23 | 1.87                     | 0.56              |
| 14:O:198:PRO:O    | 14:O:202:GLU:HG2  | 2.06                     | 0.56              |
| 35:l:119:LYS:NZ   | 54:l:712:CDL:OA3  | 2.37                     | 0.56              |
| 24:a:78:THR:OG1   | 28:e:96:SER:HB2   | 2.06                     | 0.56              |
| 40:r:14:MET:SD    | 40:r:26:ASN:HB3   | 2.46                     | 0.56              |
| 40:r:225:ILE:HG13 | 40:r:229:MET:HE2  | 1.88                     | 0.56              |
| 44:w:62:VAL:HG21  | 44:w:74:ALA:HB2   | 1.86                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:43:THR:HA     | 14:O:234:LEU:HD11 | 1.87                     | 0.56              |
| 3:C:191:ARG:O     | 3:C:195:ARG:HG3   | 2.06                     | 0.56              |
| 13:N:7:LEU:O      | 13:N:11:LEU:HG    | 2.06                     | 0.56              |
| 40:r:19:LYS:HD2   | 40:r:22:MET:HG3   | 1.86                     | 0.56              |
| 41:s:277:TYR:HE2  | 48:s:401:PEE:H58  | 1.70                     | 0.56              |
| 54:V:203:CDL:H801 | 54:V:203:CDL:H842 | 1.88                     | 0.56              |
| 25:b:104:ILE:HD13 | 27:d:18:PRO:HG3   | 1.88                     | 0.56              |
| 34:k:2:PRO:HD2    | 34:k:5:TYR:CD2    | 2.40                     | 0.56              |
| 43:v:51:LEU:O     | 43:v:52:MET:HG3   | 2.05                     | 0.56              |
| 1:A:380:GLY:O     | 1:A:386:ARG:NH1   | 2.39                     | 0.56              |
| 32:i:62:THR:HG23  | 32:i:104:MET:HE2  | 1.88                     | 0.56              |
| 22:Y:94:ASP:HB3   | 22:Y:99:ILE:HB    | 1.88                     | 0.56              |
| 44:w:80:LYS:HE3   | 44:w:270:VAL:HG21 | 1.87                     | 0.56              |
| 6:G:135:ALA:HA    | 6:G:138:LEU:HD13  | 1.87                     | 0.56              |
| 44:w:69:GLY:O     | 44:w:72:ARG:N     | 2.39                     | 0.56              |
| 2:B:64:THR:HG21   | 21:W:35:MET:HE1   | 1.88                     | 0.55              |
| 48:C:311:PEE:H27  | 48:C:311:PEE:C36  | 2.36                     | 0.55              |
| 4:E:78:VAL:O      | 4:E:82:LEU:HG     | 2.06                     | 0.55              |
| 48:V:202:PEE:H40  | 48:l:718:PEE:H47  | 1.88                     | 0.55              |
| 35:l:566:THR:O    | 35:l:570:GLN:HG2  | 2.05                     | 0.55              |
| 54:l:712:CDL:H811 | 54:l:712:CDL:H851 | 1.87                     | 0.55              |
| 1:A:375:LYS:NZ    | 14:O:33:GLY:O     | 2.40                     | 0.55              |
| 11:L:163:ASN:O    | 11:L:171:ARG:HA   | 2.07                     | 0.55              |
| 44:w:274:GLU:O    | 44:w:277:LYS:NZ   | 2.39                     | 0.55              |
| 1:A:66:LYS:NZ     | 1:A:188:GLY:O     | 2.39                     | 0.55              |
| 14:O:59:ASN:O     | 14:O:63:ILE:HG12  | 2.06                     | 0.55              |
| 33:j:64:LEU:HD13  | 36:m:165:VAL:HG22 | 1.88                     | 0.55              |
| 34:k:23:ARG:HD3   | 36:m:23:LYS:HB2   | 1.87                     | 0.55              |
| 4:E:110:THR:HG21  | 15:P:220:VAL:HG11 | 1.88                     | 0.55              |
| 12:M:51:GLN:O     | 12:M:55:LYS:HG2   | 2.06                     | 0.55              |
| 9:J:192:ARG:NH2   | 9:J:262:THR:OG1   | 2.39                     | 0.55              |
| 33:j:73:LEU:HD13  | 36:m:55:MET:HE1   | 1.86                     | 0.55              |
| 35:l:464:ALA:O    | 35:l:468:ILE:HG12 | 2.07                     | 0.55              |
| 48:l:718:PEE:C25  | 48:l:718:PEE:H34  | 2.35                     | 0.55              |
| 48:m:202:PEE:H7   | 48:m:202:PEE:O4   | 2.05                     | 0.55              |
| 18:T:119:ARG:HD3  | 18:T:122:HIS:CD2  | 2.42                     | 0.55              |
| 54:a:201:CDL:OA7  | 54:a:201:CDL:HA61 | 2.06                     | 0.55              |
| 35:l:562:LEU:HB3  | 35:l:563:PRO:HD3  | 1.89                     | 0.55              |
| 2:B:76:TYR:HE2    | 41:s:33:LEU:HB2   | 1.72                     | 0.55              |
| 6:G:75:THR:O      | 6:G:78:ALA:N      | 2.39                     | 0.55              |
| 14:O:54:ASP:OD1   | 14:O:55:PHE:N     | 2.40                     | 0.55              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:244:ASN:N     | 46:A:502:FMN:O1P  | 2.38                     | 0.55              |
| 15:P:132:LEU:HB2  | 15:P:141:ILE:HG22 | 1.88                     | 0.55              |
| 54:V:203:CDL:H322 | 54:V:203:CDL:C36  | 2.36                     | 0.55              |
| 35:l:11:THR:HG23  | 35:l:12:LEU:HD12  | 1.89                     | 0.55              |
| 44:w:185:GLU:O    | 44:w:189:GLU:HG3  | 2.06                     | 0.55              |
| 9:J:238:GLN:N     | 9:J:326:ASP:OD2   | 2.36                     | 0.55              |
| 40:r:14:MET:O     | 40:r:18:SER:OG    | 2.22                     | 0.55              |
| 43:v:46:MET:HE2   | 43:v:56:ARG:HG2   | 1.89                     | 0.55              |
| 11:L:111:LEU:HD11 | 13:N:126:PRO:HG2  | 1.89                     | 0.54              |
| 15:P:69:LEU:HD22  | 15:P:96:VAL:HG22  | 1.89                     | 0.54              |
| 16:Q:184:ILE:HG12 | 16:Q:203:MET:HE3  | 1.89                     | 0.54              |
| 22:Y:51:THR:HG22  | 22:Y:53:SER:H     | 1.72                     | 0.54              |
| 37:n:50:ARG:HB2   | 37:n:53:GLU:HB2   | 1.88                     | 0.54              |
| 40:r:398:MET:HA   | 40:r:398:MET:HE2  | 1.89                     | 0.54              |
| 5:F:46:LYS:HE2    | 12:M:674:LEU:HD21 | 1.89                     | 0.54              |
| 25:b:99:GLU:OE2   | 35:l:2:ASN:ND2    | 2.39                     | 0.54              |
| 44:w:116:LYS:NZ   | 44:w:125:ASP:OD2  | 2.39                     | 0.54              |
| 9:J:211:ASP:O     | 9:J:215:ASN:ND2   | 2.40                     | 0.54              |
| 13:N:2:GLU:HG3    | 13:N:4:VAL:HG22   | 1.89                     | 0.54              |
| 44:w:105:ASP:OD1  | 44:w:106:VAL:N    | 2.40                     | 0.54              |
| 1:A:50:ASP:O      | 1:A:59:ARG:NH2    | 2.36                     | 0.54              |
| 16:Q:127:LYS:HB3  | 16:Q:131:GLN:HB3  | 1.90                     | 0.54              |
| 18:T:119:ARG:HD3  | 18:T:122:HIS:HD2  | 1.71                     | 0.54              |
| 20:V:46:PRO:HB3   | 20:V:55:ARG:NH2   | 2.23                     | 0.54              |
| 54:a:201:CDL:H211 | 54:a:201:CDL:C25  | 2.34                     | 0.54              |
| 26:c:161:TYR:O    | 26:c:183:HIS:NE2  | 2.38                     | 0.54              |
| 35:l:419:THR:HA   | 35:l:422:TYR:CE2  | 2.43                     | 0.54              |
| 41:s:225:MET:HE2  | 56:s:403:UQ:H153  | 1.90                     | 0.54              |
| 3:C:50:LEU:HD21   | 48:C:311:PEE:H27  | 1.90                     | 0.54              |
| 13:N:6:VAL:HG12   | 13:N:9:ARG:NH2    | 2.23                     | 0.54              |
| 15:P:152:PRO:HB3  | 15:P:177:PHE:HD2  | 1.72                     | 0.54              |
| 35:l:7:LEU:HD22   | 35:l:46:LEU:HD11  | 1.89                     | 0.54              |
| 48:l:720:PEE:H5   | 48:l:720:PEE:P    | 2.30                     | 0.54              |
| 2:B:68:ARG:NH2    | 21:W:26:PRO:O     | 2.41                     | 0.54              |
| 13:N:4:VAL:HA     | 13:N:7:LEU:HD12   | 1.88                     | 0.54              |
| 20:V:70:PHE:HD1   | 20:V:94:GLY:HA2   | 1.73                     | 0.54              |
| 26:c:96:ASP:OD1   | 26:c:97:LEU:N     | 2.40                     | 0.54              |
| 44:w:132:GLN:CD   | 57:w:401:ADP:HN62 | 2.16                     | 0.54              |
| 35:l:172:ILE:O    | 35:l:176:ARG:HG2  | 2.08                     | 0.54              |
| 6:G:83:VAL:O      | 6:G:87:LEU:HD23   | 2.08                     | 0.54              |
| 20:V:81:ARG:NH2   | 20:V:88:LEU:HD22  | 2.22                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:4:TYR:HB2    | 25:b:9:LYS:HE3    | 1.88                     | 0.54              |
| 48:m:202:PEE:H25  | 48:m:202:PEE:C35  | 2.37                     | 0.54              |
| 15:P:44:ARG:HB3   | 15:P:45:PRO:CD    | 2.38                     | 0.54              |
| 42:u:49:GLU:OE1   | 42:u:135:ARG:NH2  | 2.40                     | 0.54              |
| 12:M:260:ASN:HD21 | 12:M:278:HIS:HD2  | 1.56                     | 0.53              |
| 13:N:85:GLU:HB2   | 13:N:98:PRO:HB3   | 1.89                     | 0.53              |
| 14:O:38:LEU:O     | 14:O:124:ARG:NH2  | 2.41                     | 0.53              |
| 27:d:28:ASN:HD21  | 27:d:31:THR:HG23  | 1.73                     | 0.53              |
| 33:j:30:TYR:CE2   | 41:s:59:GLU:HB2   | 2.43                     | 0.53              |
| 41:s:90:PRO:HD2   | 41:s:240:ILE:HD13 | 1.90                     | 0.53              |
| 1:A:119:GLU:O     | 1:A:119:GLU:HG3   | 2.09                     | 0.53              |
| 26:c:159:LYS:NZ   | 43:v:57:ASP:OD2   | 2.40                     | 0.53              |
| 40:r:251:ASN:HD21 | 40:r:304:GLN:HE22 | 1.55                     | 0.53              |
| 44:w:66:ILE:HD11  | 44:w:237:ILE:CD1  | 2.38                     | 0.53              |
| 16:Q:274:ASP:OD1  | 16:Q:323:ARG:NH1  | 2.41                     | 0.53              |
| 21:W:30:LEU:HD23  | 21:W:35:MET:HG2   | 1.90                     | 0.53              |
| 16:Q:102:SER:OG   | 16:Q:107:ARG:NH1  | 2.42                     | 0.53              |
| 27:d:114:GLN:HG3  | 35:l:203:MET:HG2  | 1.91                     | 0.53              |
| 27:d:144:SER:O    | 27:d:158:LYS:NZ   | 2.40                     | 0.53              |
| 33:j:73:LEU:O     | 41:s:160:TYR:OH   | 2.26                     | 0.53              |
| 49:n:101:PLX:O7   | 49:n:101:PLX:H92  | 2.07                     | 0.53              |
| 12:M:544:VAL:HG23 | 12:M:565:PHE:HB3  | 1.90                     | 0.53              |
| 44:w:63:ASP:HB3   | 44:w:241:TYR:CE1  | 2.44                     | 0.53              |
| 7:H:51:ILE:HG22   | 7:H:55:LYS:HE2    | 1.90                     | 0.53              |
| 12:M:487:THR:OG1  | 12:M:677:GLN:OE1  | 2.21                     | 0.53              |
| 30:g:36:MET:HE2   | 32:i:339:MET:HE2  | 1.90                     | 0.53              |
| 13:N:68:MET:CG    | 13:N:69:ASN:H     | 2.22                     | 0.53              |
| 16:Q:39:PRO:HB3   | 16:Q:43:TRP:CD1   | 2.44                     | 0.53              |
| 16:Q:68:ASP:O     | 32:i:49:ASN:ND2   | 2.42                     | 0.53              |
| 16:Q:182:ASN:OD1  | 16:Q:404:LYS:NZ   | 2.41                     | 0.53              |
| 22:Y:43:ARG:HG3   | 22:Y:48:PRO:HA    | 1.91                     | 0.53              |
| 54:i:401:CDL:H331 | 54:i:401:CDL:OA9  | 2.09                     | 0.53              |
| 44:w:216:SER:O    | 44:w:220:LYS:HG2  | 2.08                     | 0.53              |
| 2:B:99:GLY:O      | 2:B:169:GLU:HG3   | 2.09                     | 0.53              |
| 12:M:389:THR:O    | 12:M:390:THR:OG1  | 2.24                     | 0.53              |
| 6:X:123:GLU:HG2   | 6:X:129:GLU:HA    | 1.91                     | 0.53              |
| 44:w:214:ILE:CG2  | 44:w:234:LEU:HD13 | 2.35                     | 0.53              |
| 32:i:334:THR:HG21 | 54:r:714:CDL:H391 | 1.89                     | 0.53              |
| 35:l:86:SER:OG    | 35:l:262:ARG:NH2  | 2.42                     | 0.53              |
| 35:l:102:GLU:OE2  | 35:l:456:ARG:NH2  | 2.32                     | 0.53              |
| 9:J:257:ASP:O     | 9:J:261:LYS:NZ    | 2.40                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:224:ASP:OD2  | 12:M:291:ARG:NH2  | 2.35                     | 0.52              |
| 16:Q:206:GLU:OE2  | 16:Q:209:LYS:NZ   | 2.42                     | 0.52              |
| 27:d:26:LEU:HD12  | 27:d:27:PRO:HD2   | 1.90                     | 0.52              |
| 30:g:36:MET:HE3   | 30:g:74:GLY:HA2   | 1.90                     | 0.52              |
| 32:i:270:MET:HE1  | 32:i:282:MET:SD   | 2.49                     | 0.52              |
| 35:l:8:THR:HG23   | 35:l:82:MET:HE3   | 1.91                     | 0.52              |
| 44:w:63:ASP:OD2   | 44:w:245:PHE:CZ   | 2.61                     | 0.52              |
| 12:M:217:GLU:HG3  | 12:M:412:PRO:HB3  | 1.90                     | 0.52              |
| 12:M:638:THR:O    | 12:M:642:VAL:HG23 | 2.10                     | 0.52              |
| 34:k:11:ALA:HB1   | 36:m:17:PHE:CD2   | 2.44                     | 0.52              |
| 7:H:72:LEU:HD13   | 7:H:80:VAL:HG11   | 1.91                     | 0.52              |
| 8:I:13:ASN:HD22   | 8:I:19:ASP:HA     | 1.74                     | 0.52              |
| 24:a:96:ALA:HB2   | 27:d:61:TYR:CE2   | 2.45                     | 0.52              |
| 44:w:65:ASN:HB3   | 44:w:214:ILE:CD1  | 2.39                     | 0.52              |
| 11:L:89:SER:O     | 12:M:59:GLN:NE2   | 2.41                     | 0.52              |
| 32:i:289:ASN:HA   | 32:i:292:PHE:CE2  | 2.45                     | 0.52              |
| 35:l:5:ALA:HB2    | 35:l:61:MET:SD    | 2.49                     | 0.52              |
| 35:l:66:TRP:O     | 35:l:78:LEU:N     | 2.37                     | 0.52              |
| 37:n:30:ARG:O     | 37:n:33:GLU:HG2   | 2.10                     | 0.52              |
| 12:M:406:ASN:ND2  | 12:M:688:GLN:O    | 2.35                     | 0.52              |
| 24:a:152:LYS:HD3  | 30:g:96:VAL:HG21  | 1.91                     | 0.52              |
| 33:j:87:MET:HE1   | 41:s:309:ILE:HD11 | 1.91                     | 0.52              |
| 41:s:130:ILE:O    | 41:s:134:ARG:HG3  | 2.09                     | 0.52              |
| 14:O:171:LEU:O    | 14:O:172:ILE:HD13 | 2.10                     | 0.52              |
| 35:l:27:TYR:O     | 35:l:115:ASN:ND2  | 2.36                     | 0.52              |
| 1:A:185:ASN:C     | 1:A:187:CYS:H     | 2.18                     | 0.52              |
| 20:V:95:CYS:HB2   | 20:V:115:CYS:CA   | 2.18                     | 0.52              |
| 54:V:203:CDL:H822 | 54:V:203:CDL:H781 | 1.91                     | 0.52              |
| 23:Z:25:GLU:HA    | 23:Z:30:GLU:OE2   | 2.10                     | 0.52              |
| 34:k:23:ARG:HG2   | 36:m:23:LYS:HE2   | 1.91                     | 0.52              |
| 36:m:17:PHE:CD1   | 36:m:20:PHE:HE1   | 2.27                     | 0.52              |
| 41:s:200:LEU:HD11 | 41:s:285:LEU:HD21 | 1.90                     | 0.52              |
| 17:S:55:SER:O     | 17:S:64:LYS:NZ    | 2.43                     | 0.52              |
| 32:i:40:MET:HE3   | 32:i:44:LEU:HD21  | 1.92                     | 0.52              |
| 32:i:220:ILE:HB   | 32:i:323:MET:HE1  | 1.92                     | 0.52              |
| 32:i:347:ASN:HB3  | 49:i:705:PLX:H301 | 1.91                     | 0.52              |
| 1:A:102:MET:HG2   | 1:A:149:MET:HE2   | 1.91                     | 0.52              |
| 6:G:75:THR:O      | 6:G:76:LEU:C      | 2.53                     | 0.52              |
| 10:K:109:ARG:HH11 | 10:K:109:ARG:HG3  | 1.75                     | 0.52              |
| 11:L:112:MET:HA   | 11:L:112:MET:HE2  | 1.92                     | 0.52              |
| 34:k:37:MET:SD    | 34:k:67:ALA:HB3   | 2.50                     | 0.52              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:u:137:LEU:HD12 | 42:u:138:PRO:HD2  | 1.92                     | 0.52              |
| 4:E:39:TRP:O      | 4:E:43:VAL:HG23   | 2.10                     | 0.51              |
| 7:H:38:ILE:O      | 7:H:45:ARG:NH1    | 2.36                     | 0.51              |
| 40:r:403:THR:HA   | 40:r:406:TYR:CE2  | 2.45                     | 0.51              |
| 6:G:90:TYR:OH     | 6:G:117:GLU:OE1   | 2.25                     | 0.51              |
| 35:l:161:ARG:NH2  | 39:p:88:GLY:O     | 2.43                     | 0.51              |
| 1:A:213:ILE:HG12  | 1:A:235:VAL:HG13  | 1.92                     | 0.51              |
| 36:m:125:TRP:HA   | 36:m:128:TYR:CD2  | 2.46                     | 0.51              |
| 1:A:185:ASN:O     | 1:A:187:CYS:N     | 2.43                     | 0.51              |
| 35:l:161:ARG:NH1  | 35:l:238:GLU:OE2  | 2.40                     | 0.51              |
| 2:B:99:GLY:H      | 2:B:169:GLU:HG2   | 1.75                     | 0.51              |
| 32:i:236:LYS:HD3  | 32:i:237:MET:HE2  | 1.92                     | 0.51              |
| 54:l:712:CDL:H611 | 54:l:712:CDL:H811 | 1.92                     | 0.51              |
| 1:A:408:GLU:O     | 1:A:411:SER:HB3   | 2.11                     | 0.51              |
| 4:E:101:THR:OG1   | 15:P:219:VAL:O    | 2.19                     | 0.51              |
| 7:H:30:LYS:O      | 7:H:34:VAL:HG23   | 2.11                     | 0.51              |
| 12:M:382:ARG:HG2  | 12:M:386:LEU:HD11 | 1.93                     | 0.51              |
| 14:O:236:GLU:HG2  | 14:O:237:PRO:HD2  | 1.93                     | 0.51              |
| 48:l:718:PEE:H34  | 48:l:718:PEE:H41  | 1.91                     | 0.51              |
| 44:w:129:TYR:OH   | 44:w:186:HIS:ND1  | 2.27                     | 0.51              |
| 27:d:60:ARG:NH2   | 27:d:62:TYR:OH    | 2.43                     | 0.51              |
| 27:d:106:ILE:HG13 | 27:d:135:VAL:HG21 | 1.93                     | 0.51              |
| 44:w:295:ARG:HA   | 44:w:298:VAL:HG22 | 1.92                     | 0.51              |
| 44:w:343:TYR:HA   | 44:w:352:ILE:HD12 | 1.93                     | 0.51              |
| 8:I:8:ILE:HD11    | 54:N:202:CDL:H142 | 1.93                     | 0.51              |
| 10:K:98:MET:SD    | 10:K:98:MET:N     | 2.83                     | 0.51              |
| 49:e:201:PLX:H131 | 54:l:712:CDL:H632 | 1.93                     | 0.51              |
| 3:C:192:ILE:HG13  | 9:J:87:GLU:HG2    | 1.92                     | 0.51              |
| 8:I:40:LYS:HB3    | 21:W:7:LYS:H      | 1.76                     | 0.51              |
| 24:a:127:ASP:CG   | 49:n:101:PLX:H1C2 | 2.35                     | 0.51              |
| 2:B:37:THR:OG1    | 16:Q:317:ASP:OD1  | 2.23                     | 0.51              |
| 9:J:192:ARG:NH1   | 9:J:198:ALA:O     | 2.44                     | 0.51              |
| 43:v:27:PRO:HB2   | 43:v:34:ARG:HE    | 1.76                     | 0.51              |
| 48:C:311:PEE:C42  | 41:s:56:PHE:HD2   | 2.22                     | 0.50              |
| 21:W:93:GLU:OE1   | 31:h:92:TYR:OH    | 2.21                     | 0.50              |
| 54:a:201:CDL:H382 | 27:d:48:ALA:HB2   | 1.93                     | 0.50              |
| 25:b:85:TYR:CE1   | 48:l:720:PEE:H48  | 2.45                     | 0.50              |
| 35:l:264:TYR:CD2  | 35:l:265:PRO:HD3  | 2.46                     | 0.50              |
| 48:m:202:PEE:O4   | 48:m:202:PEE:H18  | 2.11                     | 0.50              |
| 39:p:92:GLU:HB3   | 39:p:95:GLU:HG3   | 1.92                     | 0.50              |
| 13:N:39:VAL:CG2   | 13:N:50:GLU:HG2   | 2.42                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:X:90:TYR:HE1    | 23:Z:44:PRO:HB2   | 1.76                     | 0.50              |
| 40:r:299:VAL:O    | 40:r:303:ILE:HG12 | 2.10                     | 0.50              |
| 12:M:347:ASP:HB3  | 12:M:594:ALA:HB1  | 1.92                     | 0.50              |
| 12:M:538:ARG:HG2  | 12:M:538:ARG:HH11 | 1.77                     | 0.50              |
| 35:l:76:LEU:HD21  | 35:l:196:TRP:HE3  | 1.76                     | 0.50              |
| 54:l:712:CDL:H842 | 54:l:712:CDL:C64  | 2.40                     | 0.50              |
| 48:l:719:PEE:H7   | 48:l:719:PEE:H13  | 1.90                     | 0.50              |
| 36:m:61:LEU:HD23  | 36:m:65:LEU:HD12  | 1.93                     | 0.50              |
| 43:v:39:MET:HE3   | 43:v:41:ALA:N     | 2.26                     | 0.50              |
| 15:P:119:VAL:HG12 | 15:P:121:THR:HG22 | 1.94                     | 0.50              |
| 32:i:88:LYS:HD2   | 32:i:148:SER:OG   | 2.12                     | 0.50              |
| 48:l:718:PEE:C1   | 48:l:718:PEE:H10  | 2.42                     | 0.50              |
| 36:m:125:TRP:HA   | 36:m:128:TYR:HD2  | 1.76                     | 0.50              |
| 38:o:3:PHE:CZ     | 39:p:70:GLU:HG3   | 2.46                     | 0.50              |
| 40:r:103:GLN:HE21 | 40:r:107:ILE:HD11 | 1.76                     | 0.50              |
| 5:F:44:LEU:HD22   | 5:F:91:LEU:HD21   | 1.93                     | 0.50              |
| 8:I:8:ILE:CG1     | 54:N:202:CDL:HA32 | 2.38                     | 0.50              |
| 16:Q:36:GLN:NE2   | 40:r:135:ARG:O    | 2.43                     | 0.50              |
| 19:U:14:ALA:O     | 19:U:15:LYS:HG2   | 2.12                     | 0.50              |
| 24:a:66:ARG:NH1   | 28:e:72:ASP:OD1   | 2.44                     | 0.50              |
| 54:a:201:CDL:HB21 | 48:l:720:PEE:H51  | 1.94                     | 0.50              |
| 9:J:180:TYR:O     | 9:J:183:SER:OG    | 2.28                     | 0.50              |
| 19:U:59:ASP:HA    | 19:U:63:MET:HE2   | 1.93                     | 0.50              |
| 35:l:290:LEU:O    | 35:l:293:ILE:HG22 | 2.12                     | 0.50              |
| 41:s:21:THR:CG2   | 41:s:224:PHE:HE1  | 2.25                     | 0.50              |
| 44:w:235:GLN:NE2  | 44:w:238:GLU:OE2  | 2.45                     | 0.50              |
| 13:N:106:ARG:HB2  | 13:N:109:ILE:HG13 | 1.93                     | 0.50              |
| 14:O:110:MET:O    | 14:O:114:GLU:HG3  | 2.12                     | 0.50              |
| 26:c:123:PRO:HD2  | 35:l:525:MET:HE1  | 1.93                     | 0.50              |
| 27:d:110:LEU:HD11 | 35:l:203:MET:HE2  | 1.93                     | 0.50              |
| 54:l:712:CDL:H331 | 54:l:712:CDL:OA9  | 2.10                     | 0.50              |
| 40:r:300:ALA:O    | 40:r:308:SER:HB3  | 2.12                     | 0.50              |
| 1:A:210:THR:HB    | 1:A:224:ARG:HG2   | 1.93                     | 0.50              |
| 3:C:126:GLU:O     | 3:C:128:ARG:N     | 2.45                     | 0.50              |
| 3:C:187:GLU:OE2   | 3:C:189:ARG:NH1   | 2.45                     | 0.50              |
| 20:V:65:ALA:O     | 20:V:69:ILE:HG12  | 2.12                     | 0.50              |
| 42:u:44:MET:HE3   | 42:u:48:TRP:CH2   | 2.47                     | 0.50              |
| 42:u:83:THR:HA    | 42:u:86:TRP:CD1   | 2.46                     | 0.50              |
| 14:O:179:ALA:HB3  | 14:O:185:MET:SD   | 2.52                     | 0.50              |
| 34:k:4:VAL:O      | 34:k:8:ILE:HG12   | 2.11                     | 0.50              |
| 35:l:557:TRP:O    | 35:l:561:ILE:HG12 | 2.12                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:3:SER:O       | 54:N:202:CDL:CA2  | 2.59                     | 0.49              |
| 54:N:202:CDL:C34  | 54:N:202:CDL:CA7  | 2.89                     | 0.49              |
| 14:O:206:ASP:OD1  | 14:O:207:GLU:N    | 2.45                     | 0.49              |
| 15:P:125:ARG:HH22 | 15:P:201:ASP:CG   | 2.20                     | 0.49              |
| 24:a:61:GLY:O     | 24:a:65:ARG:HG3   | 2.11                     | 0.49              |
| 24:a:168:TRP:CD2  | 30:g:2:THR:HG23   | 2.47                     | 0.49              |
| 26:c:81:ARG:NE    | 26:c:85:GLU:OE1   | 2.42                     | 0.49              |
| 26:c:166:LEU:HD22 | 26:c:169:GLU:OE2  | 2.12                     | 0.49              |
| 15:P:125:ARG:NH2  | 15:P:201:ASP:OD1  | 2.44                     | 0.49              |
| 39:p:16:VAL:HG22  | 39:p:64:LEU:HD13  | 1.93                     | 0.49              |
| 13:N:73:THR:HG22  | 13:N:73:THR:O     | 2.11                     | 0.49              |
| 54:V:203:CDL:H832 | 54:V:203:CDL:C79  | 2.18                     | 0.49              |
| 41:s:96:ILE:HG22  | 41:s:98:MET:HG3   | 1.94                     | 0.49              |
| 44:w:69:GLY:C     | 44:w:71:GLY:H     | 2.17                     | 0.49              |
| 2:B:44:ARG:HH21   | 8:I:112:TYR:HB3   | 1.77                     | 0.49              |
| 54:V:203:CDL:C79  | 54:V:203:CDL:C83  | 2.86                     | 0.49              |
| 43:v:60:ALA:O     | 43:v:64:ILE:HG12  | 2.12                     | 0.49              |
| 16:Q:431:HIS:O    | 16:Q:454:GLN:NE2  | 2.45                     | 0.49              |
| 40:r:204:MET:HG3  | 40:r:209:LEU:HB2  | 1.94                     | 0.49              |
| 40:r:251:ASN:HD21 | 40:r:304:GLN:NE2  | 2.11                     | 0.49              |
| 26:c:33:THR:OG1   | 26:c:35:ASP:OD1   | 2.26                     | 0.49              |
| 34:k:45:THR:HG23  | 36:m:52:LEU:HD13  | 1.95                     | 0.49              |
| 35:l:536:LEU:HB3  | 35:l:537:PRO:HD3  | 1.93                     | 0.49              |
| 44:w:63:ASP:O     | 44:w:206:TYR:HD1  | 1.95                     | 0.49              |
| 2:B:96:ARG:O      | 16:Q:219:GLY:HA3  | 2.13                     | 0.49              |
| 4:E:117:ASP:OD1   | 4:E:120:SER:OG    | 2.15                     | 0.49              |
| 12:M:149:ASP:OD2  | 12:M:150:ARG:NH1  | 2.46                     | 0.49              |
| 15:P:64:TYR:OH    | 15:P:103:HIS:NE2  | 2.35                     | 0.49              |
| 16:Q:176:GLU:OE2  | 16:Q:311:TYR:OH   | 2.18                     | 0.49              |
| 32:i:84:TRP:HH2   | 34:k:59:MET:HE2   | 1.77                     | 0.49              |
| 35:l:173:LEU:HD13 | 40:r:405:LEU:HD21 | 1.94                     | 0.49              |
| 41:s:170:GLU:OE2  | 42:u:98:ARG:NH2   | 2.43                     | 0.49              |
| 3:C:161:ILE:HG13  | 3:C:180:LEU:HB2   | 1.94                     | 0.49              |
| 9:J:129:LEU:HD23  | 9:J:167:ILE:HG13  | 1.95                     | 0.49              |
| 9:J:145:PHE:CD1   | 9:J:184:LYS:HE3   | 2.46                     | 0.49              |
| 41:s:235:ASN:ND2  | 41:s:266:LEU:HB3  | 2.28                     | 0.49              |
| 44:w:64:GLY:N     | 44:w:70:LYS:HD3   | 2.27                     | 0.49              |
| 35:l:49:VAL:HB    | 35:l:50:PRO:HD3   | 1.94                     | 0.49              |
| 38:o:48:LEU:HB3   | 39:p:166:LEU:HD13 | 1.95                     | 0.49              |
| 40:r:271:MET:HE2  | 40:r:271:MET:HA   | 1.94                     | 0.49              |
| 41:s:86:TRP:NE1   | 41:s:233:MET:HB2  | 2.26                     | 0.49              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:l:718:PEE:H10  | 48:l:718:PEE:H2   | 1.94                     | 0.49              |
| 37:n:13:VAL:HG13  | 40:r:14:MET:HA    | 1.95                     | 0.49              |
| 44:w:213:GLU:HG2  | 44:w:217:ARG:HD2  | 1.93                     | 0.49              |
| 7:H:69:GLU:HG2    | 7:H:77:ILE:HG12   | 1.95                     | 0.48              |
| 39:p:100:PRO:HG3  | 40:r:419:TYR:CE1  | 2.47                     | 0.48              |
| 1:A:182:ILE:HD11  | 1:A:193:PHE:HD2   | 1.78                     | 0.48              |
| 5:F:37:ILE:HD12   | 5:F:37:ILE:H      | 1.78                     | 0.48              |
| 16:Q:181:LEU:HD23 | 16:Q:207:ARG:HG2  | 1.95                     | 0.48              |
| 48:V:202:PEE:H35  | 40:r:159:PRO:HG2  | 1.94                     | 0.48              |
| 48:V:207:PEE:O4   | 48:V:207:PEE:H10  | 2.13                     | 0.48              |
| 48:l:718:PEE:H37  | 48:l:718:PEE:H60  | 1.95                     | 0.48              |
| 44:w:170:LEU:HD21 | 44:w:184:VAL:HG23 | 1.94                     | 0.48              |
| 12:M:171:THR:HG23 | 12:M:173:MET:SD   | 2.52                     | 0.48              |
| 33:j:49:LEU:N     | 33:j:50:PRO:HD2   | 2.28                     | 0.48              |
| 35:l:105:MET:HB2  | 35:l:449:LEU:HD13 | 1.95                     | 0.48              |
| 36:m:25:SER:O     | 36:m:27:ILE:N     | 2.46                     | 0.48              |
| 38:o:113:GLU:O    | 38:o:117:GLN:HG2  | 2.13                     | 0.48              |
| 44:w:110:GLY:HA2  | 44:w:134:TRP:CD2  | 2.47                     | 0.48              |
| 14:O:100:LYS:O    | 14:O:104:ILE:HG12 | 2.13                     | 0.48              |
| 35:l:221:ALA:HA   | 35:l:226:GLN:HG2  | 1.95                     | 0.48              |
| 1:A:115:VAL:HG21  | 1:A:142:CYS:SG    | 2.53                     | 0.48              |
| 3:C:67:PHE:HE2    | 3:C:103:MET:HE2   | 1.79                     | 0.48              |
| 48:C:311:PEE:H49  | 33:j:28:ASN:HD22  | 1.78                     | 0.48              |
| 11:L:174:THR:HG23 | 14:O:111:ARG:HD2  | 1.94                     | 0.48              |
| 13:N:120:THR:HG22 | 13:N:122:GLN:H    | 1.78                     | 0.48              |
| 16:Q:84:PHE:HE2   | 16:Q:444:LEU:HD11 | 1.78                     | 0.48              |
| 20:V:108:TYR:CE2  | 54:V:203:CDL:OA6  | 2.66                     | 0.48              |
| 31:h:88:LYS:HB3   | 31:h:88:LYS:HE2   | 1.63                     | 0.48              |
| 2:B:47:SER:OG     | 2:B:49:ASP:OD1    | 2.24                     | 0.48              |
| 11:L:158:LYS:NZ   | 12:M:69:LEU:O     | 2.30                     | 0.48              |
| 12:M:347:ASP:CB   | 12:M:594:ALA:HB1  | 2.43                     | 0.48              |
| 27:d:159:GLN:O    | 27:d:163:MET:HG3  | 2.12                     | 0.48              |
| 28:e:70:ASN:O     | 28:e:73:SER:HB2   | 2.14                     | 0.48              |
| 33:j:13:LEU:HD13  | 41:s:10:ILE:HG21  | 1.96                     | 0.48              |
| 34:k:25:HIS:O     | 34:k:28:SER:N     | 2.40                     | 0.48              |
| 9:J:179:ARG:O     | 9:J:183:SER:OG    | 2.30                     | 0.48              |
| 14:O:137:THR:HG22 | 14:O:138:THR:H    | 1.79                     | 0.48              |
| 16:Q:65:PRO:HB2   | 16:Q:67:ASN:O     | 2.13                     | 0.48              |
| 21:W:66:GLU:OE1   | 42:u:123:GLY:N    | 2.43                     | 0.48              |
| 6:X:93:ILE:HD11   | 6:X:110:LEU:HD11  | 1.95                     | 0.48              |
| 24:a:83:ALA:HA    | 54:a:201:CDL:H161 | 1.96                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:a:201:CDL:H772 | 54:a:201:CDL:H201 | 1.94                     | 0.48              |
| 48:l:719:PEE:C11  | 48:l:719:PEE:C3   | 2.85                     | 0.48              |
| 43:v:106:ARG:O    | 43:v:110:GLN:HG2  | 2.14                     | 0.48              |
| 48:C:311:PEE:H72  | 41:s:56:PHE:CE2   | 2.48                     | 0.48              |
| 15:P:186:ARG:NH1  | 15:P:189:THR:OG1  | 2.39                     | 0.48              |
| 25:b:106:PRO:HA   | 25:b:117:ILE:HG22 | 1.96                     | 0.48              |
| 33:j:15:SER:HA    | 41:s:76:ILE:HD12  | 1.95                     | 0.48              |
| 40:r:14:MET:HE3   | 40:r:14:MET:HB3   | 1.83                     | 0.48              |
| 44:w:148:GLU:OE1  | 44:w:301:LYS:NZ   | 2.40                     | 0.48              |
| 6:G:75:THR:HB     | 6:G:156:GLU:OE1   | 2.14                     | 0.48              |
| 9:J:163:LYS:NZ    | 9:J:253:ILE:O     | 2.42                     | 0.48              |
| 13:N:73:THR:HG22  | 13:N:77:VAL:HG12  | 1.95                     | 0.48              |
| 21:W:114:THR:OG1  | 42:u:143:HIS:ND1  | 2.35                     | 0.48              |
| 54:a:201:CDL:H191 | 54:a:201:CDL:H732 | 1.95                     | 0.48              |
| 32:i:222:SER:O    | 32:i:224:ALA:N    | 2.47                     | 0.48              |
| 41:s:277:TYR:HE2  | 48:s:401:PEE:C36  | 2.27                     | 0.48              |
| 42:u:18:VAL:HG12  | 42:u:20:VAL:HG22  | 1.96                     | 0.48              |
| 36:m:17:PHE:O     | 36:m:21:SER:HB2   | 2.14                     | 0.48              |
| 44:w:58:LYS:HZ3   | 44:w:278:CYS:HB2  | 1.79                     | 0.48              |
| 9:J:127:ILE:HD11  | 9:J:253:ILE:HD11  | 1.95                     | 0.47              |
| 16:Q:184:ILE:HD11 | 16:Q:251:PHE:CZ   | 2.49                     | 0.47              |
| 32:i:321:LYS:NZ   | 54:i:401:CDL:OA4  | 2.46                     | 0.47              |
| 42:u:114:LYS:HB2  | 42:u:115:LEU:HD12 | 1.95                     | 0.47              |
| 1:A:109:ARG:HG2   | 11:L:166:TRP:CD1  | 2.49                     | 0.47              |
| 5:F:71:PHE:CD1    | 12:M:362:ASP:HB2  | 2.49                     | 0.47              |
| 7:H:38:ILE:HB     | 7:H:45:ARG:HD2    | 1.94                     | 0.47              |
| 28:e:144:PRO:HA   | 28:e:147:ILE:HD12 | 1.96                     | 0.47              |
| 32:i:335:LEU:HD21 | 54:r:714:CDL:H402 | 1.96                     | 0.47              |
| 33:j:95:LEU:HD23  | 33:j:98:LEU:HD23  | 1.96                     | 0.47              |
| 35:l:78:LEU:HD11  | 54:l:712:CDL:H251 | 1.95                     | 0.47              |
| 35:l:152:PHE:HB2  | 35:l:172:ILE:HD11 | 1.95                     | 0.47              |
| 2:B:98:ARG:NH2    | 16:Q:224:ALA:O    | 2.44                     | 0.47              |
| 5:F:23:LEU:O      | 5:F:57:GLU:HA     | 2.14                     | 0.47              |
| 16:Q:70:ASP:OD2   | 32:i:51:ARG:NH1   | 2.48                     | 0.47              |
| 26:c:108:ASP:HB3  | 26:c:111:MET:HE2  | 1.96                     | 0.47              |
| 31:h:103:ASP:OD1  | 31:h:103:ASP:O    | 2.32                     | 0.47              |
| 44:w:132:GLN:HE22 | 57:w:401:ADP:N6   | 2.12                     | 0.47              |
| 1:A:385:CYS:HB3   | 45:A:501:SF4:S2   | 2.54                     | 0.47              |
| 3:C:50:LEU:HD23   | 48:C:311:PEE:H26  | 1.92                     | 0.47              |
| 21:W:128:ARG:NH1  | 31:h:102:GLU:OE1  | 2.38                     | 0.47              |
| 25:b:85:TYR:CD1   | 48:l:720:PEE:H48  | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:20:VAL:HG11  | 32:i:137:ALA:HB1  | 1.97                     | 0.47              |
| 35:l:166:THR:CG2  | 48:l:719:PEE:H2   | 2.44                     | 0.47              |
| 5:F:42:VAL:HG23   | 12:M:671:LEU:CD1  | 2.44                     | 0.47              |
| 16:Q:140:ASP:OD2  | 16:Q:143:SER:OG   | 2.25                     | 0.47              |
| 24:a:187:PRO:HA   | 42:u:48:TRP:CD1   | 2.49                     | 0.47              |
| 27:d:164:LEU:HD12 | 28:e:149:LEU:HD22 | 1.97                     | 0.47              |
| 33:j:17:LEU:HA    | 33:j:20:ILE:HG12  | 1.96                     | 0.47              |
| 33:j:53:MET:HG3   | 33:j:57:LEU:HD23  | 1.95                     | 0.47              |
| 35:l:372:ALA:HA   | 35:l:458:LEU:HD21 | 1.97                     | 0.47              |
| 18:T:47:ASP:O     | 18:T:52:ARG:NH1   | 2.47                     | 0.47              |
| 29:f:47:THR:HG23  | 30:g:65:LEU:HD22  | 1.96                     | 0.47              |
| 32:i:40:MET:HE1   | 32:i:129:LEU:HD23 | 1.97                     | 0.47              |
| 39:p:120:ALA:O    | 39:p:124:GLN:HG2  | 2.13                     | 0.47              |
| 41:s:85:MET:SD    | 41:s:108:MET:HB2  | 2.55                     | 0.47              |
| 1:A:98:LYS:HA     | 1:A:101:PHE:HD2   | 1.80                     | 0.47              |
| 3:C:126:GLU:HB2   | 41:s:59:GLU:OE1   | 2.15                     | 0.47              |
| 4:E:98:LYS:HB3    | 4:E:102:HIS:HB2   | 1.96                     | 0.47              |
| 4:E:98:LYS:HE2    | 4:E:102:HIS:HB3   | 1.96                     | 0.47              |
| 9:J:37:HIS:CE1    | 18:T:49:ASP:HA    | 2.49                     | 0.47              |
| 12:M:266:ARG:HB3  | 12:M:271:MET:HE3  | 1.96                     | 0.47              |
| 54:N:202:CDL:C32  | 54:N:202:CDL:C54  | 2.88                     | 0.47              |
| 20:V:81:ARG:HH22  | 20:V:88:LEU:HD22  | 1.78                     | 0.47              |
| 54:V:201:CDL:C74  | 54:V:201:CDL:C61  | 2.88                     | 0.47              |
| 25:b:14:GLN:NE2   | 39:p:157:ALA:HB3  | 2.26                     | 0.47              |
| 29:f:63:LYS:O     | 29:f:67:LEU:HD13  | 2.15                     | 0.47              |
| 34:k:58:MET:SD    | 36:m:146:LEU:HA   | 2.55                     | 0.47              |
| 41:s:62:ARG:HH11  | 41:s:64:ALA:HA    | 1.79                     | 0.47              |
| 41:s:66:SER:OG    | 41:s:122:ALA:O    | 2.17                     | 0.47              |
| 44:w:161:ARG:HD3  | 44:w:241:TYR:OH   | 2.14                     | 0.47              |
| 32:i:203:LEU:HB2  | 32:i:347:ASN:HD21 | 1.78                     | 0.47              |
| 35:l:292:ALA:HB2  | 35:l:304:PHE:HB3  | 1.97                     | 0.47              |
| 1:A:151:ALA:O     | 1:A:191:TYR:OH    | 2.25                     | 0.47              |
| 2:B:98:ARG:HB3    | 2:B:169:GLU:CD    | 2.39                     | 0.47              |
| 6:X:75:THR:OG1    | 6:X:156:GLU:O     | 2.25                     | 0.47              |
| 54:n:102:CDL:H781 | 54:n:102:CDL:H752 | 1.62                     | 0.47              |
| 40:r:122:PHE:CZ   | 40:r:206:LYS:HD3  | 2.49                     | 0.47              |
| 43:v:93:LEU:HA    | 43:v:96:VAL:HG22  | 1.97                     | 0.47              |
| 1:A:134:ASP:N     | 1:A:134:ASP:OD1   | 2.47                     | 0.47              |
| 5:F:18:GLU:OE1    | 5:F:68:ARG:NH1    | 2.48                     | 0.47              |
| 16:Q:196:ALA:O    | 16:Q:197:MET:HG2  | 2.14                     | 0.47              |
| 25:b:13:GLN:HA    | 25:b:16:ARG:HH11  | 1.80                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:b:81:ILE:HG23  | 48:l:720:PEE:H58  | 1.97                     | 0.47              |
| 27:d:82:ILE:HG23  | 27:d:83:LEU:HD22  | 1.96                     | 0.47              |
| 35:l:450:LEU:O    | 35:l:454:ILE:HG12 | 2.14                     | 0.47              |
| 44:w:86:PHE:HB2   | 44:w:159:LEU:HD23 | 1.96                     | 0.47              |
| 4:E:16:SER:HA     | 11:L:54:ALA:HA    | 1.97                     | 0.46              |
| 54:N:202:CDL:H312 | 54:N:202:CDL:C52  | 2.31                     | 0.46              |
| 17:S:1:MET:HB2    | 17:S:3:PHE:CE2    | 2.50                     | 0.46              |
| 22:Y:52:ARG:O     | 22:Y:56:ILE:HG23  | 2.15                     | 0.46              |
| 39:p:132:SER:HB2  | 39:p:163:LEU:HD13 | 1.97                     | 0.46              |
| 40:r:281:ASP:OD1  | 40:r:340:ARG:HG2  | 2.16                     | 0.46              |
| 44:w:65:ASN:HB3   | 44:w:214:ILE:HD11 | 1.97                     | 0.46              |
| 1:A:177:TYR:CD2   | 10:K:93:LEU:HD22  | 2.49                     | 0.46              |
| 8:I:12:ARG:HD3    | 8:I:20:LEU:HD22   | 1.98                     | 0.46              |
| 9:J:213:PHE:CD1   | 9:J:214:LEU:HD12  | 2.47                     | 0.46              |
| 12:M:251:ILE:HB   | 12:M:606:THR:HG22 | 1.96                     | 0.46              |
| 49:V:205:PLX:H191 | 40:r:201:MET:HE1  | 1.97                     | 0.46              |
| 6:X:143:GLU:OE1   | 25:b:9:LYS:HE2    | 2.14                     | 0.46              |
| 25:b:24:LYS:O     | 25:b:27:GLU:HG3   | 2.15                     | 0.46              |
| 35:l:245:ALA:O    | 35:l:249:SER:OG   | 2.24                     | 0.46              |
| 2:B:114:ILE:HD12  | 12:M:130:ILE:HG23 | 1.97                     | 0.46              |
| 12:M:29:SER:OG    | 12:M:30:ASN:N     | 2.48                     | 0.46              |
| 12:M:445:LEU:HD22 | 12:M:460:HIS:HE1  | 1.80                     | 0.46              |
| 41:s:233:MET:HE3  | 41:s:233:MET:HB3  | 1.78                     | 0.46              |
| 19:U:9:LEU:CD1    | 48:U:101:PEE:H68  | 2.45                     | 0.46              |
| 30:g:7:ARG:NH1    | 30:g:91:ASP:OD1   | 2.48                     | 0.46              |
| 34:k:80:MET:HE3   | 36:m:172:THR:HA   | 1.98                     | 0.46              |
| 54:n:102:CDL:C58  | 54:n:102:CDL:C54  | 2.86                     | 0.46              |
| 43:v:80:CYS:HB3   | 43:v:83:GLU:OE1   | 2.16                     | 0.46              |
| 1:A:65:THR:OG1    | 1:A:140:GLU:OE1   | 2.33                     | 0.46              |
| 14:O:168:LEU:HB3  | 14:O:169:PHE:HD1  | 1.81                     | 0.46              |
| 19:U:38:TYR:HB2   | 41:s:310:MET:O    | 2.16                     | 0.46              |
| 20:V:29:GLY:O     | 20:V:63:SER:OG    | 2.33                     | 0.46              |
| 22:Y:39:HIS:NE2   | 23:Z:10:GLY:HA2   | 2.31                     | 0.46              |
| 41:s:87:VAL:N     | 41:s:88:PRO:CD    | 2.74                     | 0.46              |
| 2:B:200:GLU:HG3   | 13:N:88:ARG:HB2   | 1.98                     | 0.46              |
| 12:M:36:VAL:HB    | 12:M:56:VAL:HG21  | 1.98                     | 0.46              |
| 54:V:201:CDL:H532 | 35:l:577:VAL:HA   | 1.96                     | 0.46              |
| 35:l:331:MET:CE   | 35:l:465:GLY:HA2  | 2.46                     | 0.46              |
| 35:l:529:TYR:HB3  | 35:l:530:PRO:HD3  | 1.98                     | 0.46              |
| 35:l:581:LYS:HB3  | 35:l:583:LEU:HD23 | 1.98                     | 0.46              |
| 39:p:63:LEU:C     | 39:p:65:ARG:H     | 2.24                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:74:LEU:HD23   | 6:G:74:LEU:N      | 2.24                     | 0.46              |
| 8:I:13:ASN:ND2    | 8:I:20:LEU:H      | 2.14                     | 0.46              |
| 25:b:86:LEU:HD11  | 35:l:9:LEU:HD12   | 1.97                     | 0.46              |
| 25:b:93:LYS:HE2   | 25:b:93:LYS:HB2   | 1.73                     | 0.46              |
| 28:e:104:THR:CG2  | 49:n:101:PLX:H212 | 2.45                     | 0.46              |
| 35:l:33:PRO:HB2   | 35:l:105:MET:HE3  | 1.98                     | 0.46              |
| 35:l:592:LEU:O    | 35:l:596:MET:HG3  | 2.15                     | 0.46              |
| 42:u:69:ASP:O     | 42:u:73:GLN:HG3   | 2.16                     | 0.46              |
| 44:w:248:GLU:O    | 44:w:251:GLU:HG2  | 2.16                     | 0.46              |
| 8:I:13:ASN:ND2    | 8:I:19:ASP:HA     | 2.30                     | 0.46              |
| 22:Y:65:MET:SD    | 35:l:375:ILE:HG12 | 2.55                     | 0.46              |
| 24:a:168:TRP:HB3  | 30:g:2:THR:O      | 2.16                     | 0.46              |
| 26:c:40:PRO:O     | 26:c:74:ASP:HB2   | 2.15                     | 0.46              |
| 40:r:41:LEU:O     | 40:r:44:GLN:NE2   | 2.49                     | 0.46              |
| 13:N:4:VAL:O      | 13:N:8:ARG:HG3    | 2.15                     | 0.46              |
| 19:U:9:LEU:HD11   | 48:U:101:PEE:C41  | 2.46                     | 0.46              |
| 32:i:72:MET:HE3   | 32:i:76:ILE:HG13  | 1.98                     | 0.46              |
| 54:l:713:CDL:H421 | 54:l:713:CDL:H391 | 1.64                     | 0.46              |
| 36:m:170:GLU:HG3  | 36:m:173:ARG:HH21 | 1.81                     | 0.46              |
| 41:s:92:PRO:HG3   | 41:s:252:PRO:CB   | 2.46                     | 0.46              |
| 44:w:214:ILE:CG2  | 44:w:215:GLN:N    | 2.79                     | 0.46              |
| 44:w:258:TYR:CE2  | 44:w:269:VAL:HG22 | 2.51                     | 0.46              |
| 5:F:68:ARG:NH2    | 12:M:364:ASP:OD1  | 2.50                     | 0.45              |
| 5:F:90:THR:HA     | 5:F:93:ASN:HD22   | 1.80                     | 0.45              |
| 12:M:382:ARG:HE   | 12:M:527:ASP:CG   | 2.24                     | 0.45              |
| 12:M:445:LEU:HD22 | 12:M:460:HIS:CE1  | 2.51                     | 0.45              |
| 20:V:8:LYS:N      | 20:V:8:LYS:HD2    | 2.31                     | 0.45              |
| 6:X:119:ILE:HG21  | 6:X:135:ALA:HB1   | 1.98                     | 0.45              |
| 26:c:55:TYR:OH    | 26:c:74:ASP:O     | 2.17                     | 0.45              |
| 41:s:22:LEU:HD12  | 41:s:22:LEU:O     | 2.15                     | 0.45              |
| 41:s:26:LYS:HE2   | 41:s:37:PRO:O     | 2.16                     | 0.45              |
| 42:u:83:THR:HA    | 42:u:86:TRP:NE1   | 2.31                     | 0.45              |
| 1:A:116:ASN:O     | 1:A:245:VAL:HG23  | 2.16                     | 0.45              |
| 8:I:4:ALA:O       | 8:I:9:GLN:NE2     | 2.38                     | 0.45              |
| 9:J:166:HIS:HB3   | 9:J:200:ILE:HD13  | 1.97                     | 0.45              |
| 26:c:165:ASP:O    | 26:c:170:ARG:NH2  | 2.48                     | 0.45              |
| 27:d:142:ARG:NH1  | 28:e:138:GLU:O    | 2.42                     | 0.45              |
| 28:e:119:ARG:O    | 28:e:123:GLU:HG3  | 2.15                     | 0.45              |
| 35:l:480:THR:HG21 | 43:v:91:GLU:HB2   | 1.97                     | 0.45              |
| 40:r:74:PRO:O     | 40:r:78:MET:HG3   | 2.16                     | 0.45              |
| 1:A:36:LYS:HB2    | 1:A:39:ASP:HB2    | 1.99                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:110:PRO:O     | 1:A:238:CYS:HB3   | 2.17                     | 0.45              |
| 9:J:207:PHE:HB2   | 9:J:214:LEU:HD13  | 1.99                     | 0.45              |
| 16:Q:204:PHE:HA   | 16:Q:207:ARG:HB2  | 1.97                     | 0.45              |
| 17:S:43:TYR:CZ    | 21:W:68:ARG:HG3   | 2.52                     | 0.45              |
| 21:W:89:GLU:OE2   | 21:W:128:ARG:NH2  | 2.37                     | 0.45              |
| 36:m:166:VAL:O    | 36:m:170:GLU:OE1  | 2.33                     | 0.45              |
| 39:p:76:HIS:O     | 39:p:78:GLN:N     | 2.49                     | 0.45              |
| 7:H:76:GLN:O      | 7:H:79:GLU:N      | 2.48                     | 0.45              |
| 10:K:106:GLN:HB2  | 10:K:110:HIS:CD2  | 2.52                     | 0.45              |
| 13:N:97:PRO:HG2   | 13:N:100:THR:HG23 | 1.97                     | 0.45              |
| 32:i:313:MET:HE2  | 32:i:313:MET:HB3  | 1.79                     | 0.45              |
| 34:k:44:SER:O     | 34:k:48:ILE:HG12  | 2.17                     | 0.45              |
| 41:s:306:SER:O    | 41:s:310:MET:HG3  | 2.17                     | 0.45              |
| 1:A:85:LEU:HD21   | 1:A:247:THR:HG23  | 1.98                     | 0.45              |
| 9:J:167:ILE:HD13  | 9:J:201:ILE:HB    | 1.99                     | 0.45              |
| 12:M:129:PRO:O    | 12:M:241:ARG:NH2  | 2.50                     | 0.45              |
| 14:O:215:LYS:HA   | 14:O:215:LYS:HD2  | 1.83                     | 0.45              |
| 16:Q:236:LEU:HD22 | 16:Q:240:LEU:HD23 | 1.99                     | 0.45              |
| 18:T:60:LYS:HG2   | 18:T:62:VAL:HG23  | 1.99                     | 0.45              |
| 27:d:99:ASP:OD2   | 27:d:142:ARG:NH2  | 2.49                     | 0.45              |
| 28:e:128:TYR:O    | 28:e:132:ASN:ND2  | 2.41                     | 0.45              |
| 40:r:12:LEU:HB2   | 40:r:13:PRO:HD3   | 1.97                     | 0.45              |
| 40:r:206:LYS:HB3  | 40:r:206:LYS:HE2  | 1.70                     | 0.45              |
| 5:F:30:SER:OG     | 5:F:63:PRO:HG3    | 2.16                     | 0.45              |
| 25:b:123:PHE:HD2  | 43:v:40:VAL:HG11  | 1.82                     | 0.45              |
| 34:k:38:LEU:O     | 34:k:42:ILE:HG12  | 2.17                     | 0.45              |
| 1:A:244:ASN:ND2   | 46:A:502:FMN:O2   | 2.49                     | 0.45              |
| 8:I:96:THR:HB     | 8:I:97:PRO:HD2    | 1.99                     | 0.45              |
| 12:M:478:SER:O    | 12:M:482:GLN:HG2  | 2.16                     | 0.45              |
| 14:O:164:THR:CG2  | 14:O:169:PHE:H    | 2.29                     | 0.45              |
| 16:Q:397:TYR:OH   | 16:Q:406:GLU:OE2  | 2.34                     | 0.45              |
| 22:Y:68:TRP:CZ2   | 22:Y:72:ARG:HD2   | 2.52                     | 0.45              |
| 32:i:222:SER:O    | 32:i:222:SER:OG   | 2.32                     | 0.45              |
| 54:l:712:CDL:H311 | 54:l:712:CDL:H762 | 1.98                     | 0.45              |
| 54:n:102:CDL:H741 | 54:n:102:CDL:H712 | 1.76                     | 0.45              |
| 40:r:457:PRO:HG2  | 40:r:458:LEU:HD12 | 1.99                     | 0.45              |
| 44:w:66:ILE:HD12  | 44:w:234:LEU:HD21 | 1.98                     | 0.45              |
| 44:w:180:ARG:NH2  | 44:w:182:GLN:OE1  | 2.50                     | 0.45              |
| 1:A:184:LYS:HD3   | 10:K:98:MET:HE1   | 1.98                     | 0.45              |
| 9:J:84:TYR:O      | 9:J:84:TYR:CG     | 2.70                     | 0.45              |
| 13:N:14:VAL:HA    | 13:N:23:TYR:CD1   | 2.52                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:124:LEU:HD11 | 48:V:202:PEE:H58  | 1.98                     | 0.45              |
| 54:V:201:CDL:H512 | 35:l:580:GLN:HE22 | 1.82                     | 0.45              |
| 21:W:68:ARG:CZ    | 21:W:72:MET:HE2   | 2.46                     | 0.45              |
| 23:Z:13:LYS:HD2   | 23:Z:13:LYS:HA    | 1.75                     | 0.45              |
| 40:r:112:ALA:HB1  | 40:r:118:PHE:HB2  | 1.98                     | 0.45              |
| 1:A:380:GLY:HA2   | 1:A:386:ARG:HB2   | 1.99                     | 0.45              |
| 3:C:188:LYS:HD3   | 3:C:191:ARG:HD3   | 1.98                     | 0.45              |
| 12:M:341:ILE:HG13 | 12:M:545:LEU:HD11 | 1.99                     | 0.45              |
| 14:O:198:PRO:O    | 14:O:201:ILE:HG22 | 2.17                     | 0.45              |
| 16:Q:372:LYS:NZ   | 18:T:94:GLY:O     | 2.39                     | 0.45              |
| 17:S:48:MET:HE1   | 21:W:143:TYR:CZ   | 2.51                     | 0.45              |
| 23:Z:19:TYR:CZ    | 23:Z:20:LYS:HE2   | 2.51                     | 0.45              |
| 25:b:32:GLU:HG3   | 39:p:115:TYR:HA   | 1.99                     | 0.45              |
| 25:b:87:LYS:NZ    | 25:b:88:TYR:OH    | 2.45                     | 0.45              |
| 32:i:250:SER:O    | 32:i:259:GLY:HA3  | 2.17                     | 0.45              |
| 54:l:713:CDL:H622 | 54:l:713:CDL:H591 | 1.50                     | 0.45              |
| 15:P:44:ARG:HB3   | 15:P:45:PRO:HD3   | 1.98                     | 0.45              |
| 33:j:104:TYR:O    | 33:j:108:GLN:HG2  | 2.17                     | 0.45              |
| 40:r:116:ILE:HG13 | 42:u:168:PHE:CD1  | 2.52                     | 0.45              |
| 40:r:357:THR:O    | 40:r:361:VAL:HG23 | 2.16                     | 0.45              |
| 41:s:248:ASP:OD2  | 41:s:251:THR:HG22 | 2.17                     | 0.45              |
| 44:w:246:LEU:N    | 44:w:247:PRO:CD   | 2.79                     | 0.45              |
| 1:A:121:GLU:HG3   | 1:A:122:PRO:CD    | 2.47                     | 0.44              |
| 6:G:123:GLU:OE1   | 6:G:129:GLU:HA    | 2.16                     | 0.44              |
| 9:J:195:PHE:HB3   | 9:J:198:ALA:HB2   | 1.99                     | 0.44              |
| 12:M:278:HIS:CE1  | 12:M:280:ASP:HB2  | 2.52                     | 0.44              |
| 6:X:134:ASP:HB3   | 6:X:147:TYR:CE2   | 2.52                     | 0.44              |
| 28:e:58:ASP:OD2   | 44:w:326:ARG:NE   | 2.38                     | 0.44              |
| 31:h:2:PRO:HA     | 32:i:140:SER:HB2  | 1.99                     | 0.44              |
| 35:l:174:TYR:CD2  | 35:l:232:TRP:HB3  | 2.52                     | 0.44              |
| 39:p:26:HIS:CD2   | 39:p:79:PRO:HB3   | 2.52                     | 0.44              |
| 44:w:180:ARG:NH1  | 44:w:316:GLU:OE2  | 2.47                     | 0.44              |
| 8:I:110:GLN:NE2   | 21:W:22:LYS:HD2   | 2.32                     | 0.44              |
| 12:M:128:CYS:SG   | 12:M:140:GLN:NE2  | 2.83                     | 0.44              |
| 22:Y:61:PHE:HA    | 22:Y:64:THR:HG22  | 1.99                     | 0.44              |
| 30:g:85:TYR:CZ    | 32:i:344:SER:HB3  | 2.52                     | 0.44              |
| 35:l:37:LYS:HD3   | 35:l:98:TRP:HE1   | 1.81                     | 0.44              |
| 35:l:190:LEU:HD22 | 40:r:383:THR:HG21 | 1.99                     | 0.44              |
| 40:r:418:LYS:HE2  | 40:r:419:TYR:CE2  | 2.52                     | 0.44              |
| 54:r:714:CDL:H392 | 54:r:714:CDL:H362 | 1.49                     | 0.44              |
| 1:A:116:ASN:ND2   | 1:A:207:GLY:O     | 2.33                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:74:LEU:HB2    | 41:s:272:TRP:CZ2  | 2.52                     | 0.44              |
| 13:N:85:GLU:HG2   | 13:N:86:TRP:H     | 1.83                     | 0.44              |
| 16:Q:393:PRO:HA   | 16:Q:413:SER:O    | 2.18                     | 0.44              |
| 26:c:80:ASP:HA    | 26:c:106:HIS:HE2  | 1.81                     | 0.44              |
| 28:e:84:LEU:HG    | 28:e:88:ARG:NH1   | 2.33                     | 0.44              |
| 32:i:254:LEU:O    | 32:i:257:LEU:HB2  | 2.17                     | 0.44              |
| 35:l:338:MET:HE2  | 35:l:338:MET:HB3  | 1.91                     | 0.44              |
| 4:E:56:VAL:HG12   | 4:E:60:ARG:HD2    | 1.98                     | 0.44              |
| 9:J:111:LYS:HE3   | 9:J:139:PHE:CE1   | 2.52                     | 0.44              |
| 15:P:103:HIS:CD2  | 15:P:105:ASN:HB2  | 2.52                     | 0.44              |
| 16:Q:150:ALA:HB2  | 16:Q:400:ILE:HG12 | 1.99                     | 0.44              |
| 23:Z:49:GLU:OE2   | 39:p:34:ARG:HB3   | 2.16                     | 0.44              |
| 25:b:81:ILE:HG23  | 48:l:720:PEE:C36  | 2.47                     | 0.44              |
| 28:e:114:MET:HB3  | 28:e:117:TRP:HB3  | 1.98                     | 0.44              |
| 32:i:338:PRO:HG3  | 54:n:102:CDL:H601 | 1.99                     | 0.44              |
| 49:C:312:PLX:H311 | 49:C:312:PLX:H281 | 1.71                     | 0.44              |
| 26:c:117:VAL:HG21 | 35:l:539:TYR:HB2  | 1.99                     | 0.44              |
| 37:n:26:TYR:CZ    | 37:n:30:ARG:HD3   | 2.53                     | 0.44              |
| 41:s:81:LEU:O     | 41:s:85:MET:HG2   | 2.17                     | 0.44              |
| 4:E:24:ASP:OD1    | 4:E:24:ASP:N      | 2.51                     | 0.44              |
| 9:J:188:GLU:C     | 9:J:188:GLU:CD    | 2.85                     | 0.44              |
| 10:K:106:GLN:HB2  | 10:K:110:HIS:HD2  | 1.82                     | 0.44              |
| 13:N:13:GLN:HE21  | 13:N:33:VAL:C     | 2.26                     | 0.44              |
| 20:V:35:ILE:HG22  | 54:V:201:CDL:H761 | 1.98                     | 0.44              |
| 1:A:154:ALA:HB2   | 1:A:193:PHE:CZ    | 2.53                     | 0.44              |
| 7:H:114:TRP:CD2   | 7:H:115:PRO:HA    | 2.53                     | 0.44              |
| 10:K:79:HIS:ND1   | 14:O:215:LYS:HE3  | 2.31                     | 0.44              |
| 13:N:26:VAL:HG13  | 13:N:33:VAL:HG12  | 1.99                     | 0.44              |
| 26:c:32:VAL:HG13  | 38:o:61:GLU:OE1   | 2.17                     | 0.44              |
| 26:c:122:THR:OG1  | 26:c:124:VAL:O    | 2.29                     | 0.44              |
| 32:i:256:PRO:HB2  | 54:n:102:CDL:H612 | 2.00                     | 0.44              |
| 35:l:65:ASN:OD1   | 35:l:66:TRP:N     | 2.48                     | 0.44              |
| 38:o:4:PRO:HD2    | 39:p:73:TYR:CE2   | 2.53                     | 0.44              |
| 43:v:34:ARG:NH1   | 43:v:36:GLU:OE1   | 2.51                     | 0.44              |
| 1:A:121:GLU:HB2   | 47:A:503:NAI:C3N  | 2.48                     | 0.44              |
| 1:A:325:PRO:HD2   | 1:A:347:THR:HA    | 2.00                     | 0.44              |
| 2:B:179:THR:OG1   | 2:B:182:GLU:OE2   | 2.34                     | 0.44              |
| 5:F:27:SER:O      | 5:F:34:ARG:NH2    | 2.51                     | 0.44              |
| 16:Q:332:CYS:O    | 16:Q:336:GLU:HG3  | 2.18                     | 0.44              |
| 16:Q:412:VAL:HB   | 16:Q:421:ARG:HB3  | 1.99                     | 0.44              |
| 19:U:26:GLY:HA3   | 48:U:101:PEE:H37  | 1.99                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:113:ALA:CB   | 48:V:207:PEE:H53  | 2.47                     | 0.44              |
| 54:V:203:CDL:OB7  | 38:o:82:PRO:O     | 2.35                     | 0.44              |
| 49:V:205:PLX:H1C3 | 49:V:205:PLX:H22  | 1.81                     | 0.44              |
| 32:i:18:MET:HE2   | 32:i:18:MET:HA    | 1.99                     | 0.44              |
| 32:i:42:PRO:HG3   | 36:m:167:VAL:HG13 | 1.99                     | 0.44              |
| 48:m:202:PEE:H18  | 48:m:202:PEE:H24  | 1.87                     | 0.44              |
| 37:n:17:VAL:HB    | 37:n:18:PRO:HD3   | 2.00                     | 0.44              |
| 39:p:150:ARG:HD2  | 39:p:150:ARG:HA   | 1.85                     | 0.44              |
| 41:s:141:SER:HB3  | 41:s:289:LEU:HD22 | 1.98                     | 0.44              |
| 42:u:38:LYS:HB3   | 42:u:39:PRO:HD3   | 1.99                     | 0.44              |
| 44:w:209:VAL:HG22 | 44:w:260:ALA:HB2  | 2.00                     | 0.44              |
| 1:A:123:GLY:N     | 14:O:180:CYS:SG   | 2.85                     | 0.44              |
| 12:M:250:SER:OG   | 12:M:251:ILE:N    | 2.44                     | 0.44              |
| 48:V:202:PEE:C46  | 40:r:201:MET:HE1  | 2.42                     | 0.44              |
| 54:V:203:CDL:H873 | 40:r:264:LEU:HD21 | 2.00                     | 0.44              |
| 48:V:207:PEE:C4   | 48:V:207:PEE:C1   | 2.85                     | 0.44              |
| 32:i:72:MET:HE3   | 32:i:76:ILE:CG1   | 2.47                     | 0.44              |
| 32:i:270:MET:HE3  | 32:i:279:PRO:HG3  | 2.00                     | 0.44              |
| 35:l:316:THR:OG1  | 35:l:395:ILE:HD12 | 2.17                     | 0.44              |
| 41:s:293:PHE:O    | 41:s:297:THR:OG1  | 2.23                     | 0.44              |
| 43:v:83:GLU:OE1   | 43:v:83:GLU:N     | 2.39                     | 0.44              |
| 3:C:66:THR:HG21   | 3:C:76:MET:HE2    | 2.00                     | 0.43              |
| 8:I:28:TYR:O      | 8:I:31:ILE:HG12   | 2.18                     | 0.43              |
| 11:L:115:SER:HB2  | 12:M:267:THR:HB   | 2.00                     | 0.43              |
| 12:M:161:GLU:OE1  | 14:O:42:ARG:NH2   | 2.51                     | 0.43              |
| 16:Q:271:ARG:HD2  | 16:Q:271:ARG:HA   | 1.77                     | 0.43              |
| 27:d:37:PHE:CE2   | 35:l:3:PRO:HB3    | 2.53                     | 0.43              |
| 35:l:554:ASP:OD2  | 40:r:288:TYR:OH   | 2.32                     | 0.43              |
| 37:n:17:VAL:HG21  | 40:r:30:HIS:CG    | 2.53                     | 0.43              |
| 54:n:102:CDL:H601 | 54:n:102:CDL:H572 | 1.75                     | 0.43              |
| 42:u:16:GLN:O     | 42:u:68:LEU:HD11  | 2.18                     | 0.43              |
| 42:u:44:MET:HB3   | 42:u:48:TRP:CZ3   | 2.48                     | 0.43              |
| 46:A:502:FMN:H9   | 46:A:502:FMN:H1'1 | 1.71                     | 0.43              |
| 9:J:88:PRO:O      | 9:J:91:THR:N      | 2.47                     | 0.43              |
| 9:J:217:PHE:HZ    | 9:J:322:VAL:HG21  | 1.82                     | 0.43              |
| 9:J:271:TYR:OH    | 9:J:346:GLU:OE1   | 2.30                     | 0.43              |
| 20:V:39:TYR:OH    | 35:l:594:THR:HG22 | 2.18                     | 0.43              |
| 54:V:201:CDL:H322 | 35:l:576:MET:HE1  | 1.99                     | 0.43              |
| 24:a:126:TYR:C    | 24:a:127:ASP:OD1  | 2.61                     | 0.43              |
| 32:i:30:TRP:O     | 32:i:34:GLU:HG2   | 2.17                     | 0.43              |
| 35:l:383:MET:SD   | 35:l:384:PRO:HD2  | 2.58                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:u:14:LYS:O     | 42:u:61:LYS:NZ    | 2.51                     | 0.43              |
| 9:J:85:ARG:HD2    | 51:J:401:NDP:C2A  | 2.48                     | 0.43              |
| 9:J:116:ILE:O     | 9:J:120:VAL:HG22  | 2.18                     | 0.43              |
| 13:N:78:ASP:OD2   | 13:N:80:SER:OG    | 2.26                     | 0.43              |
| 24:a:126:TYR:O    | 49:n:101:PLX:C1B  | 2.63                     | 0.43              |
| 32:i:280:THR:O    | 32:i:284:MET:HG2  | 2.19                     | 0.43              |
| 3:C:184:ILE:O     | 3:C:187:GLU:HG2   | 2.18                     | 0.43              |
| 4:E:17:VAL:O      | 11:L:53:ILE:HD12  | 2.18                     | 0.43              |
| 10:K:79:HIS:CE1   | 14:O:215:LYS:HB3  | 2.53                     | 0.43              |
| 10:K:87:LEU:HD11  | 14:O:66:ILE:HD11  | 2.00                     | 0.43              |
| 12:M:389:THR:HG21 | 12:M:473:MET:SD   | 2.59                     | 0.43              |
| 16:Q:63:PRO:HA    | 16:Q:64:PRO:HD3   | 1.93                     | 0.43              |
| 28:e:97:ILE:O     | 28:e:101:LEU:HB2  | 2.17                     | 0.43              |
| 32:i:226:THR:HG23 | 32:i:229:SER:H    | 1.84                     | 0.43              |
| 35:l:78:LEU:HA    | 35:l:139:GLN:HE21 | 1.82                     | 0.43              |
| 36:m:129:ASP:OD1  | 36:m:129:ASP:N    | 2.47                     | 0.43              |
| 54:n:102:CDL:H171 | 54:n:102:CDL:H201 | 1.84                     | 0.43              |
| 3:C:188:LYS:HG3   | 3:C:188:LYS:O     | 2.19                     | 0.43              |
| 6:G:75:THR:O      | 6:G:77:GLU:N      | 2.51                     | 0.43              |
| 6:G:80:LYS:HG2    | 6:G:145:VAL:HG21  | 1.99                     | 0.43              |
| 7:H:82:LEU:HA     | 7:H:85:GLU:OE2    | 2.18                     | 0.43              |
| 14:O:63:ILE:HD12  | 14:O:82:VAL:HG22  | 1.99                     | 0.43              |
| 16:Q:83:ASN:ND2   | 16:Q:96:ARG:HH21  | 2.17                     | 0.43              |
| 25:b:88:TYR:CZ    | 27:d:49:ARG:HG2   | 2.54                     | 0.43              |
| 35:l:244:SER:O    | 35:l:249:SER:HB3  | 2.18                     | 0.43              |
| 54:l:713:CDL:H181 | 54:l:713:CDL:H212 | 1.76                     | 0.43              |
| 1:A:123:GLY:O     | 1:A:353:ALA:HB1   | 2.19                     | 0.43              |
| 1:A:149:MET:HE1   | 1:A:241:THR:CB    | 2.48                     | 0.43              |
| 1:A:210:THR:O     | 1:A:214:GLU:HG2   | 2.18                     | 0.43              |
| 3:C:96:SER:HB3    | 3:C:99:GLN:CD     | 2.44                     | 0.43              |
| 9:J:36:LEU:HB3    | 12:M:304:GLN:OE1  | 2.19                     | 0.43              |
| 12:M:347:ASP:OD1  | 12:M:347:ASP:N    | 2.43                     | 0.43              |
| 16:Q:278:VAL:HG23 | 16:Q:437:LYS:NZ   | 2.33                     | 0.43              |
| 48:V:202:PEE:H32  | 48:V:202:PEE:H25  | 1.70                     | 0.43              |
| 24:a:184:LYS:O    | 24:a:185:THR:OG1  | 2.29                     | 0.43              |
| 54:i:401:CDL:OA7  | 54:i:401:CDL:HA62 | 2.16                     | 0.43              |
| 33:j:90:MET:SD    | 36:m:151:THR:HG23 | 2.58                     | 0.43              |
| 35:l:102:GLU:HA   | 35:l:105:MET:HG3  | 2.00                     | 0.43              |
| 35:l:108:MET:HE1  | 35:l:240:PRO:HB3  | 1.99                     | 0.43              |
| 36:m:3:MET:N      | 36:m:3:MET:SD     | 2.92                     | 0.43              |
| 36:m:10:SER:O     | 36:m:14:VAL:HG23  | 2.18                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:s:294:LEU:O    | 41:s:298:LEU:HG   | 2.18                     | 0.43              |
| 42:u:38:LYS:NZ    | 42:u:42:GLU:OE2   | 2.51                     | 0.43              |
| 1:A:174:ARG:HD2   | 1:A:178:GLU:OE1   | 2.17                     | 0.43              |
| 15:P:161:LYS:HA   | 15:P:161:LYS:HD3  | 1.87                     | 0.43              |
| 16:Q:431:HIS:HB3  | 16:Q:454:GLN:HG2  | 2.00                     | 0.43              |
| 18:T:37:LYS:HE3   | 18:T:37:LYS:HB2   | 1.76                     | 0.43              |
| 20:V:61:PHE:HD2   | 20:V:104:ARG:HH12 | 1.66                     | 0.43              |
| 21:W:104:TRP:CH2  | 31:h:75:ARG:HG3   | 2.54                     | 0.43              |
| 28:e:74:HIS:HB2   | 28:e:83:ASP:OD2   | 2.19                     | 0.43              |
| 32:i:57:THR:HA    | 34:k:77:LEU:HD13  | 2.01                     | 0.43              |
| 41:s:19:PHE:O     | 41:s:23:VAL:HG23  | 2.18                     | 0.43              |
| 44:w:258:TYR:HE2  | 44:w:269:VAL:HG13 | 1.83                     | 0.43              |
| 1:A:177:TYR:CD1   | 1:A:182:ILE:HG23  | 2.54                     | 0.43              |
| 1:A:432:ALA:O     | 1:A:436:GLN:HG3   | 2.19                     | 0.43              |
| 12:M:260:ASN:ND2  | 12:M:278:HIS:HB2  | 2.34                     | 0.43              |
| 21:W:128:ARG:HB3  | 21:W:132:GLU:OE2  | 2.18                     | 0.43              |
| 54:a:201:CDL:OB7  | 48:l:720:PEE:H14  | 2.19                     | 0.43              |
| 28:e:73:SER:C     | 28:e:75:GLY:H     | 2.26                     | 0.43              |
| 32:i:172:GLN:OE1  | 32:i:177:LYS:HD3  | 2.19                     | 0.43              |
| 33:j:81:THR:C     | 33:j:83:ASN:H     | 2.26                     | 0.43              |
| 39:p:65:ARG:O     | 39:p:69:GLU:HG3   | 2.19                     | 0.43              |
| 1:A:385:CYS:O     | 1:A:389:VAL:HB    | 2.19                     | 0.43              |
| 4:E:19:PRO:HA     | 11:L:53:ILE:HD11  | 2.01                     | 0.43              |
| 5:F:37:ILE:HA     | 5:F:41:TYR:HB2    | 1.99                     | 0.43              |
| 12:M:476:LEU:HD21 | 12:M:481:LEU:HD21 | 2.01                     | 0.43              |
| 24:a:95:GLU:CD    | 54:a:201:CDL:O1   | 2.56                     | 0.43              |
| 26:c:109:LEU:O    | 26:c:113:ILE:HG23 | 2.18                     | 0.43              |
| 27:d:37:PHE:CD2   | 35:l:3:PRO:HB3    | 2.54                     | 0.43              |
| 35:l:452:ASN:HA   | 35:l:455:LYS:HG2  | 2.00                     | 0.43              |
| 54:l:712:CDL:C85  | 54:l:712:CDL:C81  | 2.97                     | 0.43              |
| 39:p:20:TYR:HB2   | 39:p:48:PHE:CZ    | 2.54                     | 0.43              |
| 44:w:235:GLN:HA   | 44:w:238:GLU:CG   | 2.49                     | 0.43              |
| 3:C:190:LEU:HD23  | 3:C:190:LEU:HA    | 1.86                     | 0.43              |
| 7:H:65:VAL:O      | 7:H:69:GLU:HG3    | 2.18                     | 0.43              |
| 54:V:201:CDL:C51  | 35:l:580:GLN:HE22 | 2.31                     | 0.43              |
| 49:V:205:PLX:H301 | 49:V:205:PLX:H331 | 1.65                     | 0.43              |
| 34:k:98:CYS:SG    | 35:l:587:TYR:OH   | 2.75                     | 0.43              |
| 41:s:21:THR:HG22  | 41:s:224:PHE:CE1  | 2.54                     | 0.43              |
| 42:u:59:GLU:HA    | 42:u:62:LEU:HD12  | 2.00                     | 0.43              |
| 2:B:118:LEU:HD11  | 16:Q:382:PHE:CE2  | 2.54                     | 0.42              |
| 6:G:126:PHE:CE2   | 6:G:148:ILE:HG21  | 2.54                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:I:105:GLU:OE1   | 8:I:105:GLU:HA    | 2.19                     | 0.42              |
| 9:J:131:GLY:O     | 51:J:401:NDP:H52A | 2.19                     | 0.42              |
| 9:J:319:VAL:HA    | 9:J:322:VAL:HG12  | 2.01                     | 0.42              |
| 36:m:57:PHE:CE1   | 41:s:111:LEU:HD11 | 2.54                     | 0.42              |
| 37:n:47:ARG:HG2   | 37:n:47:ARG:HH11  | 1.84                     | 0.42              |
| 40:r:71:TRP:O     | 40:r:74:PRO:HD2   | 2.19                     | 0.42              |
| 54:r:714:CDL:H542 | 54:r:714:CDL:H511 | 1.79                     | 0.42              |
| 42:u:44:MET:HE3   | 42:u:48:TRP:CZ3   | 2.54                     | 0.42              |
| 9:J:132:ARG:HD2   | 9:J:134:TRP:CZ2   | 2.53                     | 0.42              |
| 24:a:139:ILE:HG23 | 40:r:54:LEU:HD23  | 2.01                     | 0.42              |
| 27:d:46:THR:O     | 27:d:50:GLU:HG3   | 2.20                     | 0.42              |
| 41:s:190:LEU:HD23 | 41:s:270:PHE:CD1  | 2.53                     | 0.42              |
| 56:s:403:UQ:H152  | 56:s:403:UQ:H101  | 2.01                     | 0.42              |
| 2:B:210:LEU:HD23  | 2:B:210:LEU:HA    | 1.89                     | 0.42              |
| 5:F:64:LYS:HD3    | 5:F:76:ASN:HB2    | 2.01                     | 0.42              |
| 5:F:83:SER:OG     | 5:F:86:GLN:HG3    | 2.19                     | 0.42              |
| 12:M:173:MET:HE1  | 45:M:802:SF4:S1   | 2.60                     | 0.42              |
| 12:M:538:ARG:HG2  | 12:M:538:ARG:NH1  | 2.33                     | 0.42              |
| 13:N:68:MET:SD    | 13:N:81:MET:HG2   | 2.59                     | 0.42              |
| 16:Q:139:LEU:HD23 | 16:Q:139:LEU:HA   | 1.89                     | 0.42              |
| 27:d:61:TYR:C     | 27:d:62:TYR:HD1   | 2.27                     | 0.42              |
| 27:d:117:GLU:HG3  | 27:d:124:ASN:HB2  | 2.02                     | 0.42              |
| 32:i:104:MET:HG3  | 32:i:111:PHE:HB3  | 2.01                     | 0.42              |
| 35:l:119:LYS:HZ1  | 54:l:712:CDL:H512 | 1.81                     | 0.42              |
| 49:n:101:PLX:H102 | 40:r:40:SER:HB3   | 2.01                     | 0.42              |
| 40:r:306:PRO:HA   | 40:r:458:LEU:HD22 | 2.01                     | 0.42              |
| 54:r:714:CDL:H772 | 54:r:714:CDL:H741 | 1.81                     | 0.42              |
| 1:A:162:PHE:HB3   | 1:A:165:GLU:HB2   | 1.99                     | 0.42              |
| 1:A:413:TRP:O     | 1:A:416:SER:OG    | 2.26                     | 0.42              |
| 6:G:139:MET:HA    | 6:G:139:MET:HE3   | 2.00                     | 0.42              |
| 12:M:361:VAL:HG12 | 12:M:361:VAL:O    | 2.20                     | 0.42              |
| 25:b:70:PHE:O     | 25:b:74:HIS:HB2   | 2.18                     | 0.42              |
| 54:l:713:CDL:H382 | 54:l:713:CDL:H351 | 1.74                     | 0.42              |
| 40:r:178:ILE:HD12 | 40:r:178:ILE:H    | 1.84                     | 0.42              |
| 44:w:59:VAL:HG23  | 44:w:157:VAL:HG23 | 2.01                     | 0.42              |
| 44:w:214:ILE:CG2  | 44:w:234:LEU:CD1  | 2.97                     | 0.42              |
| 46:A:502:FMN:HM71 | 46:A:502:FMN:HM83 | 1.84                     | 0.42              |
| 12:M:436:VAL:O    | 12:M:442:TYR:OH   | 2.33                     | 0.42              |
| 54:V:203:CDL:H811 | 38:o:94:GLY:HA3   | 2.00                     | 0.42              |
| 54:a:201:CDL:H211 | 54:a:201:CDL:H182 | 1.71                     | 0.42              |
| 29:f:64:GLU:OE1   | 29:f:64:GLU:HA    | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:154:MET:HE2  | 32:i:154:MET:HB2  | 1.96                     | 0.42              |
| 32:i:211:MET:HG2  | 32:i:333:SER:HB2  | 2.01                     | 0.42              |
| 33:j:5:LEU:HD23   | 41:s:2:PHE:HD2    | 1.85                     | 0.42              |
| 35:l:173:LEU:HD23 | 48:l:719:PEE:H15  | 2.01                     | 0.42              |
| 39:p:28:GLU:OE2   | 39:p:34:ARG:NH1   | 2.46                     | 0.42              |
| 44:w:211:VAL:N    | 44:w:212:PRO:CD   | 2.83                     | 0.42              |
| 1:A:161:GLU:N     | 1:A:161:GLU:OE1   | 2.52                     | 0.42              |
| 11:L:92:ASN:HB3   | 15:P:238:PRO:HA   | 2.01                     | 0.42              |
| 12:M:391:ILE:N    | 12:M:600:GLU:OE2  | 2.40                     | 0.42              |
| 12:M:605:GLN:OE1  | 12:M:643:ARG:NH1  | 2.46                     | 0.42              |
| 13:N:69:ASN:OD1   | 13:N:112:ASN:ND2  | 2.50                     | 0.42              |
| 21:W:68:ARG:NH2   | 36:m:134:GLY:HA2  | 2.34                     | 0.42              |
| 23:Z:75:PHE:O     | 23:Z:79:VAL:HG13  | 2.20                     | 0.42              |
| 26:c:97:LEU:HB3   | 26:c:99:LEU:HD12  | 2.00                     | 0.42              |
| 35:l:107:TYR:HD1  | 35:l:108:MET:HE2  | 1.85                     | 0.42              |
| 40:r:115:LEU:HD12 | 40:r:174:LEU:HD22 | 2.01                     | 0.42              |
| 41:s:126:LYS:O    | 41:s:130:ILE:HG12 | 2.18                     | 0.42              |
| 2:B:63:TRP:HB3    | 2:B:66:LEU:HD12   | 2.00                     | 0.42              |
| 2:B:99:GLY:N      | 2:B:169:GLU:HG2   | 2.34                     | 0.42              |
| 3:C:62:LEU:O      | 3:C:91:VAL:HA     | 2.19                     | 0.42              |
| 6:G:113:LEU:HA    | 6:G:116:VAL:HG12  | 2.02                     | 0.42              |
| 12:M:140:GLN:HG2  | 16:Q:379:ILE:HG23 | 2.02                     | 0.42              |
| 13:N:42:ASP:OD2   | 13:N:44:TYR:HD2   | 2.02                     | 0.42              |
| 23:Z:59:ASN:HB3   | 35:l:364:LYS:NZ   | 2.34                     | 0.42              |
| 26:c:155:PRO:HG3  | 43:v:4:HIS:CE1    | 2.54                     | 0.42              |
| 31:h:83:ARG:O     | 31:h:87:ILE:HG12  | 2.20                     | 0.42              |
| 37:n:47:ARG:HH22  | 37:n:53:GLU:CD    | 2.25                     | 0.42              |
| 40:r:445:LEU:O    | 40:r:448:THR:HG22 | 2.19                     | 0.42              |
| 1:A:263:ALA:HA    | 1:A:271:SER:HB3   | 2.01                     | 0.42              |
| 1:A:448:GLU:O     | 1:A:452:GLN:HG2   | 2.20                     | 0.42              |
| 2:B:200:GLU:HG3   | 13:N:88:ARG:HD3   | 2.02                     | 0.42              |
| 7:H:56:LEU:HA     | 7:H:59:VAL:HG12   | 2.01                     | 0.42              |
| 16:Q:97:LEU:HD11  | 16:Q:109:CYS:SG   | 2.59                     | 0.42              |
| 54:V:201:CDL:H621 | 32:i:160:LEU:HD11 | 2.01                     | 0.42              |
| 32:i:266:ILE:HG22 | 32:i:270:MET:HE2  | 2.01                     | 0.42              |
| 35:l:520:TYR:CE1  | 54:l:713:CDL:HB22 | 2.54                     | 0.42              |
| 36:m:23:LYS:N     | 36:m:24:PRO:HD3   | 2.35                     | 0.42              |
| 39:p:54:GLU:OE1   | 39:p:60:ALA:HB2   | 2.20                     | 0.42              |
| 44:w:214:ILE:HG22 | 44:w:215:GLN:N    | 2.34                     | 0.42              |
| 12:M:419:ARG:NH1  | 12:M:439:THR:O    | 2.53                     | 0.42              |
| 22:Y:84:PHE:CE2   | 43:v:89:TYR:HA    | 2.55                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 54:a:201:CDL:OB7  | 48:l:720:PEE:C11  | 2.68                     | 0.42              |
| 32:i:278:MET:HE3  | 32:i:278:MET:HB3  | 1.97                     | 0.42              |
| 33:j:91:ALA:HB1   | 41:s:305:ILE:HD13 | 2.02                     | 0.42              |
| 54:l:712:CDL:H842 | 54:l:712:CDL:H651 | 2.00                     | 0.42              |
| 54:n:102:CDL:OB7  | 42:u:170:TRP:HA   | 2.20                     | 0.42              |
| 40:r:285:LEU:HD13 | 40:r:342:MET:HE1  | 2.02                     | 0.42              |
| 1:A:46:TYR:CD1    | 14:O:226:GLU:HB3  | 2.55                     | 0.42              |
| 1:A:50:ASP:HB3    | 1:A:55:GLY:HA3    | 2.02                     | 0.42              |
| 2:B:210:LEU:HD12  | 8:I:38:PRO:HB3    | 2.01                     | 0.42              |
| 6:G:71:ALA:HB1    | 6:G:72:PRO:HD2    | 2.02                     | 0.42              |
| 7:H:26:ILE:O      | 7:H:30:LYS:HG3    | 2.19                     | 0.42              |
| 13:N:85:GLU:HG2   | 13:N:86:TRP:N     | 2.34                     | 0.42              |
| 14:O:108:PRO:HA   | 14:O:109:PRO:HD3  | 1.95                     | 0.42              |
| 16:Q:158:LEU:HD23 | 16:Q:158:LEU:HA   | 1.89                     | 0.42              |
| 21:W:51:MET:HE2   | 41:s:311:THR:HB   | 2.02                     | 0.42              |
| 24:a:147:ALA:HB2  | 40:r:173:SER:HB2  | 2.01                     | 0.42              |
| 49:j:203:PLX:H372 | 49:j:203:PLX:H342 | 1.61                     | 0.42              |
| 54:l:713:CDL:H112 | 54:l:713:CDL:H142 | 1.72                     | 0.42              |
| 56:s:403:UQ:H72   | 56:s:403:UQ:H111  | 1.88                     | 0.42              |
| 1:A:109:ARG:NH1   | 1:A:237:GLY:O     | 2.53                     | 0.41              |
| 3:C:76:MET:HE3    | 3:C:76:MET:HB3    | 1.90                     | 0.41              |
| 5:F:33:VAL:O      | 5:F:36:PHE:HB3    | 2.20                     | 0.41              |
| 12:M:260:ASN:HD21 | 12:M:278:HIS:CD2  | 2.37                     | 0.41              |
| 16:Q:52:MET:HE3   | 16:Q:52:MET:HB3   | 1.84                     | 0.41              |
| 16:Q:278:VAL:HG12 | 16:Q:329:ARG:HH21 | 1.85                     | 0.41              |
| 54:V:201:CDL:H512 | 35:l:580:GLN:NE2  | 2.34                     | 0.41              |
| 24:a:50:HIS:HB3   | 24:a:52:LYS:HE2   | 2.02                     | 0.41              |
| 24:a:136:THR:HG21 | 40:r:48:ASN:ND2   | 2.35                     | 0.41              |
| 26:c:169:GLU:HA   | 27:d:123:GLN:HB2  | 2.02                     | 0.41              |
| 27:d:149:HIS:HD2  | 40:r:304:GLN:NE2  | 2.17                     | 0.41              |
| 30:g:48:ASN:HB3   | 30:g:55:VAL:HA    | 2.02                     | 0.41              |
| 34:k:60:PRO:O     | 34:k:63:LEU:HB3   | 2.19                     | 0.41              |
| 41:s:89:LEU:HA    | 41:s:90:PRO:HD3   | 1.90                     | 0.41              |
| 41:s:197:PRO:HB3  | 41:s:278:PRO:O    | 2.20                     | 0.41              |
| 14:O:130:TYR:HA   | 14:O:189:ASN:ND2  | 2.35                     | 0.41              |
| 16:Q:188:THR:HB   | 16:Q:200:PHE:HA   | 2.02                     | 0.41              |
| 48:U:101:PEE:H35  | 48:U:101:PEE:H30  | 1.50                     | 0.41              |
| 21:W:105:LYS:HE2  | 21:W:105:LYS:HB2  | 1.90                     | 0.41              |
| 24:a:106:VAL:HG13 | 37:n:50:ARG:NH2   | 2.35                     | 0.41              |
| 27:d:9:VAL:O      | 27:d:109:ARG:NH2  | 2.45                     | 0.41              |
| 49:e:201:PLX:H301 | 49:e:201:PLX:H331 | 1.60                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:207:ILE:O    | 32:i:211:MET:HG3  | 2.20                     | 0.41              |
| 32:i:283:ALA:HB1  | 40:r:158:LEU:HD13 | 2.00                     | 0.41              |
| 33:j:55:PHE:HB2   | 36:m:74:MET:HE1   | 2.01                     | 0.41              |
| 35:l:303:ALA:O    | 35:l:306:THR:HG22 | 2.20                     | 0.41              |
| 35:l:468:ILE:O    | 35:l:472:ILE:HG12 | 2.21                     | 0.41              |
| 54:l:712:CDL:H241 | 48:l:720:PEE:H33  | 2.02                     | 0.41              |
| 40:r:121:LEU:O    | 40:r:125:THR:HG23 | 2.20                     | 0.41              |
| 44:w:170:LEU:HD22 | 44:w:187:TYR:CD1  | 2.54                     | 0.41              |
| 44:w:223:ASN:O    | 44:w:227:MET:HG3  | 2.20                     | 0.41              |
| 1:A:338:ASP:O     | 1:A:342:LEU:HB2   | 2.20                     | 0.41              |
| 6:G:106:LYS:H     | 6:G:106:LYS:HG2   | 1.73                     | 0.41              |
| 9:J:36:LEU:N      | 12:M:304:GLN:HE22 | 2.17                     | 0.41              |
| 12:M:94:MET:HE2   | 12:M:94:MET:HB2   | 1.90                     | 0.41              |
| 15:P:108:PHE:O    | 15:P:160:TYR:OH   | 2.32                     | 0.41              |
| 16:Q:144:MET:HE3  | 16:Q:222:MET:HB2  | 2.01                     | 0.41              |
| 54:V:201:CDL:H342 | 54:V:201:CDL:H371 | 1.92                     | 0.41              |
| 32:i:5:ILE:HG21   | 36:m:170:GLU:OE2  | 2.20                     | 0.41              |
| 54:l:712:CDL:H851 | 54:l:712:CDL:C81  | 2.50                     | 0.41              |
| 41:s:98:MET:HE1   | 41:s:104:PHE:CG   | 2.56                     | 0.41              |
| 44:w:167:PHE:O    | 44:w:170:LEU:HB3  | 2.19                     | 0.41              |
| 1:A:329:LYS:HA    | 1:A:332:CYS:SG    | 2.61                     | 0.41              |
| 2:B:86:TYR:CD1    | 2:B:87:PRO:HA     | 2.55                     | 0.41              |
| 13:N:132:LYS:NZ   | 13:N:136:GLU:OE1  | 2.53                     | 0.41              |
| 15:P:107:GLN:NE2  | 15:P:136:ARG:HG2  | 2.36                     | 0.41              |
| 26:c:81:ARG:HB3   | 26:c:85:GLU:OE1   | 2.20                     | 0.41              |
| 27:d:33:LEU:HD23  | 27:d:33:LEU:HA    | 1.85                     | 0.41              |
| 29:f:72:ARG:HE    | 30:g:22:SER:HB3   | 1.85                     | 0.41              |
| 31:h:17:TRP:CD1   | 31:h:17:TRP:H     | 2.39                     | 0.41              |
| 32:i:245:MET:HE3  | 32:i:245:MET:HB3  | 1.92                     | 0.41              |
| 1:A:208:GLU:OE1   | 1:A:210:THR:OG1   | 2.30                     | 0.41              |
| 1:A:317:VAL:HG23  | 1:A:356:VAL:HG12  | 2.02                     | 0.41              |
| 19:U:78:LEU:HD23  | 19:U:78:LEU:HA    | 1.94                     | 0.41              |
| 20:V:124:LEU:CD1  | 48:V:202:PEE:H58  | 2.51                     | 0.41              |
| 32:i:112:HIS:HB2  | 32:i:184:ILE:HD13 | 2.01                     | 0.41              |
| 49:j:203:PLX:H312 | 49:j:203:PLX:H282 | 1.83                     | 0.41              |
| 48:l:720:PEE:H3   | 48:l:720:PEE:O4   | 2.20                     | 0.41              |
| 44:w:54:THR:C     | 44:w:56:THR:H     | 2.27                     | 0.41              |
| 44:w:346:ASP:OD1  | 44:w:347:VAL:N    | 2.53                     | 0.41              |
| 2:B:66:LEU:HB3    | 41:s:277:TYR:OH   | 2.20                     | 0.41              |
| 2:B:151:LYS:HA    | 3:C:141:GLY:HA2   | 2.01                     | 0.41              |
| 12:M:42:MET:HE3   | 12:M:42:MET:HA    | 2.01                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:698:ASP:N    | 12:M:698:ASP:OD1  | 2.53                     | 0.41              |
| 15:P:183:ASP:OD1  | 15:P:185:ARG:NE   | 2.53                     | 0.41              |
| 16:Q:198:THR:HB   | 16:Q:199:PRO:HD3  | 2.02                     | 0.41              |
| 22:Y:51:THR:O     | 22:Y:54:GLN:HG2   | 2.20                     | 0.41              |
| 32:i:129:LEU:HD13 | 54:i:401:CDL:H341 | 2.01                     | 0.41              |
| 35:l:44:PHE:HB2   | 35:l:94:LEU:HB3   | 2.02                     | 0.41              |
| 35:l:107:TYR:CD1  | 35:l:108:MET:HE2  | 2.55                     | 0.41              |
| 35:l:562:LEU:HG   | 48:l:718:PEE:H32  | 2.02                     | 0.41              |
| 37:n:47:ARG:NH2   | 37:n:53:GLU:OE2   | 2.46                     | 0.41              |
| 40:r:233:ALA:HA   | 40:r:320:GLY:HA2  | 2.03                     | 0.41              |
| 41:s:21:THR:CG2   | 41:s:224:PHE:CE1  | 3.03                     | 0.41              |
| 41:s:142:TYR:O    | 41:s:145:THR:HG22 | 2.21                     | 0.41              |
| 42:u:60:GLY:O     | 42:u:63:VAL:HG22  | 2.21                     | 0.41              |
| 8:I:8:ILE:HG13    | 54:N:202:CDL:CA3  | 2.44                     | 0.41              |
| 12:M:185:PHE:CZ   | 12:M:221:ASN:HB2  | 2.56                     | 0.41              |
| 12:M:625:ALA:O    | 12:M:629:ILE:HG12 | 2.21                     | 0.41              |
| 16:Q:198:THR:HG22 | 16:Q:202:TRP:CE2  | 2.56                     | 0.41              |
| 27:d:77:CYS:SG    | 27:d:84:CYS:HB3   | 2.60                     | 0.41              |
| 32:i:291:TYR:HA   | 40:r:151:PHE:HZ   | 1.85                     | 0.41              |
| 35:l:105:MET:HE2  | 35:l:105:MET:HB3  | 1.93                     | 0.41              |
| 35:l:211:MET:N    | 35:l:212:PRO:HD2  | 2.36                     | 0.41              |
| 35:l:423:SER:O    | 35:l:427:ILE:HG12 | 2.20                     | 0.41              |
| 36:m:51:PHE:CZ    | 36:m:55:MET:HE3   | 2.56                     | 0.41              |
| 36:m:124:ASP:N    | 36:m:124:ASP:OD1  | 2.48                     | 0.41              |
| 40:r:216:LEU:HD23 | 40:r:287:ALA:HB1  | 2.01                     | 0.41              |
| 40:r:243:MET:HB3  | 40:r:301:ILE:HG21 | 2.03                     | 0.41              |
| 1:A:121:GLU:HA    | 1:A:122:PRO:HD3   | 1.82                     | 0.41              |
| 2:B:76:TYR:CE2    | 41:s:33:LEU:HD13  | 2.56                     | 0.41              |
| 2:B:99:GLY:O      | 2:B:169:GLU:CG    | 2.69                     | 0.41              |
| 9:J:72:HIS:NE2    | 15:P:215:GLU:OE2  | 2.54                     | 0.41              |
| 11:L:154:LYS:HE2  | 11:L:154:LYS:HB3  | 1.79                     | 0.41              |
| 6:X:136:GLU:O     | 25:b:2:SER:OG     | 2.38                     | 0.41              |
| 32:i:45:MET:HE1   | 36:m:171:ILE:HG23 | 2.02                     | 0.41              |
| 32:i:344:SER:C    | 32:i:346:LEU:H    | 2.29                     | 0.41              |
| 35:l:123:LEU:CD1  | 54:l:712:CDL:OA7  | 2.68                     | 0.41              |
| 40:r:369:LEU:HD12 | 40:r:370:PRO:HD2  | 2.02                     | 0.41              |
| 41:s:245:ALA:HB3  | 41:s:255:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:99:TRP:N      | 1:A:99:TRP:CD1    | 2.87                     | 0.41              |
| 48:C:311:PEE:H20  | 48:C:311:PEE:H28  | 2.02                     | 0.41              |
| 5:F:56:ARG:HB3    | 12:M:651:PRO:HD2  | 2.03                     | 0.41              |
| 6:G:130:ILE:HG22  | 6:G:135:ALA:HB2   | 2.03                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:167:PRO:HD2  | 12:M:215:MET:HE1  | 2.03                     | 0.41              |
| 12:M:372:PHE:H    | 12:M:532:PRO:HB2  | 1.86                     | 0.41              |
| 16:Q:226:TYR:OH   | 16:Q:234:GLN:O    | 2.22                     | 0.41              |
| 23:Z:24:ILE:HG23  | 23:Z:29:LEU:HB2   | 2.02                     | 0.41              |
| 49:e:201:PLX:H382 | 40:r:67:VAL:HG12  | 2.02                     | 0.41              |
| 29:f:55:TRP:O     | 29:f:59:ILE:HG12  | 2.20                     | 0.41              |
| 30:g:2:THR:HG22   | 30:g:4:MET:HG3    | 2.03                     | 0.41              |
| 30:g:60:LEU:HD13  | 44:w:353:TRP:HB2  | 2.03                     | 0.41              |
| 35:l:10:THR:O     | 35:l:14:ILE:HG12  | 2.21                     | 0.41              |
| 35:l:94:LEU:HD23  | 35:l:94:LEU:HA    | 1.92                     | 0.41              |
| 35:l:169:LEU:HD12 | 35:l:169:LEU:HA   | 1.88                     | 0.41              |
| 35:l:559:GLU:OE2  | 40:r:148:TYR:OH   | 2.26                     | 0.41              |
| 49:n:101:PLX:H111 | 49:n:101:PLX:H81  | 1.60                     | 0.41              |
| 38:o:84:PRO:O     | 38:o:88:LEU:HG    | 2.21                     | 0.41              |
| 39:p:29:SER:HB3   | 39:p:76:HIS:CD2   | 2.52                     | 0.41              |
| 40:r:235:LEU:HD23 | 40:r:235:LEU:HA   | 1.92                     | 0.41              |
| 54:r:714:CDL:H812 | 54:r:714:CDL:H241 | 2.03                     | 0.41              |
| 4:E:115:PRO:HB2   | 4:E:120:SER:OG    | 2.21                     | 0.41              |
| 5:F:89:ARG:O      | 5:F:93:ASN:ND2    | 2.54                     | 0.41              |
| 7:H:76:GLN:O      | 7:H:79:GLU:HG2    | 2.21                     | 0.41              |
| 9:J:84:TYR:HD2    | 9:J:86:CYS:O      | 2.04                     | 0.41              |
| 12:M:245:THR:HA   | 12:M:265:THR:O    | 2.21                     | 0.41              |
| 12:M:402:LEU:HD23 | 12:M:475:VAL:HB   | 2.03                     | 0.41              |
| 12:M:624:ARG:HH12 | 12:M:628:GLU:HG3  | 1.86                     | 0.41              |
| 54:V:203:CDL:C36  | 54:V:203:CDL:C32  | 2.98                     | 0.41              |
| 6:X:82:ARG:O      | 6:X:86:VAL:HG23   | 2.21                     | 0.41              |
| 27:d:74:ILE:HG23  | 27:d:156:LEU:HD22 | 2.02                     | 0.41              |
| 27:d:90:MET:SD    | 40:r:47:GLU:HB3   | 2.61                     | 0.41              |
| 31:h:65:GLU:OE2   | 31:h:71:LYS:HB2   | 2.21                     | 0.41              |
| 32:i:72:MET:HG2   | 34:k:12:PHE:CE2   | 2.56                     | 0.41              |
| 48:m:202:PEE:H25  | 48:m:202:PEE:H56  | 2.03                     | 0.41              |
| 42:u:47:ARG:NH2   | 42:u:53:PRO:HG3   | 2.36                     | 0.41              |
| 1:A:75:TRP:CH2    | 1:A:79:GLU:HG3    | 2.55                     | 0.40              |
| 1:A:122:PRO:HA    | 14:O:176:CYS:SG   | 2.60                     | 0.40              |
| 1:A:272:GLY:O     | 1:A:292:MET:HB2   | 2.20                     | 0.40              |
| 2:B:90:LYS:HG3    | 13:N:91:HIS:CE1   | 2.56                     | 0.40              |
| 7:H:54:GLU:O      | 7:H:58:MET:HG3    | 2.21                     | 0.40              |
| 25:b:32:GLU:HG3   | 39:p:115:TYR:CD1  | 2.56                     | 0.40              |
| 35:l:137:LEU:HD23 | 35:l:137:LEU:HA   | 1.96                     | 0.40              |
| 44:w:243:LYS:HD3  | 44:w:243:LYS:HA   | 1.88                     | 0.40              |
| 44:w:350:LYS:HA   | 44:w:350:LYS:HD3  | 1.86                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:158:ILE:HG23  | 1:A:199:ARG:HG2   | 2.04                     | 0.40              |
| 1:A:279:SER:OG    | 1:A:280:GLY:N     | 2.54                     | 0.40              |
| 2:B:177:THR:CG2   | 2:B:182:GLU:HB2   | 2.50                     | 0.40              |
| 6:G:93:ILE:HG23   | 6:G:108:LEU:HD22  | 2.01                     | 0.40              |
| 9:J:199:THR:OG1   | 9:J:258:ALA:O     | 2.39                     | 0.40              |
| 11:L:53:ILE:HG22  | 11:L:55:VAL:HB    | 2.02                     | 0.40              |
| 16:Q:383:LYS:HD2  | 16:Q:383:LYS:HA   | 1.92                     | 0.40              |
| 19:U:42:ALA:HB2   | 41:s:312:ALA:HA   | 2.03                     | 0.40              |
| 20:V:41:ILE:HD13  | 20:V:55:ARG:HH11  | 1.86                     | 0.40              |
| 25:b:100:ARG:HB3  | 35:l:60:GLU:HB2   | 2.03                     | 0.40              |
| 32:i:125:GLN:HG3  | 54:i:401:CDL:OA3  | 2.20                     | 0.40              |
| 32:i:155:LEU:HD22 | 32:i:278:MET:HE2  | 2.03                     | 0.40              |
| 35:l:572:LYS:HA   | 35:l:572:LYS:HD2  | 1.91                     | 0.40              |
| 39:p:159:LYS:HE3  | 39:p:159:LYS:HB2  | 1.84                     | 0.40              |
| 6:G:84:LEU:HB3    | 6:G:88:LYS:HZ3    | 1.86                     | 0.40              |
| 8:I:34:ARG:HB2    | 13:N:95:ASP:OD1   | 2.22                     | 0.40              |
| 12:M:133:GLN:O    | 12:M:137:CYS:HB2  | 2.22                     | 0.40              |
| 16:Q:345:SER:HB2  | 21:W:19:ILE:HD12  | 2.02                     | 0.40              |
| 32:i:78:LEU:HD22  | 32:i:84:TRP:CZ2   | 2.57                     | 0.40              |
| 33:j:6:THR:O      | 33:j:10:ASN:ND2   | 2.54                     | 0.40              |
| 35:l:327:LEU:O    | 35:l:331:MET:HG2  | 2.21                     | 0.40              |
| 40:r:22:MET:HE3   | 40:r:22:MET:HB3   | 1.85                     | 0.40              |
| 44:w:132:GLN:NE2  | 57:w:401:ADP:HN62 | 2.20                     | 0.40              |
| 1:A:147:ARG:HA    | 1:A:147:ARG:HD2   | 1.90                     | 0.40              |
| 1:A:209:GLU:HB2   | 1:A:242:VAL:HG21  | 2.02                     | 0.40              |
| 1:A:267:ARG:HG3   | 1:A:293:SER:OG    | 2.20                     | 0.40              |
| 2:B:38:TYR:CZ     | 8:I:106:LEU:HD13  | 2.57                     | 0.40              |
| 2:B:44:ARG:HD3    | 2:B:45:GLU:H      | 1.86                     | 0.40              |
| 13:N:3:LEU:HD23   | 13:N:7:LEU:HD11   | 2.02                     | 0.40              |
| 14:O:63:ILE:HD12  | 14:O:82:VAL:HG13  | 2.04                     | 0.40              |
| 16:Q:133:LEU:HD22 | 16:Q:228:ARG:HD3  | 2.03                     | 0.40              |
| 54:V:201:CDL:OA5  | 48:V:207:PEE:H12  | 2.21                     | 0.40              |
| 27:d:101:GLU:OE1  | 28:e:119:ARG:NH1  | 2.52                     | 0.40              |
| 32:i:49:ASN:ND2   | 32:i:51:ARG:HB2   | 2.37                     | 0.40              |
| 32:i:258:SER:OG   | 32:i:336:VAL:HG22 | 2.22                     | 0.40              |
| 33:j:19:LEU:O     | 33:j:23:TRP:HD1   | 2.04                     | 0.40              |
| 35:l:396:ILE:HA   | 35:l:399:VAL:HG12 | 2.04                     | 0.40              |
| 35:l:562:LEU:HG   | 48:l:718:PEE:C20  | 2.52                     | 0.40              |
| 40:r:202:ALA:O    | 40:r:205:VAL:HG12 | 2.22                     | 0.40              |
| 40:r:403:THR:O    | 40:r:404:ALA:C    | 2.65                     | 0.40              |
| 41:s:98:MET:HE2   | 41:s:101:GLY:HA2  | 2.02                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:79:ARG:NH2    | 8:I:20:LEU:HD21   | 2.37                     | 0.40              |
| 9:J:201:ILE:HG22  | 9:J:203:PRO:HD3   | 2.02                     | 0.40              |
| 14:O:186:VAL:HG22 | 14:O:196:LEU:HD11 | 2.03                     | 0.40              |
| 20:V:140:LYS:H    | 20:V:140:LYS:HG2  | 1.75                     | 0.40              |
| 48:V:207:PEE:H20  | 48:V:207:PEE:H14  | 1.56                     | 0.40              |
| 6:X:133:ILE:HD11  | 39:p:6:PRO:HA     | 2.03                     | 0.40              |
| 27:d:43:ARG:O     | 27:d:47:LEU:HG    | 2.21                     | 0.40              |
| 32:i:54:GLU:OE2   | 34:k:95:LEU:HB2   | 2.22                     | 0.40              |
| 35:l:184:LEU:HD13 | 40:r:393:ILE:HG21 | 2.03                     | 0.40              |
| 54:l:713:CDL:H201 | 54:l:713:CDL:H232 | 1.96                     | 0.40              |
| 44:w:165:SER:O    | 44:w:168:VAL:HG22 | 2.22                     | 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     | 429/431 (100%) | 414 (96%) | 15 (4%)  | 0        | 100         | 100 |
| 2   | B     | 174/176 (99%)  | 172 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 3   | C     | 154/156 (99%)  | 146 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 4   | E     | 113/115 (98%)  | 111 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 5   | F     | 84/86 (98%)    | 81 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 6   | G     | 86/88 (98%)    | 84 (98%)  | 1 (1%)   | 1 (1%)   | 10          | 37  |
| 6   | X     | 86/88 (98%)    | 83 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 7   | H     | 110/112 (98%)  | 102 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 8   | I     | 93/112 (83%)   | 82 (88%)  | 11 (12%) | 0        | 100         | 100 |
| 9   | J     | 289/341 (85%)  | 271 (94%) | 16 (6%)  | 2 (1%)   | 18          | 49  |
| 10  | K     | 40/42 (95%)    | 40 (100%) | 0        | 0        | 100         | 100 |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 11  | L     | 123/125 (98%)  | 121 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 12  | M     | 688/690 (100%) | 662 (96%) | 25 (4%)  | 1 (0%)   | 48          | 78  |
| 13  | N     | 142/144 (99%)  | 137 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 14  | O     | 215/217 (99%)  | 205 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 15  | P     | 206/208 (99%)  | 196 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 16  | Q     | 412/430 (96%)  | 401 (97%) | 11 (3%)  | 0        | 100         | 100 |
| 17  | S     | 68/70 (97%)    | 63 (93%)  | 5 (7%)   | 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%)  | 132 (96%) | 5 (4%)   | 1 (1%)   | 18          | 49  |
| 21  | W     | 140/142 (99%)  | 136 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 22  | Y     | 68/70 (97%)    | 64 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 23  | Z     | 82/84 (98%)    | 78 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 24  | a     | 138/140 (99%)  | 135 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 25  | b     | 99/126 (79%)   | 95 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 26  | c     | 154/156 (99%)  | 145 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 27  | d     | 173/175 (99%)  | 172 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 28  | e     | 105/107 (98%)  | 101 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 29  | f     | 40/42 (95%)    | 39 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 30  | g     | 119/121 (98%)  | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 31  | h     | 103/105 (98%)  | 98 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 32  | i     | 345/347 (99%)  | 328 (95%) | 15 (4%)  | 2 (1%)   | 21          | 52  |
| 33  | j     | 95/113 (84%)   | 89 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 34  | k     | 96/98 (98%)    | 87 (91%)  | 9 (9%)   | 0        | 100         | 100 |
| 35  | l     | 601/603 (100%) | 575 (96%) | 26 (4%)  | 0        | 100         | 100 |
| 36  | m     | 125/175 (71%)  | 112 (90%) | 13 (10%) | 0        | 100         | 100 |
| 37  | n     | 54/56 (96%)    | 54 (100%) | 0        | 0        | 100         | 100 |
| 38  | o     | 126/128 (98%)  | 120 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 39  | p     | 176/178 (99%)  | 163 (93%) | 13 (7%)  | 0        | 100         | 100 |
| 40  | r     | 457/459 (100%) | 441 (96%) | 16 (4%)  | 0        | 100         | 100 |
| 41  | s     | 299/318 (94%)  | 285 (95%) | 13 (4%)  | 1 (0%)   | 36          | 67  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 42  | u     | 169/171 (99%)   | 162 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 43  | v     | 122/125 (98%)   | 115 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 44  | w     | 318/320 (99%)   | 302 (95%)  | 15 (5%)  | 1 (0%)   | 36          | 67  |
| All | All   | 8029/8309 (97%) | 7684 (96%) | 336 (4%) | 9 (0%)   | 49          | 78  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | i     | 93  | VAL  |
| 44  | w     | 70  | LYS  |
| 9   | J     | 38  | HIS  |
| 32  | i     | 92  | PRO  |
| 6   | G     | 76  | LEU  |
| 20  | V     | 46  | PRO  |
| 12  | M     | 283 | GLU  |
| 9   | J     | 83  | PRO  |
| 41  | s     | 90  | PRO  |

### 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     | 345/345 (100%) | 343 (99%)  | 2 (1%)   | 78          | 83  |
| 2   | B     | 151/151 (100%) | 151 (100%) | 0        | 100         | 100 |
| 3   | C     | 132/132 (100%) | 132 (100%) | 0        | 100         | 100 |
| 4   | E     | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 5   | F     | 76/76 (100%)   | 76 (100%)  | 0        | 100         | 100 |
| 6   | G     | 76/81 (94%)    | 76 (100%)  | 0        | 100         | 100 |
| 6   | X     | 77/81 (95%)    | 77 (100%)  | 0        | 100         | 100 |
| 7   | H     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 8   | I     | 87/97 (90%)    | 87 (100%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 9   | J     | 255/295 (86%)  | 255 (100%) | 0        | 100         | 100 |
| 10  | K     | 41/41 (100%)   | 41 (100%)  | 0        | 100         | 100 |
| 11  | L     | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 12  | M     | 580/580 (100%) | 580 (100%) | 0        | 100         | 100 |
| 13  | N     | 130/130 (100%) | 130 (100%) | 0        | 100         | 100 |
| 14  | O     | 183/183 (100%) | 183 (100%) | 0        | 100         | 100 |
| 15  | P     | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 16  | Q     | 361/370 (98%)  | 361 (100%) | 0        | 100         | 100 |
| 17  | S     | 58/58 (100%)   | 58 (100%)  | 0        | 100         | 100 |
| 18  | T     | 79/79 (100%)   | 79 (100%)  | 0        | 100         | 100 |
| 19  | U     | 69/69 (100%)   | 69 (100%)  | 0        | 100         | 100 |
| 20  | V     | 101/101 (100%) | 101 (100%) | 0        | 100         | 100 |
| 21  | W     | 122/123 (99%)  | 122 (100%) | 0        | 100         | 100 |
| 22  | Y     | 63/63 (100%)   | 63 (100%)  | 0        | 100         | 100 |
| 23  | Z     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 24  | a     | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 25  | b     | 98/119 (82%)   | 98 (100%)  | 0        | 100         | 100 |
| 26  | c     | 141/141 (100%) | 141 (100%) | 0        | 100         | 100 |
| 27  | d     | 155/155 (100%) | 155 (100%) | 0        | 100         | 100 |
| 28  | e     | 99/99 (100%)   | 99 (100%)  | 0        | 100         | 100 |
| 29  | f     | 35/38 (92%)    | 35 (100%)  | 0        | 100         | 100 |
| 30  | g     | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 31  | h     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 32  | i     | 311/311 (100%) | 311 (100%) | 0        | 100         | 100 |
| 33  | j     | 88/99 (89%)    | 88 (100%)  | 0        | 100         | 100 |
| 34  | k     | 85/85 (100%)   | 85 (100%)  | 0        | 100         | 100 |
| 35  | l     | 537/537 (100%) | 537 (100%) | 0        | 100         | 100 |
| 36  | m     | 99/141 (70%)   | 99 (100%)  | 0        | 100         | 100 |
| 37  | n     | 53/53 (100%)   | 53 (100%)  | 0        | 100         | 100 |
| 38  | o     | 113/113 (100%) | 113 (100%) | 0        | 100         | 100 |
| 39  | p     | 159/159 (100%) | 159 (100%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 40  | r     | 410/410 (100%)  | 410 (100%)  | 0        | 100         | 100 |
| 41  | s     | 263/275 (96%)   | 263 (100%)  | 0        | 100         | 100 |
| 42  | u     | 153/153 (100%)  | 153 (100%)  | 0        | 100         | 100 |
| 43  | v     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 44  | w     | 281/283 (99%)   | 279 (99%)   | 2 (1%)   | 76          | 82  |
| All | All   | 7064/7234 (98%) | 7060 (100%) | 4 (0%)   | 87          | 90  |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 124 | THR  |
| 1   | A     | 125 | CYS  |
| 44  | w     | 214 | ILE  |
| 44  | w     | 246 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 136 | HIS  |
| 1   | A     | 244 | ASN  |
| 1   | A     | 283 | ASN  |
| 1   | A     | 457 | HIS  |
| 4   | E     | 58  | GLN  |
| 5   | F     | 81  | ASN  |
| 6   | G     | 142 | GLN  |
| 7   | H     | 21  | HIS  |
| 7   | H     | 76  | GLN  |
| 8   | I     | 13  | ASN  |
| 8   | I     | 110 | GLN  |
| 9   | J     | 122 | HIS  |
| 9   | J     | 376 | ASN  |
| 12  | M     | 123 | ASN  |
| 12  | M     | 260 | ASN  |
| 12  | M     | 300 | GLN  |
| 12  | M     | 388 | ASN  |
| 12  | M     | 498 | GLN  |
| 12  | M     | 604 | GLN  |
| 12  | M     | 663 | ASN  |
| 13  | N     | 13  | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | N     | 135 | GLN  |
| 14  | O     | 69  | ASN  |
| 14  | O     | 133 | GLN  |
| 15  | P     | 63  | GLN  |
| 15  | P     | 107 | GLN  |
| 15  | P     | 131 | ASN  |
| 15  | P     | 181 | HIS  |
| 16  | Q     | 183 | HIS  |
| 16  | Q     | 234 | GLN  |
| 16  | Q     | 250 | ASN  |
| 16  | Q     | 306 | GLN  |
| 16  | Q     | 454 | GLN  |
| 17  | S     | 27  | HIS  |
| 17  | S     | 46  | ASN  |
| 20  | V     | 129 | GLN  |
| 22  | Y     | 83  | HIS  |
| 24  | a     | 170 | GLN  |
| 24  | a     | 181 | HIS  |
| 26  | c     | 164 | ASN  |
| 30  | g     | 119 | HIS  |
| 32  | i     | 49  | ASN  |
| 32  | i     | 63  | GLN  |
| 32  | i     | 150 | ASN  |
| 32  | i     | 174 | GLN  |
| 32  | i     | 221 | HIS  |
| 33  | j     | 82  | ASN  |
| 33  | j     | 108 | GLN  |
| 34  | k     | 57  | ASN  |
| 35  | l     | 139 | GLN  |
| 35  | l     | 192 | HIS  |
| 35  | l     | 354 | GLN  |
| 35  | l     | 580 | GLN  |
| 37  | n     | 3   | ASN  |
| 37  | n     | 11  | HIS  |
| 38  | o     | 52  | ASN  |
| 38  | o     | 75  | ASN  |
| 40  | r     | 81  | GLN  |
| 40  | r     | 103 | GLN  |
| 40  | r     | 144 | ASN  |
| 40  | r     | 175 | ASN  |
| 40  | r     | 192 | ASN  |
| 40  | r     | 251 | ASN  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | r     | 304 | GLN  |
| 40  | r     | 366 | ASN  |
| 41  | s     | 47  | GLN  |
| 41  | s     | 124 | ASN  |
| 41  | s     | 235 | ASN  |
| 41  | s     | 250 | HIS  |
| 41  | s     | 317 | GLN  |
| 42  | u     | 30  | HIS  |
| 42  | u     | 163 | HIS  |
| 43  | v     | 47  | ASN  |
| 43  | v     | 85  | HIS  |
| 44  | w     | 127 | ASN  |
| 44  | w     | 219 | GLN  |
| 44  | w     | 344 | 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     | 2.00 | 1 (10%)     | 5,13,15     | 6.21 | 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   | -       | 2/10/13/15 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 16  | Q     | 118 | 2MR  | CZ-NE | 5.58 | 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  | 12.76 | 131.18      | 119.48   |
| 16  | Q     | 118 | 2MR  | CD-NE-CZ   | 4.41  | 131.65      | 123.36   |
| 16  | Q     | 118 | 2MR  | CQ2-NH2-CZ | 3.08  | 130.26      | 123.65   |

There are no chirality outliers.

All (2) 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 |

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 41 ligands modelled in this entry, 2 are monoatomic - leaving 39 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 | $\# Z  > 2$ |
| 48  | PEE  | m     | 202 | -    | 40,40,50     | 1.16 | 5 (12%)     | 43,45,55    | 1.05 | 2 (4%)      |
| 52  | FES  | M     | 803 | 12   | 0,4,4        | -    | -           | -           |      |             |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 54  | CDL  | r     | 714 | -    | 96,96,99     | 1.11 | 8 (8%)   | 102,108,111 | 0.89 | 4 (3%)   |
| 54  | CDL  | a     | 201 | -    | 90,90,99     | 0.97 | 4 (4%)   | 96,102,111  | 1.07 | 6 (6%)   |
| 48  | PEE  | U     | 101 | -    | 50,50,50     | 1.17 | 6 (12%)  | 53,55,55    | 0.96 | 2 (3%)   |
| 48  | PEE  | l     | 720 | -    | 45,45,50     | 1.24 | 6 (13%)  | 48,50,55    | 1.02 | 2 (4%)   |
| 51  | NDP  | J     | 401 | -    | 51,52,52     | 4.25 | 25 (49%) | 71,80,80    | 2.21 | 14 (19%) |
| 45  | SF4  | B     | 301 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 49  | PLX  | e     | 201 | -    | 51,51,51     | 1.20 | 5 (9%)   | 53,59,59    | 0.63 | 1 (1%)   |
| 49  | PLX  | V     | 205 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.62 | 1 (1%)   |
| 50  | 8Q1  | G     | 201 | -    | 32,34,34     | 2.24 | 7 (21%)  | 39,43,43    | 1.69 | 11 (28%) |
| 46  | FMN  | A     | 502 | -    | 33,33,33     | 1.09 | 2 (6%)   | 48,50,50    | 1.28 | 8 (16%)  |
| 48  | PEE  | l     | 719 | -    | 45,45,50     | 1.24 | 6 (13%)  | 48,50,55    | 1.02 | 2 (4%)   |
| 49  | PLX  | n     | 101 | -    | 51,51,51     | 0.60 | 0        | 53,59,59    | 0.70 | 0        |
| 57  | ADP  | w     | 401 | -    | 28,29,29     | 3.16 | 9 (32%)  | 43,45,45    | 1.91 | 9 (20%)  |
| 48  | PEE  | V     | 207 | -    | 39,39,50     | 1.33 | 6 (15%)  | 42,44,55    | 1.10 | 3 (7%)   |
| 49  | PLX  | i     | 705 | -    | 51,51,51     | 1.18 | 3 (5%)   | 53,59,59    | 0.67 | 1 (1%)   |
| 48  | PEE  | V     | 202 | -    | 50,50,50     | 1.17 | 6 (12%)  | 53,55,55    | 1.02 | 2 (3%)   |
| 54  | CDL  | N     | 202 | -    | 50,50,99     | 1.27 | 4 (8%)   | 56,62,111   | 1.32 | 7 (12%)  |
| 45  | SF4  | A     | 501 | 1    | 0,12,12      | -    | -        | -           |      |          |
| 45  | SF4  | M     | 801 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 49  | PLX  | C     | 312 | -    | 51,51,51     | 1.19 | 3 (5%)   | 53,59,59    | 0.63 | 1 (1%)   |
| 48  | PEE  | l     | 718 | -    | 46,46,50     | 1.22 | 6 (13%)  | 49,51,55    | 1.02 | 3 (6%)   |
| 54  | CDL  | n     | 102 | -    | 77,77,99     | 1.02 | 4 (5%)   | 83,89,111   | 1.16 | 7 (8%)   |
| 56  | UQ   | s     | 403 | -    | 28,28,63     | 3.30 | 7 (25%)  | 36,37,79    | 2.77 | 11 (30%) |
| 54  | CDL  | l     | 712 | -    | 98,98,99     | 0.92 | 4 (4%)   | 104,110,111 | 1.17 | 9 (8%)   |
| 47  | NAI  | A     | 503 | -    | 47,48,48     | 4.01 | 22 (46%) | 64,73,73    | 1.68 | 12 (18%) |
| 48  | PEE  | s     | 401 | -    | 50,50,50     | 1.18 | 6 (12%)  | 53,55,55    | 0.98 | 2 (3%)   |
| 54  | CDL  | i     | 401 | -    | 65,65,99     | 1.14 | 4 (6%)   | 71,77,111   | 1.21 | 5 (7%)   |
| 54  | CDL  | l     | 713 | -    | 99,99,99     | 1.11 | 8 (8%)   | 105,111,111 | 0.84 | 4 (3%)   |
| 50  | 8Q1  | X     | 201 | -    | 32,34,34     | 2.27 | 7 (21%)  | 39,43,43    | 1.73 | 10 (25%) |
| 54  | CDL  | V     | 203 | -    | 67,67,99     | 1.11 | 4 (5%)   | 73,79,111   | 1.20 | 6 (8%)   |
| 45  | SF4  | B     | 302 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 54  | CDL  | V     | 201 | -    | 93,93,99     | 0.95 | 4 (4%)   | 99,105,111  | 1.08 | 5 (5%)   |
| 49  | PLX  | j     | 203 | -    | 51,51,51     | 1.21 | 4 (7%)   | 53,59,59    | 0.61 | 1 (1%)   |
| 45  | SF4  | M     | 802 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 48  | PEE  | C     | 311 | -    | 46,46,50     | 1.23 | 6 (13%)  | 49,51,55    | 0.97 | 2 (4%)   |
| 45  | SF4  | C     | 301 | 3    | 0,12,12      | -    | -        | -           |      |          |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 52  | FES  | O     | 301 | 14   | 0,4,4        | -    | -        | -           |      |          |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 48  | PEE  | m     | 202 | -    | -       | 18/44/44/54    | -       |
| 52  | FES  | M     | 803 | 12   | -       | -              | 0/1/1/1 |
| 45  | SF4  | M     | 802 | 12   | -       | -              | 0/6/5/5 |
| 54  | CDL  | r     | 714 | -    | -       | 63/107/107/110 | -       |
| 48  | PEE  | C     | 311 | -    | -       | 24/50/50/54    | -       |
| 54  | CDL  | a     | 201 | -    | -       | 26/101/101/110 | -       |
| 48  | PEE  | U     | 101 | -    | -       | 24/54/54/54    | -       |
| 48  | PEE  | l     | 720 | -    | -       | 26/49/49/54    | -       |
| 51  | NDP  | J     | 401 | -    | -       | 12/34/77/77    | 0/5/5/5 |
| 45  | SF4  | B     | 301 | 2    | -       | -              | 0/6/5/5 |
| 49  | PLX  | V     | 205 | -    | -       | 32/55/55/55    | -       |
| 50  | 8Q1  | G     | 201 | -    | -       | 19/41/41/41    | -       |
| 46  | FMN  | A     | 502 | -    | -       | 6/18/18/18     | 0/3/3/3 |
| 48  | PEE  | l     | 719 | -    | -       | 20/49/49/54    | -       |
| 57  | ADP  | w     | 401 | -    | -       | 3/16/32/32     | 0/3/3/3 |
| 48  | PEE  | V     | 207 | -    | -       | 21/43/43/54    | -       |
| 49  | PLX  | i     | 705 | -    | -       | 23/55/55/55    | -       |
| 48  | PEE  | V     | 202 | -    | -       | 21/54/54/54    | -       |
| 54  | CDL  | N     | 202 | -    | -       | 22/61/61/110   | -       |
| 45  | SF4  | A     | 501 | 1    | -       | -              | 0/6/5/5 |
| 45  | SF4  | M     | 801 | 12   | -       | -              | 0/6/5/5 |
| 49  | PLX  | C     | 312 | -    | -       | 34/55/55/55    | -       |
| 48  | PEE  | l     | 718 | -    | -       | 22/50/50/54    | -       |
| 54  | CDL  | n     | 102 | -    | -       | 28/88/88/110   | -       |
| 56  | UQ   | s     | 403 | -    | -       | 9/21/45/87     | 0/1/1/1 |
| 54  | CDL  | l     | 712 | -    | -       | 39/109/109/110 | -       |
| 47  | NAI  | A     | 503 | -    | -       | 5/29/72/72     | 0/5/5/5 |
| 48  | PEE  | s     | 401 | -    | -       | 22/54/54/54    | -       |
| 54  | CDL  | i     | 401 | -    | -       | 30/76/76/110   | -       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 54  | CDL  | l     | 713 | -    | -       | 65/110/110/110 | -       |
| 50  | 8Q1  | X     | 201 | -    | -       | 23/41/41/41    | -       |
| 54  | CDL  | V     | 203 | -    | -       | 33/78/78/110   | -       |
| 45  | SF4  | B     | 302 | 2    | -       | -              | 0/6/5/5 |
| 54  | CDL  | V     | 201 | -    | -       | 37/104/104/110 | -       |
| 49  | PLX  | j     | 203 | -    | -       | 24/55/55/55    | -       |
| 49  | PLX  | e     | 201 | -    | -       | 38/55/55/55    | -       |
| 49  | PLX  | n     | 101 | -    | -       | 15/55/55/55    | -       |
| 45  | SF4  | C     | 301 | 3    | -       | -              | 0/6/5/5 |
| 52  | FES  | O     | 301 | 14   | -       | -              | 0/1/1/1 |

All (195) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 51  | J     | 401 | NDP  | C3B-C2B | -13.06 | 1.24        | 1.53     |
| 51  | J     | 401 | NDP  | O4D-C4D | 10.66  | 1.68        | 1.45     |
| 47  | A     | 503 | NAI  | C3D-C4D | -10.38 | 1.26        | 1.53     |
| 51  | J     | 401 | NDP  | C3D-C4D | -10.03 | 1.27        | 1.53     |
| 56  | s     | 403 | UQ   | C13-C14 | 9.59   | 1.55        | 1.33     |
| 47  | A     | 503 | NAI  | O4B-C1B | 9.27   | 1.63        | 1.42     |
| 56  | s     | 403 | UQ   | C8-C9   | 9.12   | 1.54        | 1.33     |
| 57  | w     | 401 | ADP  | C3'-C4' | -8.95  | 1.30        | 1.53     |
| 47  | A     | 503 | NAI  | O4B-C4B | -8.35  | 1.26        | 1.45     |
| 51  | J     | 401 | NDP  | O4B-C4B | -7.96  | 1.27        | 1.45     |
| 56  | s     | 403 | UQ   | C18-C19 | 7.94   | 1.56        | 1.32     |
| 50  | G     | 201 | 8Q1  | P24-O27 | 7.86   | 1.85        | 1.60     |
| 47  | A     | 503 | NAI  | C2D-C1D | -7.74  | 1.29        | 1.53     |
| 57  | w     | 401 | ADP  | O4'-C4' | 7.65   | 1.62        | 1.45     |
| 50  | X     | 201 | 8Q1  | P24-O27 | 7.64   | 1.84        | 1.60     |
| 47  | A     | 503 | NAI  | C2B-C1B | -7.43  | 1.30        | 1.53     |
| 51  | J     | 401 | NDP  | C2N-C3N | 7.40   | 1.55        | 1.35     |
| 51  | J     | 401 | NDP  | C6N-C5N | 7.26   | 1.55        | 1.33     |
| 47  | A     | 503 | NAI  | O4D-C4D | 6.90   | 1.60        | 1.45     |
| 57  | w     | 401 | ADP  | PA-O3A  | 6.45   | 1.66        | 1.59     |
| 51  | J     | 401 | NDP  | PN-O3   | 6.20   | 1.66        | 1.59     |
| 47  | A     | 503 | NAI  | PA-O3   | 6.18   | 1.66        | 1.59     |
| 47  | A     | 503 | NAI  | C2D-C3D | 5.96   | 1.69        | 1.53     |
| 51  | J     | 401 | NDP  | C6A-N6A | 5.77   | 1.48        | 1.34     |
| 51  | J     | 401 | NDP  | P2B-O2B | 5.66   | 1.69        | 1.59     |
| 47  | A     | 503 | NAI  | O4D-C1D | 5.65   | 1.55        | 1.42     |
| 50  | G     | 201 | 8Q1  | C28-C29 | 5.48   | 1.61        | 1.52     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 50  | X     | 201 | 8Q1  | C28-C29 | 5.43  | 1.61        | 1.52     |
| 47  | A     | 503 | NAI  | PN-O3   | 5.40  | 1.65        | 1.59     |
| 57  | w     | 401 | ADP  | C6-N6   | 5.39  | 1.48        | 1.34     |
| 47  | A     | 503 | NAI  | C7N-N7N | 5.32  | 1.48        | 1.33     |
| 47  | A     | 503 | NAI  | C4N-C3N | -5.31 | 1.40        | 1.50     |
| 51  | J     | 401 | NDP  | PA-O3   | 5.21  | 1.65        | 1.59     |
| 51  | J     | 401 | NDP  | C3B-C4B | 5.17  | 1.66        | 1.53     |
| 51  | J     | 401 | NDP  | O4D-C1D | -5.09 | 1.30        | 1.42     |
| 47  | A     | 503 | NAI  | C6A-N6A | 5.06  | 1.47        | 1.34     |
| 51  | J     | 401 | NDP  | C6N-N1N | 5.01  | 1.49        | 1.37     |
| 51  | J     | 401 | NDP  | O4B-C1B | 4.77  | 1.53        | 1.42     |
| 51  | J     | 401 | NDP  | C1B-N9A | -4.64 | 1.33        | 1.46     |
| 57  | w     | 401 | ADP  | O4'-C1' | -4.59 | 1.31        | 1.42     |
| 47  | A     | 503 | NAI  | O2B-C2B | 4.36  | 1.53        | 1.43     |
| 54  | i     | 401 | CDL  | OA8-CA7 | 4.30  | 1.45        | 1.33     |
| 54  | V     | 203 | CDL  | OA8-CA7 | 4.29  | 1.45        | 1.33     |
| 54  | a     | 201 | CDL  | OA8-CA7 | 4.29  | 1.45        | 1.33     |
| 54  | N     | 202 | CDL  | OB8-CB7 | 4.28  | 1.45        | 1.33     |
| 54  | i     | 401 | CDL  | OA6-CA5 | 4.28  | 1.46        | 1.34     |
| 54  | l     | 712 | CDL  | OA8-CA7 | 4.27  | 1.45        | 1.33     |
| 54  | V     | 201 | CDL  | OA8-CA7 | 4.27  | 1.45        | 1.33     |
| 54  | i     | 401 | CDL  | OB8-CB7 | 4.26  | 1.45        | 1.33     |
| 54  | n     | 102 | CDL  | OB8-CB7 | 4.26  | 1.45        | 1.33     |
| 54  | V     | 201 | CDL  | OB8-CB7 | 4.25  | 1.45        | 1.33     |
| 54  | V     | 203 | CDL  | OB8-CB7 | 4.24  | 1.45        | 1.33     |
| 54  | l     | 712 | CDL  | OB8-CB7 | 4.21  | 1.45        | 1.33     |
| 54  | N     | 202 | CDL  | OA8-CA7 | 4.20  | 1.45        | 1.33     |
| 54  | V     | 201 | CDL  | OA6-CA5 | 4.19  | 1.46        | 1.34     |
| 54  | a     | 201 | CDL  | OB8-CB7 | 4.19  | 1.45        | 1.33     |
| 54  | i     | 401 | CDL  | OB6-CB5 | 4.16  | 1.46        | 1.34     |
| 54  | a     | 201 | CDL  | OB6-CB5 | 4.15  | 1.46        | 1.34     |
| 54  | N     | 202 | CDL  | OA6-CA5 | 4.13  | 1.46        | 1.34     |
| 54  | n     | 102 | CDL  | OA8-CA7 | 4.13  | 1.45        | 1.33     |
| 54  | V     | 201 | CDL  | OB6-CB5 | 4.12  | 1.45        | 1.34     |
| 54  | V     | 203 | CDL  | OA6-CA5 | 4.11  | 1.45        | 1.34     |
| 54  | a     | 201 | CDL  | OA6-CA5 | 4.07  | 1.45        | 1.34     |
| 54  | n     | 102 | CDL  | OA6-CA5 | 4.01  | 1.45        | 1.34     |
| 54  | l     | 712 | CDL  | OA6-CA5 | 3.98  | 1.45        | 1.34     |
| 54  | V     | 203 | CDL  | OB6-CB5 | 3.98  | 1.45        | 1.34     |
| 54  | l     | 712 | CDL  | OB6-CB5 | 3.98  | 1.45        | 1.34     |
| 54  | N     | 202 | CDL  | OB6-CB5 | 3.97  | 1.45        | 1.34     |
| 54  | n     | 102 | CDL  | OB6-CB5 | 3.90  | 1.45        | 1.34     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 51  | J     | 401 | NDP  | O2D-C2D | -3.90 | 1.33        | 1.43     |
| 50  | X     | 201 | 8Q1  | C1-S44  | 3.88  | 1.85        | 1.76     |
| 48  | m     | 202 | PEE  | C18-C19 | 3.84  | 1.53        | 1.31     |
| 51  | J     | 401 | NDP  | C7N-N7N | 3.83  | 1.44        | 1.33     |
| 48  | C     | 311 | PEE  | C18-C19 | 3.83  | 1.53        | 1.31     |
| 48  | V     | 207 | PEE  | C18-C19 | 3.82  | 1.53        | 1.31     |
| 50  | G     | 201 | 8Q1  | C1-S44  | 3.82  | 1.85        | 1.76     |
| 48  | s     | 401 | PEE  | C18-C19 | 3.82  | 1.53        | 1.31     |
| 48  | V     | 202 | PEE  | C18-C19 | 3.81  | 1.53        | 1.31     |
| 48  | l     | 719 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | l     | 720 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | l     | 718 | PEE  | C18-C19 | 3.79  | 1.53        | 1.31     |
| 48  | U     | 101 | PEE  | C18-C19 | 3.75  | 1.53        | 1.31     |
| 48  | C     | 311 | PEE  | C39-C38 | 3.75  | 1.53        | 1.31     |
| 48  | V     | 202 | PEE  | C39-C38 | 3.74  | 1.52        | 1.31     |
| 48  | l     | 719 | PEE  | C39-C38 | 3.73  | 1.52        | 1.31     |
| 48  | l     | 718 | PEE  | C39-C38 | 3.73  | 1.52        | 1.31     |
| 48  | V     | 207 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | l     | 720 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | U     | 101 | PEE  | C39-C38 | 3.70  | 1.52        | 1.31     |
| 48  | s     | 401 | PEE  | C39-C38 | 3.70  | 1.52        | 1.31     |
| 47  | A     | 503 | NAI  | C7N-C3N | 3.50  | 1.56        | 1.48     |
| 54  | l     | 713 | CDL  | OA8-CA7 | 3.47  | 1.43        | 1.33     |
| 47  | A     | 503 | NAI  | C4N-C5N | -3.42 | 1.40        | 1.49     |
| 57  | w     | 401 | ADP  | C8-N9   | -3.37 | 1.31        | 1.37     |
| 50  | X     | 201 | 8Q1  | O27-C28 | -3.37 | 1.33        | 1.43     |
| 54  | r     | 714 | CDL  | OA8-CA7 | 3.36  | 1.43        | 1.33     |
| 50  | X     | 201 | 8Q1  | C34-N36 | 3.34  | 1.41        | 1.33     |
| 50  | G     | 201 | 8Q1  | O27-C28 | -3.31 | 1.33        | 1.43     |
| 51  | J     | 401 | NDP  | C8A-N9A | -3.31 | 1.31        | 1.37     |
| 46  | A     | 502 | FMN  | C4A-N5  | 3.29  | 1.37        | 1.30     |
| 50  | G     | 201 | 8Q1  | C34-N36 | 3.28  | 1.41        | 1.33     |
| 51  | J     | 401 | NDP  | C5A-N7A | -3.20 | 1.33        | 1.39     |
| 50  | X     | 201 | 8Q1  | C6-C1   | 3.18  | 1.54        | 1.50     |
| 57  | w     | 401 | ADP  | O2'-C2' | -3.09 | 1.35        | 1.43     |
| 57  | w     | 401 | ADP  | O3'-C3' | 3.07  | 1.50        | 1.43     |
| 54  | r     | 714 | CDL  | OB6-CB5 | 3.06  | 1.42        | 1.34     |
| 50  | X     | 201 | 8Q1  | C39-N41 | 3.04  | 1.40        | 1.33     |
| 54  | l     | 713 | CDL  | OB6-CB5 | 3.00  | 1.42        | 1.34     |
| 54  | l     | 713 | CDL  | OA6-CA5 | 2.98  | 1.42        | 1.34     |
| 54  | l     | 713 | CDL  | OB8-CB7 | 2.97  | 1.42        | 1.33     |
| 51  | J     | 401 | NDP  | O3D-C3D | 2.95  | 1.50        | 1.43     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 54  | r     | 714 | CDL  | OB8-CB7 | 2.93  | 1.41        | 1.33     |
| 49  | C     | 312 | PLX  | O6-C4   | -2.93 | 1.40        | 1.44     |
| 49  | e     | 201 | PLX  | O6-C4   | -2.89 | 1.40        | 1.44     |
| 51  | J     | 401 | NDP  | C7N-C3N | 2.87  | 1.54        | 1.48     |
| 49  | i     | 705 | PLX  | O6-C4   | -2.86 | 1.40        | 1.44     |
| 50  | G     | 201 | 8Q1  | C6-C1   | 2.82  | 1.53        | 1.50     |
| 54  | r     | 714 | CDL  | OA6-CA5 | 2.79  | 1.42        | 1.34     |
| 48  | s     | 401 | PEE  | O2-C2   | -2.75 | 1.40        | 1.46     |
| 54  | r     | 714 | CDL  | OA6-CA4 | -2.72 | 1.40        | 1.46     |
| 49  | j     | 203 | PLX  | O6-C4   | -2.72 | 1.41        | 1.44     |
| 47  | A     | 503 | NAI  | C8A-N9A | -2.72 | 1.32        | 1.37     |
| 48  | V     | 202 | PEE  | O2-C2   | -2.67 | 1.40        | 1.46     |
| 48  | l     | 719 | PEE  | O2-C2   | -2.67 | 1.40        | 1.46     |
| 51  | J     | 401 | NDP  | O2B-C2B | 2.66  | 1.53        | 1.44     |
| 48  | l     | 718 | PEE  | O2-C2   | -2.66 | 1.40        | 1.46     |
| 49  | V     | 205 | PLX  | O6-C4   | -2.63 | 1.41        | 1.44     |
| 48  | U     | 101 | PEE  | O2-C2   | -2.63 | 1.40        | 1.46     |
| 54  | l     | 713 | CDL  | OA6-CA4 | -2.62 | 1.40        | 1.46     |
| 56  | s     | 403 | UQ   | C6-C1   | 2.60  | 1.53        | 1.46     |
| 50  | G     | 201 | 8Q1  | C39-N41 | 2.59  | 1.39        | 1.33     |
| 48  | C     | 311 | PEE  | O2-C2   | -2.54 | 1.40        | 1.46     |
| 48  | l     | 720 | PEE  | O2-C2   | -2.54 | 1.40        | 1.46     |
| 48  | C     | 311 | PEE  | O3-C30  | 2.53  | 1.40        | 1.33     |
| 48  | l     | 718 | PEE  | O3-C30  | 2.53  | 1.40        | 1.33     |
| 51  | J     | 401 | NDP  | C2D-C3D | 2.52  | 1.60        | 1.53     |
| 48  | l     | 720 | PEE  | O3-C30  | 2.48  | 1.40        | 1.33     |
| 48  | V     | 207 | PEE  | O3-C30  | 2.47  | 1.40        | 1.33     |
| 47  | A     | 503 | NAI  | C6N-C5N | 2.45  | 1.40        | 1.33     |
| 49  | V     | 205 | PLX  | C7-C6   | 2.44  | 1.55        | 1.50     |
| 48  | V     | 207 | PEE  | O2-C2   | -2.44 | 1.40        | 1.46     |
| 48  | m     | 202 | PEE  | O2-C2   | -2.43 | 1.40        | 1.46     |
| 54  | l     | 713 | CDL  | OB6-CB4 | -2.42 | 1.40        | 1.46     |
| 48  | s     | 401 | PEE  | O3-C30  | 2.41  | 1.40        | 1.33     |
| 47  | A     | 503 | NAI  | PN-O5D  | 2.41  | 1.68        | 1.59     |
| 48  | U     | 101 | PEE  | O3-C30  | 2.41  | 1.40        | 1.33     |
| 57  | w     | 401 | ADP  | C5-N7   | -2.40 | 1.34        | 1.39     |
| 48  | l     | 719 | PEE  | O3-C30  | 2.37  | 1.40        | 1.33     |
| 48  | V     | 202 | PEE  | O3-C30  | 2.37  | 1.40        | 1.33     |
| 49  | i     | 705 | PLX  | C7-C6   | 2.36  | 1.55        | 1.50     |
| 47  | A     | 503 | NAI  | C5B-C4B | 2.36  | 1.58        | 1.51     |
| 47  | A     | 503 | NAI  | O3B-C3B | -2.36 | 1.37        | 1.43     |
| 49  | e     | 201 | PLX  | C7-C6   | 2.34  | 1.55        | 1.50     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 48  | m     | 202 | PEE  | O3-C30  | 2.32  | 1.40        | 1.33     |
| 48  | l     | 720 | PEE  | O2-C10  | 2.30  | 1.40        | 1.34     |
| 48  | C     | 311 | PEE  | O2-C10  | 2.30  | 1.40        | 1.34     |
| 48  | m     | 202 | PEE  | O2-C10  | 2.29  | 1.40        | 1.34     |
| 48  | V     | 207 | PEE  | O2-C10  | 2.28  | 1.40        | 1.34     |
| 48  | m     | 202 | PEE  | O3-C3   | -2.27 | 1.40        | 1.45     |
| 46  | A     | 502 | FMN  | C10-N1  | 2.27  | 1.37        | 1.33     |
| 49  | j     | 203 | PLX  | C7-C6   | 2.25  | 1.55        | 1.50     |
| 48  | U     | 101 | PEE  | O2-C10  | 2.25  | 1.40        | 1.34     |
| 48  | U     | 101 | PEE  | O3-C3   | -2.24 | 1.40        | 1.45     |
| 49  | j     | 203 | PLX  | P1-O4   | 2.23  | 1.68        | 1.59     |
| 54  | l     | 713 | CDL  | PB2-OB2 | 2.23  | 1.68        | 1.59     |
| 51  | J     | 401 | NDP  | O7N-C7N | -2.22 | 1.19        | 1.24     |
| 48  | V     | 202 | PEE  | O3-C3   | -2.22 | 1.40        | 1.45     |
| 54  | r     | 714 | CDL  | PB2-OB5 | 2.22  | 1.68        | 1.59     |
| 48  | l     | 719 | PEE  | O3-C3   | -2.21 | 1.40        | 1.45     |
| 54  | r     | 714 | CDL  | PB2-OB2 | 2.20  | 1.68        | 1.59     |
| 56  | s     | 403 | UQ   | O4-C4   | -2.20 | 1.18        | 1.23     |
| 54  | r     | 714 | CDL  | OB6-CB4 | -2.19 | 1.41        | 1.46     |
| 48  | l     | 719 | PEE  | O2-C10  | 2.18  | 1.40        | 1.34     |
| 54  | l     | 713 | CDL  | PB2-OB5 | 2.18  | 1.67        | 1.59     |
| 48  | l     | 720 | PEE  | O3-C3   | -2.17 | 1.40        | 1.45     |
| 48  | V     | 202 | PEE  | O2-C10  | 2.17  | 1.40        | 1.34     |
| 49  | V     | 205 | PLX  | P1-O4   | 2.16  | 1.67        | 1.59     |
| 49  | C     | 312 | PLX  | C7-C6   | 2.16  | 1.55        | 1.50     |
| 56  | s     | 403 | UQ   | O3-CM3  | -2.15 | 1.40        | 1.45     |
| 48  | l     | 718 | PEE  | O2-C10  | 2.14  | 1.40        | 1.34     |
| 48  | s     | 401 | PEE  | O3-C3   | -2.14 | 1.40        | 1.45     |
| 49  | e     | 201 | PLX  | P1-O4   | 2.14  | 1.67        | 1.59     |
| 47  | A     | 503 | NAI  | C5A-N7A | -2.12 | 1.35        | 1.39     |
| 48  | s     | 401 | PEE  | O2-C10  | 2.11  | 1.40        | 1.34     |
| 49  | j     | 203 | PLX  | P1-O1   | 2.11  | 1.67        | 1.59     |
| 48  | V     | 207 | PEE  | O3-C3   | -2.10 | 1.40        | 1.45     |
| 48  | C     | 311 | PEE  | O3-C3   | -2.09 | 1.40        | 1.45     |
| 49  | C     | 312 | PLX  | P1-O4   | 2.09  | 1.67        | 1.59     |
| 56  | s     | 403 | UQ   | O1-C1   | -2.07 | 1.18        | 1.23     |
| 48  | l     | 718 | PEE  | O3-C3   | -2.06 | 1.40        | 1.45     |
| 49  | i     | 705 | PLX  | P1-O4   | 2.05  | 1.67        | 1.59     |
| 51  | J     | 401 | NDP  | PA-O5B  | 2.03  | 1.67        | 1.59     |
| 49  | V     | 205 | PLX  | P1-O1   | 2.03  | 1.67        | 1.59     |
| 49  | e     | 201 | PLX  | C1-C2   | 2.02  | 1.57        | 1.51     |
| 49  | e     | 201 | PLX  | P1-O1   | 2.01  | 1.67        | 1.59     |

All (153) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | s     | 403 | UQ   | C7-C8-C9    | -9.66 | 110.19      | 126.83   |
| 51  | J     | 401 | NDP  | C3N-C2N-N1N | -7.68 | 111.92      | 123.20   |
| 51  | J     | 401 | NDP  | C1D-N1N-C2N | -6.92 | 109.73      | 121.14   |
| 51  | J     | 401 | NDP  | C6N-N1N-C2N | -6.71 | 112.14      | 119.32   |
| 56  | s     | 403 | UQ   | C12-C13-C14 | -6.19 | 113.45      | 127.62   |
| 51  | J     | 401 | NDP  | C5A-C4A-N3A | -5.58 | 119.03      | 126.72   |
| 57  | w     | 401 | ADP  | C5-C4-N3    | -5.45 | 119.21      | 126.72   |
| 47  | A     | 503 | NAI  | C5A-C4A-N3A | -5.43 | 119.25      | 126.72   |
| 51  | J     | 401 | NDP  | C1D-N1N-C6N | -5.30 | 109.56      | 120.77   |
| 54  | l     | 712 | CDL  | OA6-CA5-C11 | 4.86  | 121.99      | 111.48   |
| 56  | s     | 403 | UQ   | C10-C9-C8   | -4.82 | 111.24      | 123.63   |
| 50  | X     | 201 | 8Q1  | C6-C1-S44   | 4.66  | 118.96      | 113.40   |
| 57  | w     | 401 | ADP  | N3-C2-N1    | -4.58 | 121.64      | 128.58   |
| 47  | A     | 503 | NAI  | N3A-C2A-N1A | -4.44 | 121.86      | 128.58   |
| 54  | n     | 102 | CDL  | OA6-CA5-C11 | 4.40  | 121.00      | 111.48   |
| 56  | s     | 403 | UQ   | C11-C9-C8   | -4.39 | 111.31      | 121.17   |
| 50  | G     | 201 | 8Q1  | C6-C1-S44   | 4.37  | 118.60      | 113.40   |
| 54  | i     | 401 | CDL  | OA6-CA5-C11 | 4.35  | 120.89      | 111.48   |
| 57  | w     | 401 | ADP  | N3-C4-N9    | 4.25  | 134.40      | 127.17   |
| 48  | V     | 202 | PEE  | O2-C10-C11  | 4.22  | 120.61      | 111.48   |
| 48  | m     | 202 | PEE  | O2-C10-C11  | 4.21  | 120.58      | 111.48   |
| 54  | V     | 203 | CDL  | OB6-CB5-C51 | 4.20  | 120.56      | 111.48   |
| 51  | J     | 401 | NDP  | N3A-C2A-N1A | -4.12 | 122.34      | 128.58   |
| 54  | r     | 714 | CDL  | OB6-CB5-C51 | 4.11  | 120.37      | 111.48   |
| 54  | N     | 202 | CDL  | OB6-CB5-C51 | 4.09  | 120.34      | 111.48   |
| 48  | l     | 719 | PEE  | O2-C10-C11  | 4.07  | 120.28      | 111.48   |
| 56  | s     | 403 | UQ   | C17-C18-C19 | -4.07 | 114.08      | 127.64   |
| 56  | s     | 403 | UQ   | C15-C14-C13 | -4.06 | 113.20      | 123.63   |
| 48  | l     | 718 | PEE  | O2-C10-C11  | 4.01  | 120.16      | 111.48   |
| 54  | N     | 202 | CDL  | OA6-CA5-C11 | 4.00  | 120.13      | 111.48   |
| 48  | l     | 720 | PEE  | O2-C10-C11  | 3.98  | 120.10      | 111.48   |
| 51  | J     | 401 | NDP  | N3A-C4A-N9A | 3.97  | 133.92      | 127.17   |
| 54  | a     | 201 | CDL  | OB6-CB5-C51 | 3.97  | 120.07      | 111.48   |
| 54  | V     | 201 | CDL  | OB6-CB5-C51 | 3.97  | 120.07      | 111.48   |
| 54  | i     | 401 | CDL  | OB6-CB5-C51 | 3.92  | 119.96      | 111.48   |
| 54  | l     | 712 | CDL  | CA4-OA6-CA5 | -3.91 | 108.44      | 117.80   |
| 48  | V     | 207 | PEE  | O2-C10-C11  | 3.88  | 119.87      | 111.48   |
| 54  | V     | 203 | CDL  | OA6-CA5-C11 | 3.87  | 119.84      | 111.48   |
| 48  | C     | 311 | PEE  | O2-C10-C11  | 3.86  | 119.84      | 111.48   |
| 48  | s     | 401 | PEE  | O2-C10-C11  | 3.86  | 119.83      | 111.48   |
| 47  | A     | 503 | NAI  | N3A-C4A-N9A | 3.86  | 133.73      | 127.17   |
| 54  | l     | 713 | CDL  | OA6-CA5-C11 | 3.85  | 119.82      | 111.48   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 54  | l     | 712 | CDL  | OB6-CB5-C51 | 3.85  | 119.81      | 111.48   |
| 54  | r     | 714 | CDL  | OA6-CA5-C11 | 3.84  | 119.80      | 111.48   |
| 54  | V     | 201 | CDL  | OA6-CA5-C11 | 3.78  | 119.66      | 111.48   |
| 48  | U     | 101 | PEE  | O2-C10-C11  | 3.76  | 119.62      | 111.48   |
| 54  | l     | 713 | CDL  | OB6-CB5-C51 | 3.76  | 119.61      | 111.48   |
| 47  | A     | 503 | NAI  | C2A-N3A-C4A | 3.68  | 120.82      | 111.83   |
| 54  | a     | 201 | CDL  | OA6-CA5-C11 | 3.68  | 119.44      | 111.48   |
| 51  | J     | 401 | NDP  | C2A-N3A-C4A | 3.62  | 120.66      | 111.83   |
| 57  | w     | 401 | ADP  | C2-N3-C4    | 3.57  | 120.55      | 111.83   |
| 54  | n     | 102 | CDL  | OB6-CB5-C51 | 3.57  | 119.20      | 111.48   |
| 56  | s     | 403 | UQ   | C16-C14-C13 | -3.53 | 113.25      | 121.17   |
| 57  | w     | 401 | ADP  | N9-C8-N7    | -3.50 | 108.97      | 113.94   |
| 50  | X     | 201 | 8Q1  | C43-S44-C1  | 3.49  | 112.16      | 101.84   |
| 46  | A     | 502 | FMN  | C4-N3-C2    | -3.45 | 119.52      | 125.64   |
| 50  | G     | 201 | 8Q1  | O35-C34-N36 | -3.41 | 115.76      | 122.98   |
| 50  | X     | 201 | 8Q1  | O35-C34-N36 | -3.36 | 115.87      | 122.98   |
| 47  | A     | 503 | NAI  | C4A-C5A-N7A | -3.34 | 106.76      | 110.58   |
| 50  | G     | 201 | 8Q1  | C43-S44-C1  | 3.34  | 111.71      | 101.84   |
| 47  | A     | 503 | NAI  | C5A-N7A-C8A | 3.31  | 108.65      | 103.45   |
| 57  | w     | 401 | ADP  | C5-N7-C8    | 3.21  | 108.49      | 103.45   |
| 47  | A     | 503 | NAI  | N9A-C8A-N7A | -3.20 | 109.39      | 113.94   |
| 51  | J     | 401 | NDP  | C4A-C5A-N7A | -3.20 | 106.93      | 110.58   |
| 54  | l     | 712 | CDL  | OB8-CB7-C71 | 3.17  | 121.50      | 111.83   |
| 56  | s     | 403 | UQ   | C21-C19-C18 | -3.16 | 113.16      | 122.66   |
| 51  | J     | 401 | NDP  | N9A-C8A-N7A | -3.16 | 109.45      | 113.94   |
| 47  | A     | 503 | NAI  | C4D-O4D-C1D | -3.15 | 102.51      | 109.47   |
| 57  | w     | 401 | ADP  | C4-N9-C8    | 3.15  | 109.04      | 105.74   |
| 56  | s     | 403 | UQ   | C7-C6-C5    | -3.14 | 119.51      | 124.89   |
| 54  | a     | 201 | CDL  | OB8-CB7-C71 | 3.12  | 121.34      | 111.83   |
| 51  | J     | 401 | NDP  | C5A-N7A-C8A | 3.09  | 108.31      | 103.45   |
| 54  | V     | 201 | CDL  | OB8-CB7-C71 | 3.09  | 121.25      | 111.83   |
| 47  | A     | 503 | NAI  | C3D-C2D-C1D | 3.04  | 107.22      | 101.46   |
| 57  | w     | 401 | ADP  | C4-C5-N7    | -3.04 | 107.11      | 110.58   |
| 48  | s     | 401 | PEE  | O3-C30-C31  | 3.03  | 121.07      | 111.83   |
| 54  | a     | 201 | CDL  | OA8-CA7-C31 | 3.03  | 121.07      | 111.83   |
| 54  | V     | 203 | CDL  | CB4-OB6-CB5 | -3.02 | 110.58      | 117.80   |
| 54  | i     | 401 | CDL  | OA8-CA7-C31 | 3.01  | 121.03      | 111.83   |
| 56  | s     | 403 | UQ   | CM5-C5-C6   | -3.00 | 119.52      | 124.45   |
| 54  | N     | 202 | CDL  | OA8-CA7-C31 | 2.95  | 120.82      | 111.83   |
| 48  | V     | 202 | PEE  | O3-C30-C31  | 2.93  | 120.76      | 111.83   |
| 50  | X     | 201 | 8Q1  | C32-C34-N36 | 2.89  | 121.98      | 116.48   |
| 48  | l     | 719 | PEE  | O3-C30-C31  | 2.88  | 120.61      | 111.83   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 54  | V     | 203 | CDL  | OA8-CA7-C31 | 2.87  | 120.57      | 111.83   |
| 49  | e     | 201 | PLX  | C1A-N1-C1   | 2.84  | 121.20      | 109.91   |
| 56  | s     | 403 | UQ   | C20-C19-C18 | -2.83 | 114.17      | 122.66   |
| 54  | V     | 201 | CDL  | OA8-CA7-C31 | 2.82  | 120.43      | 111.83   |
| 54  | V     | 201 | CDL  | CB4-OB6-CB5 | -2.77 | 111.16      | 117.80   |
| 48  | V     | 207 | PEE  | O3-C30-C31  | 2.74  | 120.19      | 111.83   |
| 54  | n     | 102 | CDL  | OA8-CA7-C31 | 2.73  | 120.17      | 111.83   |
| 54  | N     | 202 | CDL  | OB8-CB7-C71 | 2.73  | 120.16      | 111.83   |
| 50  | X     | 201 | 8Q1  | O2-P24-O27  | -2.72 | 99.57       | 106.67   |
| 54  | l     | 712 | CDL  | OA8-CA7-C31 | 2.71  | 120.11      | 111.83   |
| 48  | l     | 720 | PEE  | O3-C30-C31  | 2.70  | 120.05      | 111.83   |
| 54  | l     | 713 | CDL  | OA8-CA7-C31 | 2.69  | 120.04      | 111.83   |
| 46  | A     | 502 | FMN  | C5A-C9A-N10 | 2.68  | 120.39      | 117.97   |
| 54  | r     | 714 | CDL  | OA8-CA7-C31 | 2.66  | 119.95      | 111.83   |
| 48  | l     | 718 | PEE  | O3-C30-C31  | 2.66  | 119.95      | 111.83   |
| 48  | m     | 202 | PEE  | O3-C30-C31  | 2.66  | 119.93      | 111.83   |
| 54  | r     | 714 | CDL  | OB8-CB7-C71 | 2.64  | 119.88      | 111.83   |
| 48  | U     | 101 | PEE  | O3-C30-C31  | 2.64  | 119.87      | 111.83   |
| 54  | l     | 713 | CDL  | OB8-CB7-C71 | 2.62  | 119.83      | 111.83   |
| 50  | X     | 201 | 8Q1  | C37-C38-C39 | 2.61  | 116.75      | 112.39   |
| 54  | n     | 102 | CDL  | OB8-CB7-C71 | 2.61  | 119.79      | 111.83   |
| 48  | C     | 311 | PEE  | O3-C30-C31  | 2.60  | 119.76      | 111.83   |
| 46  | A     | 502 | FMN  | C4A-C4-N3   | 2.60  | 119.86      | 113.25   |
| 54  | V     | 203 | CDL  | OB8-CB7-C71 | 2.59  | 119.75      | 111.83   |
| 46  | A     | 502 | FMN  | C4A-C10-N10 | 2.59  | 120.19      | 116.48   |
| 50  | G     | 201 | 8Q1  | O2-P24-O27  | -2.58 | 99.94       | 106.67   |
| 54  | i     | 401 | CDL  | OB8-CB7-C71 | 2.58  | 119.69      | 111.83   |
| 47  | A     | 503 | NAI  | C2D-C3D-C4D | 2.57  | 107.58      | 102.61   |
| 50  | G     | 201 | 8Q1  | O40-C39-N41 | -2.56 | 118.00      | 123.03   |
| 49  | V     | 205 | PLX  | C1A-N1-C1   | 2.55  | 120.06      | 109.91   |
| 54  | N     | 202 | CDL  | CB4-OB6-CB5 | -2.54 | 111.71      | 117.80   |
| 49  | i     | 705 | PLX  | C1A-N1-C1   | 2.51  | 119.87      | 109.91   |
| 54  | l     | 712 | CDL  | CB4-OB6-CB5 | -2.49 | 111.83      | 117.80   |
| 50  | X     | 201 | 8Q1  | O4-C1-S44   | -2.45 | 119.57      | 122.68   |
| 49  | j     | 203 | PLX  | C1A-N1-C1   | 2.44  | 119.62      | 109.91   |
| 54  | l     | 712 | CDL  | OA6-CA5-OA7 | -2.44 | 118.00      | 123.70   |
| 50  | G     | 201 | 8Q1  | C37-C38-C39 | 2.44  | 116.45      | 112.39   |
| 46  | A     | 502 | FMN  | O4-C4-C4A   | -2.43 | 120.13      | 126.53   |
| 50  | G     | 201 | 8Q1  | C32-C34-N36 | 2.42  | 121.08      | 116.48   |
| 51  | J     | 401 | NDP  | C4A-N9A-C8A | 2.40  | 108.26      | 105.74   |
| 48  | V     | 207 | PEE  | C20-C19-C18 | -2.37 | 112.14      | 126.42   |
| 50  | G     | 201 | 8Q1  | O1-P24-O2   | 2.36  | 116.67      | 107.80   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 50  | X     | 201 | 8Q1  | O1-P24-O2   | 2.36  | 116.65      | 107.80   |
| 47  | A     | 503 | NAI  | C4A-N9A-C8A | 2.32  | 108.17      | 105.74   |
| 50  | G     | 201 | 8Q1  | O4-C1-S44   | -2.29 | 119.77      | 122.68   |
| 50  | G     | 201 | 8Q1  | O27-P24-O3  | -2.26 | 100.32      | 106.44   |
| 46  | A     | 502 | FMN  | C9A-C5A-N5  | -2.24 | 120.08      | 122.45   |
| 54  | i     | 401 | CDL  | CA4-OA6-CA5 | -2.23 | 112.45      | 117.80   |
| 54  | n     | 102 | CDL  | OA6-CA5-OA7 | -2.23 | 118.49      | 123.70   |
| 54  | n     | 102 | CDL  | CA4-OA6-CA5 | -2.23 | 112.46      | 117.80   |
| 51  | J     | 401 | NDP  | O4B-C1B-C2B | -2.22 | 102.76      | 106.59   |
| 49  | C     | 312 | PLX  | C1A-N1-C1   | 2.22  | 118.74      | 109.91   |
| 57  | w     | 401 | ADP  | C4'-O4'-C1' | -2.22 | 104.56      | 109.47   |
| 51  | J     | 401 | NDP  | C2D-C3D-C4D | 2.18  | 106.82      | 102.61   |
| 50  | X     | 201 | 8Q1  | O4-C1-C6    | -2.18 | 121.47      | 123.98   |
| 54  | l     | 712 | CDL  | OB8-CB7-OB9 | -2.18 | 118.19      | 123.63   |
| 46  | A     | 502 | FMN  | C10-C4A-N5  | -2.17 | 120.37      | 124.81   |
| 54  | N     | 202 | CDL  | OB6-CB5-OB7 | -2.12 | 118.76      | 123.70   |
| 54  | V     | 203 | CDL  | OB6-CB5-OB7 | -2.11 | 118.78      | 123.70   |
| 47  | A     | 503 | NAI  | C6N-N1N-C2N | 2.09  | 121.56      | 119.32   |
| 54  | a     | 201 | CDL  | OB8-CB7-OB9 | -2.08 | 118.43      | 123.63   |
| 46  | A     | 502 | FMN  | C4A-C10-N1  | -2.07 | 119.50      | 124.59   |
| 54  | a     | 201 | CDL  | CB4-OB6-CB5 | -2.07 | 112.84      | 117.80   |
| 50  | G     | 201 | 8Q1  | O4-C1-C6    | -2.04 | 121.62      | 123.98   |
| 54  | n     | 102 | CDL  | CA6-CA4-CA3 | -2.03 | 107.04      | 111.78   |
| 54  | l     | 712 | CDL  | OB6-CB5-OB7 | -2.02 | 118.97      | 123.70   |
| 48  | l     | 718 | PEE  | C2-O2-C10   | -2.02 | 112.96      | 117.80   |
| 50  | X     | 201 | 8Q1  | O40-C39-N41 | -2.01 | 119.09      | 123.03   |
| 54  | N     | 202 | CDL  | OA8-CA7-OA9 | -2.01 | 118.61      | 123.63   |

There are no chirality outliers.

All (784) 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' |
| 48  | C     | 311 | PEE  | O4P-C4-C5-N     |
| 48  | U     | 101 | PEE  | C1-O3P-P-O1P    |
| 48  | U     | 101 | PEE  | C4-O4P-P-O3P    |
| 48  | U     | 101 | PEE  | C4-O4P-P-O2P    |
| 48  | U     | 101 | PEE  | C4-O4P-P-O1P    |
| 48  | V     | 202 | PEE  | C11-C10-O2-C2   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 48  | V     | 202 | PEE  | C4-O4P-P-O3P   |
| 48  | V     | 202 | PEE  | C4-O4P-P-O2P   |
| 48  | V     | 202 | PEE  | C4-O4P-P-O1P   |
| 48  | V     | 207 | PEE  | C11-C10-O2-C2  |
| 48  | V     | 207 | PEE  | C1-O3P-P-O1P   |
| 48  | V     | 207 | PEE  | C1-O3P-P-O4P   |
| 48  | l     | 718 | PEE  | C4-O4P-P-O3P   |
| 48  | l     | 718 | PEE  | C4-O4P-P-O2P   |
| 48  | l     | 718 | PEE  | C4-O4P-P-O1P   |
| 48  | l     | 719 | PEE  | C11-C10-O2-C2  |
| 48  | l     | 719 | PEE  | O4-C10-O2-C2   |
| 48  | l     | 719 | PEE  | C4-O4P-P-O3P   |
| 48  | l     | 719 | PEE  | C4-O4P-P-O2P   |
| 48  | l     | 719 | PEE  | C4-O4P-P-O1P   |
| 48  | m     | 202 | PEE  | C4-O4P-P-O3P   |
| 48  | m     | 202 | PEE  | C4-O4P-P-O1P   |
| 49  | C     | 312 | PLX  | O7-C6-C7-C8    |
| 49  | C     | 312 | PLX  | O4-C3-C4-O6    |
| 49  | C     | 312 | PLX  | C3-O4-P1-O1    |
| 49  | C     | 312 | PLX  | C3-O4-P1-O2    |
| 49  | C     | 312 | PLX  | C3-O4-P1-O3    |
| 49  | C     | 312 | PLX  | C2-O1-P1-O2    |
| 49  | C     | 312 | PLX  | O9-C24-O8-C5   |
| 49  | V     | 205 | PLX  | O7-C6-O6-C4    |
| 49  | V     | 205 | PLX  | C3-C4-O6-C6    |
| 49  | V     | 205 | PLX  | C3-O4-P1-O1    |
| 49  | V     | 205 | PLX  | C3-O4-P1-O2    |
| 49  | V     | 205 | PLX  | C3-O4-P1-O3    |
| 49  | V     | 205 | PLX  | O9-C24-O8-C5   |
| 49  | e     | 201 | PLX  | O7-C6-O6-C4    |
| 49  | e     | 201 | PLX  | C3-O4-P1-O1    |
| 49  | e     | 201 | PLX  | C2-O1-P1-O4    |
| 49  | e     | 201 | PLX  | C2-O1-P1-O2    |
| 49  | e     | 201 | PLX  | C2-O1-P1-O3    |
| 49  | e     | 201 | PLX  | O9-C24-C25-C26 |
| 49  | i     | 705 | PLX  | O7-C6-O6-C4    |
| 49  | i     | 705 | PLX  | C3-O4-P1-O1    |
| 49  | i     | 705 | PLX  | C3-O4-P1-O2    |
| 49  | i     | 705 | PLX  | C25-C24-O8-C5  |
| 49  | j     | 203 | PLX  | O7-C6-C7-C8    |
| 49  | j     | 203 | PLX  | O7-C6-O6-C4    |
| 49  | n     | 101 | PLX  | O7-C6-O6-C4    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | n     | 101 | PLX  | C3-O4-P1-O1     |
| 49  | n     | 101 | PLX  | C3-O4-P1-O3     |
| 49  | n     | 101 | PLX  | O9-C24-O8-C5    |
| 50  | G     | 201 | 8Q1  | O4-C1-S44-C43   |
| 50  | G     | 201 | 8Q1  | C6-C1-S44-C43   |
| 50  | G     | 201 | 8Q1  | O27-C28-C29-C30 |
| 50  | G     | 201 | 8Q1  | O27-C28-C29-C31 |
| 50  | G     | 201 | 8Q1  | O27-C28-C29-C32 |
| 50  | G     | 201 | 8Q1  | N36-C37-C38-C39 |
| 50  | G     | 201 | 8Q1  | N41-C42-C43-S44 |
| 50  | G     | 201 | 8Q1  | C42-C43-S44-C1  |
| 50  | G     | 201 | 8Q1  | C28-O27-P24-O2  |
| 50  | G     | 201 | 8Q1  | C28-O27-P24-O1  |
| 50  | X     | 201 | 8Q1  | O4-C1-C6-C7     |
| 50  | X     | 201 | 8Q1  | S44-C1-C6-C7    |
| 50  | X     | 201 | 8Q1  | O4-C1-S44-C43   |
| 50  | X     | 201 | 8Q1  | C6-C1-S44-C43   |
| 50  | X     | 201 | 8Q1  | C28-C29-C32-C34 |
| 50  | X     | 201 | 8Q1  | C28-C29-C32-O33 |
| 50  | X     | 201 | 8Q1  | C30-C29-C32-C34 |
| 50  | X     | 201 | 8Q1  | C30-C29-C32-O33 |
| 50  | X     | 201 | 8Q1  | C31-C29-C32-C34 |
| 50  | X     | 201 | 8Q1  | C29-C32-C34-N36 |
| 50  | X     | 201 | 8Q1  | C29-C32-C34-O35 |
| 50  | X     | 201 | 8Q1  | O33-C32-C34-N36 |
| 50  | X     | 201 | 8Q1  | N36-C37-C38-C39 |
| 50  | X     | 201 | 8Q1  | C42-C43-S44-C1  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O3  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O2  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O1  |
| 51  | J     | 401 | NDP  | O4D-C4D-C5D-O5D |
| 51  | J     | 401 | NDP  | C2N-C3N-C7N-N7N |
| 54  | N     | 202 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | N     | 202 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | N     | 202 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | N     | 202 | CDL  | CA3-OA5-PA1-OA4 |
| 54  | N     | 202 | CDL  | C11-CA5-OA6-CA4 |
| 54  | N     | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | N     | 202 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | N     | 202 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | V     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | V     | 201 | CDL  | CA3-OA5-PA1-OA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | V     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | V     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | V     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | V     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | V     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | V     | 201 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | V     | 203 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | V     | 203 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | V     | 203 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | V     | 203 | CDL  | CA3-OA5-PA1-OA3 |
| 54  | V     | 203 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | V     | 203 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | V     | 203 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | V     | 203 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | V     | 203 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | a     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 54  | a     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | a     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | a     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | a     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 54  | a     | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | i     | 401 | CDL  | CB2-C1-CA2-OA2  |
| 54  | i     | 401 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | i     | 401 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | i     | 401 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | i     | 401 | CDL  | CA3-OA5-PA1-OA4 |
| 54  | i     | 401 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | i     | 401 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | i     | 401 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | l     | 712 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | l     | 712 | CDL  | CA3-OA5-PA1-OA3 |
| 54  | l     | 712 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | l     | 712 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | l     | 713 | CDL  | O1-C1-CA2-OA2   |
| 54  | l     | 713 | CDL  | CA2-OA2-PA1-OA3 |
| 54  | l     | 713 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | l     | 713 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | l     | 713 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | l     | 713 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | l     | 713 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | l     | 713 | CDL  | OB6-CB4-CB6-OB8 |
| 54  | n     | 102 | CDL  | CA2-OA2-PA1-OA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | n     | 102 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | n     | 102 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | n     | 102 | CDL  | CA3-OA5-PA1-OA3 |
| 54  | n     | 102 | CDL  | CA3-OA5-PA1-OA4 |
| 54  | n     | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | n     | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | n     | 102 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | r     | 714 | CDL  | CA2-OA2-PA1-OA3 |
| 54  | r     | 714 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | r     | 714 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | r     | 714 | CDL  | OA6-CA4-CA6-OA8 |
| 54  | r     | 714 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | r     | 714 | CDL  | C51-CB5-OB6-CB4 |
| 56  | s     | 403 | UQ   | C7-C8-C9-C10    |
| 56  | s     | 403 | UQ   | C7-C8-C9-C11    |
| 56  | s     | 403 | UQ   | C12-C13-C14-C16 |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O2A  |
| 56  | s     | 403 | UQ   | C17-C18-C19-C21 |
| 48  | V     | 202 | PEE  | O4-C10-O2-C2    |
| 48  | V     | 207 | PEE  | O4-C10-O2-C2    |
| 54  | N     | 202 | CDL  | OA7-CA5-OA6-CA4 |
| 54  | r     | 714 | CDL  | OB7-CB5-OB6-CB4 |
| 56  | s     | 403 | UQ   | C12-C11-C9-C10  |
| 56  | s     | 403 | UQ   | C13-C14-C16-C17 |
| 54  | l     | 712 | CDL  | C31-CA7-OA8-CA6 |
| 54  | r     | 714 | CDL  | C71-CB7-OB8-CB6 |
| 54  | l     | 712 | CDL  | OA9-CA7-OA8-CA6 |
| 54  | r     | 714 | CDL  | OB9-CB7-OB8-CB6 |
| 54  | N     | 202 | CDL  | O1-C1-CB2-OB2   |
| 54  | l     | 712 | CDL  | O1-C1-CA2-OA2   |
| 54  | n     | 102 | CDL  | O1-C1-CA2-OA2   |
| 48  | l     | 720 | PEE  | C31-C30-O3-C3   |
| 48  | m     | 202 | PEE  | C31-C30-O3-C3   |
| 54  | l     | 713 | CDL  | C71-CB7-OB8-CB6 |
| 54  | l     | 713 | CDL  | C59-C60-C61-C62 |
| 48  | C     | 311 | PEE  | C11-C10-O2-C2   |
| 48  | U     | 101 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 718 | PEE  | C11-C10-O2-C2   |
| 54  | N     | 202 | CDL  | C51-CB5-OB6-CB4 |
| 54  | V     | 203 | CDL  | C51-CB5-OB6-CB4 |
| 48  | l     | 720 | PEE  | O5-C30-O3-C3    |
| 48  | U     | 101 | PEE  | C19-C20-C21-C22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | l     | 713 | CDL  | OB9-CB7-OB8-CB6 |
| 48  | l     | 718 | PEE  | O4-C10-O2-C2    |
| 56  | s     | 403 | UQ   | C14-C16-C17-C18 |
| 48  | m     | 202 | PEE  | O5-C30-O3-C3    |
| 54  | V     | 203 | CDL  | C31-CA7-OA8-CA6 |
| 49  | V     | 205 | PLX  | C9-C10-C11-C12  |
| 54  | l     | 713 | CDL  | C11-C12-C13-C14 |
| 48  | U     | 101 | PEE  | C17-C18-C19-C20 |
| 48  | l     | 720 | PEE  | C37-C38-C39-C40 |
| 54  | V     | 201 | CDL  | C11-CA5-OA6-CA4 |
| 48  | U     | 101 | PEE  | C30-C31-C32-C33 |
| 49  | e     | 201 | PLX  | C30-C31-C32-C33 |
| 48  | C     | 311 | PEE  | O4-C10-O2-C2    |
| 48  | U     | 101 | PEE  | O4-C10-O2-C2    |
| 54  | V     | 201 | CDL  | CA2-C1-CB2-OB2  |
| 54  | i     | 401 | CDL  | CA2-C1-CB2-OB2  |
| 54  | r     | 714 | CDL  | CB2-C1-CA2-OA2  |
| 54  | i     | 401 | CDL  | C31-CA7-OA8-CA6 |
| 49  | C     | 312 | PLX  | C28-C29-C30-C31 |
| 49  | V     | 205 | PLX  | C30-C31-C32-C33 |
| 54  | l     | 713 | CDL  | C35-C36-C37-C38 |
| 54  | l     | 713 | CDL  | C54-C55-C56-C57 |
| 49  | j     | 203 | PLX  | C28-C29-C30-C31 |
| 49  | n     | 101 | PLX  | C11-C10-C9-C8   |
| 49  | i     | 705 | PLX  | C7-C8-C9-C10    |
| 54  | V     | 201 | CDL  | O1-C1-CB2-OB2   |
| 54  | i     | 401 | CDL  | O1-C1-CA2-OA2   |
| 54  | l     | 713 | CDL  | O1-C1-CB2-OB2   |
| 54  | i     | 401 | CDL  | OA9-CA7-OA8-CA6 |
| 54  | r     | 714 | CDL  | C36-C37-C38-C39 |
| 54  | V     | 203 | CDL  | OB5-CB3-CB4-OB6 |
| 54  | i     | 401 | CDL  | OB6-CB4-CB6-OB8 |
| 54  | l     | 712 | CDL  | C58-C59-C60-C61 |
| 51  | J     | 401 | NDP  | C2D-C1D-N1N-C6N |
| 48  | U     | 101 | PEE  | C32-C33-C34-C35 |
| 48  | V     | 207 | PEE  | C17-C18-C19-C20 |
| 48  | l     | 719 | PEE  | C37-C38-C39-C40 |
| 48  | V     | 207 | PEE  | C10-C11-C12-C13 |
| 48  | l     | 720 | PEE  | C10-C11-C12-C13 |
| 48  | l     | 719 | PEE  | C31-C30-O3-C3   |
| 54  | l     | 713 | CDL  | C39-C40-C41-C42 |
| 54  | r     | 714 | CDL  | CB5-C51-C52-C53 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | N     | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 54  | V     | 203 | CDL  | C51-C52-C53-C54 |
| 54  | a     | 201 | CDL  | C31-C32-C33-C34 |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1C    |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1A    |
| 54  | l     | 713 | CDL  | CB5-C51-C52-C53 |
| 54  | r     | 714 | CDL  | CB7-C71-C72-C73 |
| 48  | V     | 202 | PEE  | C30-C31-C32-C33 |
| 54  | l     | 713 | CDL  | CB7-C71-C72-C73 |
| 54  | r     | 714 | CDL  | CA5-C11-C12-C13 |
| 49  | e     | 201 | PLX  | C12-C13-C14-C15 |
| 48  | V     | 207 | PEE  | C11-C12-C13-C14 |
| 54  | V     | 201 | CDL  | C59-C60-C61-C62 |
| 54  | r     | 714 | CDL  | C13-C14-C15-C16 |
| 54  | i     | 401 | CDL  | O1-C1-CB2-OB2   |
| 54  | r     | 714 | CDL  | O1-C1-CA2-OA2   |
| 54  | V     | 201 | CDL  | OA7-CA5-OA6-CA4 |
| 54  | V     | 203 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | s     | 401 | PEE  | C37-C38-C39-C40 |
| 54  | V     | 203 | CDL  | OA9-CA7-OA8-CA6 |
| 46  | A     | 502 | FMN  | O2'-C2'-C3'-C4' |
| 48  | C     | 311 | PEE  | C14-C15-C16-C17 |
| 48  | l     | 719 | PEE  | O5-C30-O3-C3    |
| 54  | N     | 202 | CDL  | CB5-C51-C52-C53 |
| 54  | l     | 712 | CDL  | CB2-C1-CA2-OA2  |
| 54  | l     | 713 | CDL  | CB2-C1-CA2-OA2  |
| 54  | V     | 203 | CDL  | C32-C33-C34-C35 |
| 54  | V     | 203 | CDL  | C80-C81-C82-C83 |
| 51  | J     | 401 | NDP  | C3D-C4D-C5D-O5D |
| 49  | C     | 312 | PLX  | O6-C6-C7-C8     |
| 54  | l     | 712 | CDL  | C11-CA5-OA6-CA4 |
| 54  | n     | 102 | CDL  | C11-CA5-OA6-CA4 |
| 54  | N     | 202 | CDL  | CA6-CA4-OA6-CA5 |
| 54  | V     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 49  | j     | 203 | PLX  | C34-C35-C36-C37 |
| 54  | n     | 102 | CDL  | OA7-CA5-OA6-CA4 |
| 48  | V     | 202 | PEE  | C10-C11-C12-C13 |
| 54  | r     | 714 | CDL  | C74-C75-C76-C77 |
| 54  | r     | 714 | CDL  | CA7-C31-C32-C33 |
| 49  | C     | 312 | PLX  | C17-C18-C19-C20 |
| 54  | l     | 713 | CDL  | C57-C58-C59-C60 |
| 49  | C     | 312 | PLX  | C33-C34-C35-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | j     | 203 | PLX  | C12-C13-C14-C15 |
| 54  | r     | 714 | CDL  | C73-C74-C75-C76 |
| 49  | e     | 201 | PLX  | C33-C34-C35-C36 |
| 49  | C     | 312 | PLX  | O9-C24-C25-C26  |
| 49  | V     | 205 | PLX  | C7-C8-C9-C10    |
| 49  | j     | 203 | PLX  | C10-C11-C12-C13 |
| 54  | l     | 713 | CDL  | C72-C73-C74-C75 |
| 49  | i     | 705 | PLX  | C27-C28-C29-C30 |
| 54  | r     | 714 | CDL  | C71-C72-C73-C74 |
| 48  | l     | 720 | PEE  | C11-C10-O2-C2   |
| 48  | m     | 202 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 719 | PEE  | C31-C32-C33-C34 |
| 48  | C     | 311 | PEE  | C42-C43-C44-C45 |
| 54  | l     | 713 | CDL  | C53-C54-C55-C56 |
| 47  | A     | 503 | NAI  | C3D-C4D-C5D-O5D |
| 49  | V     | 205 | PLX  | C10-C11-C12-C13 |
| 48  | l     | 720 | PEE  | C2-C3-O3-C30    |
| 49  | j     | 203 | PLX  | C13-C14-C15-C16 |
| 49  | i     | 705 | PLX  | C33-C34-C35-C36 |
| 48  | s     | 401 | PEE  | C31-C30-O3-C3   |
| 54  | r     | 714 | CDL  | C55-C56-C57-C58 |
| 46  | A     | 502 | FMN  | O2'-C2'-C3'-O3' |
| 48  | V     | 202 | PEE  | C12-C13-C14-C15 |
| 49  | i     | 705 | PLX  | C28-C29-C30-C31 |
| 49  | j     | 203 | PLX  | C25-C26-C27-C28 |
| 48  | l     | 720 | PEE  | C13-C14-C15-C16 |
| 54  | l     | 712 | CDL  | C52-C53-C54-C55 |
| 54  | r     | 714 | CDL  | C41-C42-C43-C44 |
| 48  | l     | 720 | PEE  | C22-C23-C24-C25 |
| 50  | X     | 201 | 8Q1  | C12-C13-C14-C15 |
| 48  | l     | 720 | PEE  | C31-C32-C33-C34 |
| 54  | V     | 201 | CDL  | C52-C53-C54-C55 |
| 54  | l     | 713 | CDL  | C33-C34-C35-C36 |
| 54  | l     | 713 | CDL  | C58-C59-C60-C61 |
| 48  | s     | 401 | PEE  | C35-C36-C37-C38 |
| 48  | U     | 101 | PEE  | C31-C30-O3-C3   |
| 49  | C     | 312 | PLX  | C16-C17-C18-C19 |
| 54  | r     | 714 | CDL  | C75-C76-C77-C78 |
| 48  | U     | 101 | PEE  | C41-C42-C43-C44 |
| 48  | V     | 202 | PEE  | C20-C21-C22-C23 |
| 54  | l     | 713 | CDL  | C56-C57-C58-C59 |
| 48  | s     | 401 | PEE  | C33-C34-C35-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | e     | 201 | PLX  | C31-C32-C33-C34 |
| 48  | l     | 720 | PEE  | O4-C10-O2-C2    |
| 48  | m     | 202 | PEE  | O4-C10-O2-C2    |
| 54  | l     | 712 | CDL  | OA7-CA5-OA6-CA4 |
| 49  | V     | 205 | PLX  | C28-C29-C30-C31 |
| 49  | i     | 705 | PLX  | C11-C10-C9-C8   |
| 49  | e     | 201 | PLX  | C11-C10-C9-C8   |
| 48  | U     | 101 | PEE  | C22-C23-C24-C25 |
| 49  | C     | 312 | PLX  | C13-C14-C15-C16 |
| 54  | l     | 713 | CDL  | C14-C15-C16-C17 |
| 54  | l     | 713 | CDL  | C60-C61-C62-C63 |
| 49  | C     | 312 | PLX  | C7-C8-C9-C10    |
| 54  | r     | 714 | CDL  | C35-C36-C37-C38 |
| 54  | r     | 714 | CDL  | C62-C63-C64-C65 |
| 49  | e     | 201 | PLX  | C15-C16-C17-C18 |
| 54  | r     | 714 | CDL  | C17-C18-C19-C20 |
| 54  | r     | 714 | CDL  | C43-C44-C45-C46 |
| 48  | s     | 401 | PEE  | C21-C22-C23-C24 |
| 49  | C     | 312 | PLX  | C11-C12-C13-C14 |
| 49  | j     | 203 | PLX  | C27-C28-C29-C30 |
| 54  | V     | 201 | CDL  | O1-C1-CA2-OA2   |
| 49  | V     | 205 | PLX  | C15-C16-C17-C18 |
| 54  | V     | 203 | CDL  | C11-CA5-OA6-CA4 |
| 54  | n     | 102 | CDL  | C75-C76-C77-C78 |
| 49  | e     | 201 | PLX  | C32-C33-C34-C35 |
| 54  | l     | 713 | CDL  | CA7-C31-C32-C33 |
| 54  | l     | 712 | CDL  | C51-C52-C53-C54 |
| 48  | C     | 311 | PEE  | C37-C38-C39-C40 |
| 49  | V     | 205 | PLX  | C16-C17-C18-C19 |
| 49  | V     | 205 | PLX  | C31-C32-C33-C34 |
| 54  | l     | 713 | CDL  | C52-C53-C54-C55 |
| 49  | e     | 201 | PLX  | C2-C1-N1-C1B    |
| 48  | m     | 202 | PEE  | C12-C13-C14-C15 |
| 48  | s     | 401 | PEE  | O5-C30-O3-C3    |
| 48  | l     | 718 | PEE  | C34-C35-C36-C37 |
| 54  | l     | 713 | CDL  | C31-C32-C33-C34 |
| 48  | l     | 720 | PEE  | C14-C15-C16-C17 |
| 49  | V     | 205 | PLX  | C12-C13-C14-C15 |
| 49  | i     | 705 | PLX  | C10-C11-C12-C13 |
| 48  | U     | 101 | PEE  | O5-C30-O3-C3    |
| 54  | a     | 201 | CDL  | CA7-C31-C32-C33 |
| 54  | l     | 713 | CDL  | OA6-CA4-CA6-OA8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | e     | 201 | PLX  | C14-C15-C16-C17 |
| 48  | V     | 207 | PEE  | C31-C30-O3-C3   |
| 49  | e     | 201 | PLX  | C28-C29-C30-C31 |
| 54  | l     | 713 | CDL  | C55-C56-C57-C58 |
| 54  | l     | 713 | CDL  | C74-C75-C76-C77 |
| 48  | U     | 101 | PEE  | C36-C37-C38-C39 |
| 54  | i     | 401 | CDL  | C11-C12-C13-C14 |
| 54  | a     | 201 | CDL  | CB5-C51-C52-C53 |
| 49  | V     | 205 | PLX  | C27-C28-C29-C30 |
| 50  | G     | 201 | 8Q1  | C10-C11-C12-C13 |
| 54  | l     | 713 | CDL  | C40-C41-C42-C43 |
| 49  | i     | 705 | PLX  | C25-C26-C27-C28 |
| 54  | l     | 713 | CDL  | C37-C38-C39-C40 |
| 48  | V     | 207 | PEE  | C32-C33-C34-C35 |
| 48  | l     | 719 | PEE  | C21-C22-C23-C24 |
| 49  | j     | 203 | PLX  | C7-C8-C9-C10    |
| 48  | C     | 311 | PEE  | C39-C40-C41-C42 |
| 48  | m     | 202 | PEE  | C19-C20-C21-C22 |
| 48  | l     | 718 | PEE  | C31-C32-C33-C34 |
| 48  | l     | 720 | PEE  | C32-C33-C34-C35 |
| 49  | C     | 312 | PLX  | O4-C3-C4-C5     |
| 49  | i     | 705 | PLX  | C9-C10-C11-C12  |
| 48  | V     | 202 | PEE  | C31-C30-O3-C3   |
| 54  | r     | 714 | CDL  | C31-CA7-OA8-CA6 |
| 48  | V     | 202 | PEE  | C17-C18-C19-C20 |
| 48  | C     | 311 | PEE  | C1-C2-C3-O3     |
| 48  | l     | 720 | PEE  | C1-C2-C3-O3     |
| 49  | V     | 205 | PLX  | C3-C4-C5-O8     |
| 49  | e     | 201 | PLX  | C3-C4-C5-O8     |
| 49  | j     | 203 | PLX  | C3-C4-C5-O8     |
| 54  | l     | 713 | CDL  | CA3-CA4-CA6-OA8 |
| 54  | l     | 713 | CDL  | CB3-CB4-CB6-OB8 |
| 54  | n     | 102 | CDL  | CA3-CA4-CA6-OA8 |
| 54  | r     | 714 | CDL  | CB3-CB4-CB6-OB8 |
| 48  | C     | 311 | PEE  | C15-C16-C17-C18 |
| 48  | l     | 719 | PEE  | C15-C16-C17-C18 |
| 48  | s     | 401 | PEE  | C15-C16-C17-C18 |
| 48  | s     | 401 | PEE  | C39-C40-C41-C42 |
| 49  | C     | 312 | PLX  | C30-C31-C32-C33 |
| 49  | j     | 203 | PLX  | C14-C15-C16-C17 |
| 48  | l     | 718 | PEE  | C22-C23-C24-C25 |
| 48  | V     | 202 | PEE  | C21-C22-C23-C24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | C     | 312 | PLX  | C31-C32-C33-C34 |
| 48  | V     | 207 | PEE  | O5-C30-O3-C3    |
| 50  | G     | 201 | 8Q1  | C11-C12-C13-C14 |
| 50  | X     | 201 | 8Q1  | C7-C8-C9-C10    |
| 54  | V     | 201 | CDL  | C62-C63-C64-C65 |
| 50  | G     | 201 | 8Q1  | C28-O27-P24-O3  |
| 54  | l     | 713 | CDL  | C62-C63-C64-C65 |
| 49  | V     | 205 | PLX  | C18-C19-C20-C21 |
| 49  | V     | 205 | PLX  | C34-C35-C36-C37 |
| 54  | r     | 714 | CDL  | C11-C12-C13-C14 |
| 48  | l     | 720 | PEE  | C33-C34-C35-C36 |
| 54  | r     | 714 | CDL  | C63-C64-C65-C66 |
| 48  | V     | 207 | PEE  | C35-C36-C37-C38 |
| 48  | m     | 202 | PEE  | C22-C23-C24-C25 |
| 49  | e     | 201 | PLX  | C7-C8-C9-C10    |
| 49  | e     | 201 | PLX  | C25-C26-C27-C28 |
| 49  | j     | 203 | PLX  | C30-C31-C32-C33 |
| 56  | s     | 403 | UQ   | C12-C11-C9-C8   |
| 48  | V     | 207 | PEE  | C33-C34-C35-C36 |
| 49  | V     | 205 | PLX  | C13-C14-C15-C16 |
| 54  | l     | 712 | CDL  | C35-C36-C37-C38 |
| 49  | C     | 312 | PLX  | C25-C26-C27-C28 |
| 48  | m     | 202 | PEE  | O2-C2-C3-O3     |
| 54  | V     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 54  | i     | 401 | CDL  | OA6-CA4-CA6-OA8 |
| 54  | r     | 714 | CDL  | OB6-CB4-CB6-OB8 |
| 49  | V     | 205 | PLX  | C33-C34-C35-C36 |
| 50  | X     | 201 | 8Q1  | C31-C29-C32-O33 |
| 50  | X     | 201 | 8Q1  | C13-C14-C15-C16 |
| 48  | s     | 401 | PEE  | C14-C15-C16-C17 |
| 54  | l     | 713 | CDL  | C64-C65-C66-C67 |
| 48  | l     | 718 | PEE  | C24-C25-C26-C27 |
| 48  | V     | 202 | PEE  | O5-C30-O3-C3    |
| 54  | l     | 712 | CDL  | CB5-C51-C52-C53 |
| 54  | a     | 201 | CDL  | C37-C38-C39-C40 |
| 48  | m     | 202 | PEE  | C17-C18-C19-C20 |
| 48  | s     | 401 | PEE  | C17-C18-C19-C20 |
| 49  | e     | 201 | PLX  | C10-C11-C12-C13 |
| 49  | n     | 101 | PLX  | C34-C35-C36-C37 |
| 54  | i     | 401 | CDL  | C37-C38-C39-C40 |
| 54  | n     | 102 | CDL  | C53-C54-C55-C56 |
| 48  | s     | 401 | PEE  | C20-C21-C22-C23 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | r     | 714 | CDL  | C33-C34-C35-C36 |
| 54  | r     | 714 | CDL  | C60-C61-C62-C63 |
| 54  | r     | 714 | CDL  | OA9-CA7-OA8-CA6 |
| 54  | r     | 714 | CDL  | C59-C60-C61-C62 |
| 54  | V     | 203 | CDL  | C79-C80-C81-C82 |
| 54  | l     | 712 | CDL  | C79-C80-C81-C82 |
| 48  | l     | 718 | PEE  | O3P-C1-C2-C3    |
| 54  | i     | 401 | CDL  | OB5-CB3-CB4-CB6 |
| 48  | s     | 401 | PEE  | C11-C10-O2-C2   |
| 49  | n     | 101 | PLX  | C7-C8-C9-C10    |
| 50  | G     | 201 | 8Q1  | C29-C32-C34-N36 |
| 54  | l     | 713 | CDL  | C81-C82-C83-C84 |
| 54  | r     | 714 | CDL  | C64-C65-C66-C67 |
| 54  | l     | 712 | CDL  | C37-C38-C39-C40 |
| 49  | e     | 201 | PLX  | C13-C14-C15-C16 |
| 54  | r     | 714 | CDL  | C51-C52-C53-C54 |
| 54  | V     | 203 | CDL  | OA7-CA5-OA6-CA4 |
| 48  | l     | 719 | PEE  | C13-C14-C15-C16 |
| 54  | V     | 201 | CDL  | C37-C38-C39-C40 |
| 48  | l     | 720 | PEE  | C23-C24-C25-C26 |
| 54  | r     | 714 | CDL  | C37-C38-C39-C40 |
| 48  | l     | 718 | PEE  | C1-C2-C3-O3     |
| 48  | C     | 311 | PEE  | C43-C44-C45-C46 |
| 48  | V     | 202 | PEE  | C44-C45-C46-C47 |
| 49  | i     | 705 | PLX  | C32-C33-C34-C35 |
| 48  | l     | 719 | PEE  | C30-C31-C32-C33 |
| 49  | n     | 101 | PLX  | C14-C15-C16-C17 |
| 49  | i     | 705 | PLX  | C13-C14-C15-C16 |
| 48  | m     | 202 | PEE  | C33-C34-C35-C36 |
| 49  | j     | 203 | PLX  | C33-C34-C35-C36 |
| 54  | r     | 714 | CDL  | C57-C58-C59-C60 |
| 49  | n     | 101 | PLX  | C10-C11-C12-C13 |
| 54  | r     | 714 | CDL  | C76-C77-C78-C79 |
| 48  | s     | 401 | PEE  | C34-C35-C36-C37 |
| 48  | V     | 207 | PEE  | O3P-C1-C2-O2    |
| 54  | V     | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 54  | a     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 54  | i     | 401 | CDL  | OB5-CB3-CB4-OB6 |
| 54  | l     | 712 | CDL  | OA5-CA3-CA4-OA6 |
| 54  | l     | 713 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | l     | 719 | PEE  | C33-C34-C35-C36 |
| 54  | l     | 712 | CDL  | CB7-C71-C72-C73 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | C     | 312 | PLX  | C36-C37-C38-C39 |
| 54  | l     | 713 | CDL  | C44-C45-C46-C47 |
| 49  | C     | 312 | PLX  | O6-C4-C5-O8     |
| 48  | l     | 720 | PEE  | C34-C35-C36-C37 |
| 49  | e     | 201 | PLX  | C11-C12-C13-C14 |
| 54  | l     | 713 | CDL  | C18-C19-C20-C21 |
| 54  | l     | 712 | CDL  | C14-C15-C16-C17 |
| 49  | C     | 312 | PLX  | O8-C24-C25-C26  |
| 48  | V     | 202 | PEE  | C24-C25-C26-C27 |
| 47  | A     | 503 | NAI  | PN-O3-PA-O5B    |
| 50  | X     | 201 | 8Q1  | C1-C6-C7-C8     |
| 48  | m     | 202 | PEE  | C20-C21-C22-C23 |
| 48  | V     | 202 | PEE  | C13-C14-C15-C16 |
| 54  | r     | 714 | CDL  | C31-C32-C33-C34 |
| 48  | U     | 101 | PEE  | C38-C39-C40-C41 |
| 48  | V     | 202 | PEE  | C36-C37-C38-C39 |
| 48  | l     | 720 | PEE  | C16-C17-C18-C19 |
| 54  | N     | 202 | CDL  | CA2-C1-CB2-OB2  |
| 54  | l     | 713 | CDL  | CA2-C1-CB2-OB2  |
| 54  | n     | 102 | CDL  | CB2-C1-CA2-OA2  |
| 48  | l     | 718 | PEE  | C11-C12-C13-C14 |
| 49  | j     | 203 | PLX  | O4-C3-C4-C5     |
| 54  | V     | 203 | CDL  | OB5-CB3-CB4-CB6 |
| 54  | i     | 401 | CDL  | OA5-CA3-CA4-CA6 |
| 48  | m     | 202 | PEE  | C13-C14-C15-C16 |
| 48  | l     | 718 | PEE  | C18-C19-C20-C21 |
| 49  | n     | 101 | PLX  | C25-C26-C27-C28 |
| 50  | G     | 201 | 8Q1  | C6-C7-C8-C9     |
| 49  | C     | 312 | PLX  | C14-C15-C16-C17 |
| 54  | r     | 714 | CDL  | C80-C81-C82-C83 |
| 49  | j     | 203 | PLX  | C24-C25-C26-C27 |
| 54  | r     | 714 | CDL  | C78-C79-C80-C81 |
| 48  | s     | 401 | PEE  | O4-C10-O2-C2    |
| 49  | e     | 201 | PLX  | C16-C17-C18-C19 |
| 54  | V     | 203 | CDL  | CA6-CA4-OA6-CA5 |
| 48  | U     | 101 | PEE  | C44-C45-C46-C47 |
| 48  | l     | 718 | PEE  | O3P-C1-C2-O2    |
| 54  | i     | 401 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | s     | 401 | PEE  | C31-C32-C33-C34 |
| 54  | V     | 203 | CDL  | C75-C76-C77-C78 |
| 54  | l     | 712 | CDL  | C20-C21-C22-C23 |
| 54  | i     | 401 | CDL  | CB3-CB4-CB6-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | r     | 714 | CDL  | CA3-CA4-CA6-OA8 |
| 56  | s     | 403 | UQ   | C9-C11-C12-C13  |
| 54  | V     | 201 | CDL  | C78-C79-C80-C81 |
| 48  | V     | 207 | PEE  | C31-C32-C33-C34 |
| 54  | r     | 714 | CDL  | C12-C13-C14-C15 |
| 54  | i     | 401 | CDL  | C36-C37-C38-C39 |
| 54  | l     | 712 | CDL  | C76-C77-C78-C79 |
| 48  | l     | 720 | PEE  | C5-C4-O4P-P     |
| 48  | C     | 311 | PEE  | C13-C14-C15-C16 |
| 48  | C     | 311 | PEE  | C12-C13-C14-C15 |
| 54  | a     | 201 | CDL  | C54-C55-C56-C57 |
| 48  | C     | 311 | PEE  | O2-C2-C3-O3     |
| 48  | l     | 720 | PEE  | O2-C2-C3-O3     |
| 49  | e     | 201 | PLX  | O6-C4-C5-O8     |
| 54  | n     | 102 | CDL  | OA6-CA4-CA6-OA8 |
| 48  | l     | 718 | PEE  | C32-C33-C34-C35 |
| 49  | C     | 312 | PLX  | C9-C10-C11-C12  |
| 49  | e     | 201 | PLX  | C26-C27-C28-C29 |
| 48  | U     | 101 | PEE  | C42-C43-C44-C45 |
| 48  | C     | 311 | PEE  | C10-C11-C12-C13 |
| 54  | V     | 203 | CDL  | C72-C73-C74-C75 |
| 54  | l     | 713 | CDL  | C12-C13-C14-C15 |
| 54  | l     | 712 | CDL  | CA4-CA3-OA5-PA1 |
| 49  | C     | 312 | PLX  | N1-C1-C2-O1     |
| 49  | n     | 101 | PLX  | N1-C1-C2-O1     |
| 54  | V     | 203 | CDL  | C78-C79-C80-C81 |
| 48  | l     | 718 | PEE  | C21-C22-C23-C24 |
| 48  | C     | 311 | PEE  | C33-C34-C35-C36 |
| 49  | e     | 201 | PLX  | O7-C6-C7-C8     |
| 48  | V     | 202 | PEE  | C41-C42-C43-C44 |
| 49  | e     | 201 | PLX  | C25-C24-O8-C5   |
| 49  | j     | 203 | PLX  | C25-C24-O8-C5   |
| 54  | l     | 713 | CDL  | C15-C16-C17-C18 |
| 54  | l     | 713 | CDL  | C43-C44-C45-C46 |
| 54  | V     | 201 | CDL  | C58-C59-C60-C61 |
| 54  | N     | 202 | CDL  | OA5-CA3-CA4-CA6 |
| 54  | r     | 714 | CDL  | OB5-CB3-CB4-CB6 |
| 50  | X     | 201 | 8Q1  | C10-C11-C12-C13 |
| 48  | s     | 401 | PEE  | C23-C24-C25-C26 |
| 48  | V     | 207 | PEE  | C38-C39-C40-C41 |
| 48  | s     | 401 | PEE  | C22-C23-C24-C25 |
| 49  | e     | 201 | PLX  | O8-C24-C25-C26  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | j     | 203 | PLX  | O4-C3-C4-O6     |
| 54  | r     | 714 | CDL  | OB5-CB3-CB4-OB6 |
| 54  | l     | 712 | CDL  | C51-CB5-OB6-CB4 |
| 51  | J     | 401 | NDP  | C2N-C3N-C7N-O7N |
| 48  | C     | 311 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 720 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 719 | PEE  | C22-C23-C24-C25 |
| 48  | l     | 718 | PEE  | O2-C2-C3-O3     |
| 49  | V     | 205 | PLX  | O6-C4-C5-O8     |
| 49  | j     | 203 | PLX  | O6-C4-C5-O8     |
| 48  | m     | 202 | PEE  | C1-C2-C3-O3     |
| 49  | C     | 312 | PLX  | C3-C4-C5-O8     |
| 54  | V     | 201 | CDL  | CA3-CA4-CA6-OA8 |
| 54  | V     | 201 | CDL  | CB3-CB4-CB6-OB8 |
| 47  | A     | 503 | NAI  | O4D-C4D-C5D-O5D |
| 48  | C     | 311 | PEE  | C4-O4P-P-O2P    |
| 48  | U     | 101 | PEE  | C1-O3P-P-O2P    |
| 48  | U     | 101 | PEE  | C1-O3P-P-O4P    |
| 48  | V     | 207 | PEE  | C4-O4P-P-O1P    |
| 49  | C     | 312 | PLX  | C2-O1-P1-O4     |
| 49  | C     | 312 | PLX  | C2-O1-P1-O3     |
| 49  | V     | 205 | PLX  | C5-C4-O6-C6     |
| 49  | V     | 205 | PLX  | C2-O1-P1-O4     |
| 49  | V     | 205 | PLX  | C2-O1-P1-O2     |
| 49  | V     | 205 | PLX  | C2-O1-P1-O3     |
| 49  | e     | 201 | PLX  | C3-C4-O6-C6     |
| 49  | e     | 201 | PLX  | C5-C4-O6-C6     |
| 49  | e     | 201 | PLX  | C3-O4-P1-O2     |
| 49  | n     | 101 | PLX  | C2-O1-P1-O2     |
| 51  | J     | 401 | NDP  | C5D-O5D-PN-O3   |
| 51  | J     | 401 | NDP  | C5D-O5D-PN-O1N  |
| 51  | J     | 401 | NDP  | C5D-O5D-PN-O2N  |
| 54  | N     | 202 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | V     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 54  | V     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 54  | V     | 203 | CDL  | CA3-OA5-PA1-OA4 |
| 54  | V     | 203 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | a     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | a     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | a     | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | i     | 401 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | l     | 712 | CDL  | CA2-OA2-PA1-OA3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | l     | 712 | CDL  | CA3-OA5-PA1-OA2 |
| 54  | l     | 713 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | l     | 713 | CDL  | CB3-OB5-PB2-OB2 |
| 54  | l     | 713 | CDL  | CB3-OB5-PB2-OB3 |
| 54  | l     | 713 | CDL  | CB3-OB5-PB2-OB4 |
| 54  | r     | 714 | CDL  | CB2-OB2-PB2-OB3 |
| 54  | r     | 714 | CDL  | CB2-OB2-PB2-OB4 |
| 54  | r     | 714 | CDL  | CB2-OB2-PB2-OB5 |
| 54  | r     | 714 | CDL  | CB3-OB5-PB2-OB3 |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O1A  |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O3A  |
| 49  | j     | 203 | PLX  | C9-C10-C11-C12  |
| 48  | V     | 207 | PEE  | C2-C1-O3P-P     |
| 54  | r     | 714 | CDL  | CB4-CB3-OB5-PB2 |
| 49  | C     | 312 | PLX  | C35-C36-C37-C38 |
| 54  | a     | 201 | CDL  | C71-C72-C73-C74 |
| 49  | n     | 101 | PLX  | C15-C16-C17-C18 |
| 48  | C     | 311 | PEE  | C16-C17-C18-C19 |
| 48  | l     | 718 | PEE  | C38-C39-C40-C41 |
| 54  | l     | 712 | CDL  | C24-C25-C26-C27 |
| 49  | i     | 705 | PLX  | C16-C17-C18-C19 |
| 54  | l     | 712 | CDL  | CA6-CA4-OA6-CA5 |
| 54  | n     | 102 | CDL  | CA6-CA4-OA6-CA5 |
| 49  | V     | 205 | PLX  | C14-C15-C16-C17 |
| 54  | r     | 714 | CDL  | C44-C45-C46-C47 |
| 48  | s     | 401 | PEE  | O3P-C1-C2-C3    |
| 54  | a     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 54  | l     | 712 | CDL  | OA5-CA3-CA4-CA6 |
| 54  | l     | 713 | CDL  | OA5-CA3-CA4-CA6 |
| 50  | G     | 201 | 8Q1  | C7-C8-C9-C10    |
| 48  | s     | 401 | PEE  | O3P-C1-C2-O2    |
| 54  | V     | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | m     | 202 | PEE  | O3-C30-C31-C32  |
| 54  | V     | 201 | CDL  | CA5-C11-C12-C13 |
| 49  | e     | 201 | PLX  | C36-C37-C38-C39 |
| 49  | i     | 705 | PLX  | C36-C37-C38-C39 |
| 54  | l     | 712 | CDL  | C36-C37-C38-C39 |
| 54  | l     | 712 | CDL  | OB7-CB5-OB6-CB4 |
| 54  | l     | 713 | CDL  | C73-C74-C75-C76 |
| 48  | C     | 311 | PEE  | C19-C20-C21-C22 |
| 54  | i     | 401 | CDL  | CA3-CA4-CA6-OA8 |
| 51  | J     | 401 | NDP  | PN-O3-PA-O2A    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | V     | 201 | CDL  | C51-CB5-OB6-CB4 |
| 54  | l     | 712 | CDL  | C56-C57-C58-C59 |
| 50  | G     | 201 | 8Q1  | C29-C32-C34-O35 |
| 54  | a     | 201 | CDL  | C75-C76-C77-C78 |
| 49  | V     | 205 | PLX  | O9-C24-C25-C26  |
| 49  | i     | 705 | PLX  | O8-C24-C25-C26  |
| 49  | V     | 205 | PLX  | C20-C21-C22-C23 |
| 54  | r     | 714 | CDL  | C20-C21-C22-C23 |
| 54  | r     | 714 | CDL  | C56-C57-C58-C59 |
| 54  | n     | 102 | CDL  | CB7-C71-C72-C73 |
| 51  | J     | 401 | NDP  | O4D-C1D-N1N-C6N |
| 54  | a     | 201 | CDL  | C18-C19-C20-C21 |
| 48  | l     | 718 | PEE  | C10-C11-C12-C13 |
| 54  | l     | 713 | CDL  | C41-C42-C43-C44 |
| 54  | l     | 713 | CDL  | C21-C22-C23-C24 |
| 54  | i     | 401 | CDL  | C71-C72-C73-C74 |
| 49  | e     | 201 | PLX  | C18-C19-C20-C21 |
| 54  | N     | 202 | CDL  | O1-C1-CA2-OA2   |
| 54  | a     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 49  | j     | 203 | PLX  | C15-C16-C17-C18 |
| 54  | l     | 712 | CDL  | C83-C84-C85-C86 |
| 48  | U     | 101 | PEE  | C23-C24-C25-C26 |
| 54  | V     | 203 | CDL  | OA6-CA4-CA6-OA8 |
| 54  | a     | 201 | CDL  | C39-C40-C41-C42 |
| 49  | e     | 201 | PLX  | C24-C25-C26-C27 |
| 54  | V     | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 54  | l     | 712 | CDL  | C82-C83-C84-C85 |
| 48  | l     | 720 | PEE  | C38-C39-C40-C41 |
| 48  | l     | 719 | PEE  | C2-C1-O3P-P     |
| 54  | i     | 401 | CDL  | C33-C34-C35-C36 |
| 54  | a     | 201 | CDL  | CA5-C11-C12-C13 |
| 49  | i     | 705 | PLX  | C12-C13-C14-C15 |
| 48  | C     | 311 | PEE  | C38-C39-C40-C41 |
| 48  | l     | 719 | PEE  | C38-C39-C40-C41 |
| 48  | l     | 719 | PEE  | C3-C2-O2-C10    |
| 54  | a     | 201 | CDL  | CA6-CA4-OA6-CA5 |
| 54  | i     | 401 | CDL  | CA6-CA4-OA6-CA5 |
| 54  | V     | 203 | CDL  | C33-C34-C35-C36 |
| 54  | V     | 203 | CDL  | C32-C31-CA7-OA8 |
| 49  | j     | 203 | PLX  | C35-C36-C37-C38 |
| 49  | i     | 705 | PLX  | C30-C31-C32-C33 |
| 48  | V     | 202 | PEE  | O3P-C1-C2-O2    |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | V     | 201 | CDL  | C1-CB2-OB2-PB2  |
| 50  | G     | 201 | 8Q1  | C12-C13-C14-C15 |
| 54  | V     | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 48  | l     | 720 | PEE  | C36-C37-C38-C39 |
| 49  | C     | 312 | PLX  | C27-C28-C29-C30 |
| 47  | A     | 503 | NAI  | O4D-C1D-N1N-C2N |
| 49  | n     | 101 | PLX  | C35-C36-C37-C38 |
| 48  | l     | 718 | PEE  | C35-C36-C37-C38 |
| 49  | e     | 201 | PLX  | C27-C28-C29-C30 |
| 49  | j     | 203 | PLX  | O6-C6-C7-C8     |
| 49  | V     | 205 | PLX  | C26-C27-C28-C29 |
| 54  | r     | 714 | CDL  | C23-C24-C25-C26 |
| 48  | l     | 718 | PEE  | C2-C1-O3P-P     |
| 54  | V     | 201 | CDL  | C44-C45-C46-C47 |
| 48  | l     | 719 | PEE  | C16-C17-C18-C19 |
| 49  | n     | 101 | PLX  | O9-C24-C25-C26  |
| 47  | A     | 503 | NAI  | C2D-C1D-N1N-C2N |
| 54  | n     | 102 | CDL  | OA5-CA3-CA4-OA6 |
| 54  | i     | 401 | CDL  | C14-C15-C16-C17 |
| 54  | i     | 401 | CDL  | C31-C32-C33-C34 |
| 54  | l     | 712 | CDL  | C54-C55-C56-C57 |
| 48  | m     | 202 | PEE  | C18-C19-C20-C21 |
| 49  | C     | 312 | PLX  | C26-C27-C28-C29 |
| 54  | a     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 54  | l     | 713 | CDL  | C42-C43-C44-C45 |
| 48  | V     | 207 | PEE  | O3P-C1-C2-C3    |
| 54  | V     | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 49  | V     | 205 | PLX  | C4-C3-O4-P1     |
| 54  | l     | 712 | CDL  | C39-C40-C41-C42 |
| 54  | n     | 102 | CDL  | C58-C59-C60-C61 |
| 48  | C     | 311 | PEE  | C32-C33-C34-C35 |
| 54  | l     | 712 | CDL  | C55-C56-C57-C58 |
| 54  | l     | 713 | CDL  | C17-C18-C19-C20 |
| 54  | l     | 712 | CDL  | C81-C82-C83-C84 |
| 54  | n     | 102 | CDL  | C77-C78-C79-C80 |
| 48  | m     | 202 | PEE  | C16-C17-C18-C19 |
| 54  | l     | 713 | CDL  | C34-C35-C36-C37 |
| 48  | V     | 207 | PEE  | C37-C38-C39-C40 |
| 48  | C     | 311 | PEE  | C36-C37-C38-C39 |
| 54  | n     | 102 | CDL  | C19-C20-C21-C22 |
| 48  | l     | 719 | PEE  | O3P-C1-C2-O2    |
| 51  | J     | 401 | NDP  | O4B-C4B-C5B-O5B |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | C     | 312 | PLX  | C15-C16-C17-C18 |
| 54  | n     | 102 | CDL  | C71-C72-C73-C74 |
| 48  | U     | 101 | PEE  | C34-C35-C36-C37 |
| 48  | V     | 207 | PEE  | C16-C17-C18-C19 |
| 48  | l     | 718 | PEE  | C36-C37-C38-C39 |
| 48  | s     | 401 | PEE  | C36-C37-C38-C39 |
| 54  | N     | 202 | CDL  | C52-C51-CB5-OB6 |
| 48  | V     | 202 | PEE  | O3P-C1-C2-C3    |
| 54  | r     | 714 | CDL  | OA5-CA3-CA4-CA6 |
| 54  | l     | 713 | CDL  | C12-C11-CA5-OA6 |
| 54  | n     | 102 | CDL  | C55-C56-C57-C58 |
| 54  | r     | 714 | CDL  | C42-C43-C44-C45 |
| 48  | l     | 720 | PEE  | O2-C10-C11-C12  |
| 54  | n     | 102 | CDL  | C14-C15-C16-C17 |
| 51  | J     | 401 | NDP  | PN-O3-PA-O1A    |
| 50  | G     | 201 | 8Q1  | C9-C10-C11-C12  |
| 49  | j     | 203 | PLX  | C18-C19-C20-C21 |
| 54  | a     | 201 | CDL  | C17-C18-C19-C20 |
| 48  | V     | 202 | PEE  | C39-C40-C41-C42 |
| 54  | l     | 713 | CDL  | OA9-CA7-OA8-CA6 |
| 54  | N     | 202 | CDL  | OA5-CA3-CA4-OA6 |
| 48  | s     | 401 | PEE  | C13-C14-C15-C16 |
| 54  | l     | 713 | CDL  | C32-C31-CA7-OA8 |
| 48  | V     | 207 | PEE  | C13-C14-C15-C16 |
| 54  | l     | 713 | CDL  | C51-C52-C53-C54 |
| 54  | V     | 201 | CDL  | CB4-CB3-OB5-PB2 |
| 54  | n     | 102 | CDL  | C54-C55-C56-C57 |
| 49  | C     | 312 | PLX  | C25-C24-O8-C5   |
| 54  | N     | 202 | CDL  | OB6-CB4-CB6-OB8 |
| 54  | V     | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | s     | 401 | PEE  | C42-C43-C44-C45 |
| 54  | V     | 201 | CDL  | C41-C42-C43-C44 |
| 54  | l     | 713 | CDL  | C31-CA7-OA8-CA6 |
| 48  | l     | 720 | PEE  | O3-C30-C31-C32  |
| 54  | r     | 714 | CDL  | C79-C80-C81-C82 |
| 54  | a     | 201 | CDL  | C22-C23-C24-C25 |
| 48  | U     | 101 | PEE  | O2-C10-C11-C12  |
| 54  | r     | 714 | CDL  | C32-C33-C34-C35 |
| 48  | C     | 311 | PEE  | C40-C41-C42-C43 |
| 54  | r     | 714 | CDL  | C72-C73-C74-C75 |
| 49  | i     | 705 | PLX  | O6-C6-C7-C8     |
| 54  | V     | 201 | CDL  | C72-C73-C74-C75 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 54  | V     | 201 | CDL  | C35-C36-C37-C38 |
| 54  | l     | 713 | CDL  | C12-C11-CA5-OA7 |
| 49  | e     | 201 | PLX  | O9-C24-O8-C5    |
| 49  | i     | 705 | PLX  | O9-C24-O8-C5    |
| 48  | l     | 720 | PEE  | O4-C10-C11-C12  |
| 54  | V     | 201 | CDL  | C39-C40-C41-C42 |
| 49  | V     | 205 | PLX  | C6-C7-C8-C9     |
| 54  | N     | 202 | CDL  | C52-C51-CB5-OB7 |
| 54  | l     | 713 | CDL  | C32-C31-CA7-OA9 |
| 54  | n     | 102 | CDL  | C12-C11-CA5-OA6 |
| 48  | U     | 101 | PEE  | O4-C10-C11-C12  |
| 54  | r     | 714 | CDL  | C1-CA2-OA2-PA1  |
| 48  | C     | 311 | PEE  | O3-C30-C31-C32  |
| 49  | i     | 705 | PLX  | C6-C7-C8-C9     |
| 49  | i     | 705 | PLX  | O4-C3-C4-C5     |
| 54  | l     | 712 | CDL  | C23-C24-C25-C26 |
| 54  | n     | 102 | CDL  | C22-C23-C24-C25 |
| 48  | l     | 720 | PEE  | O5-C30-C31-C32  |

There are no ring outliers.

32 monomers are involved in 286 short contacts:

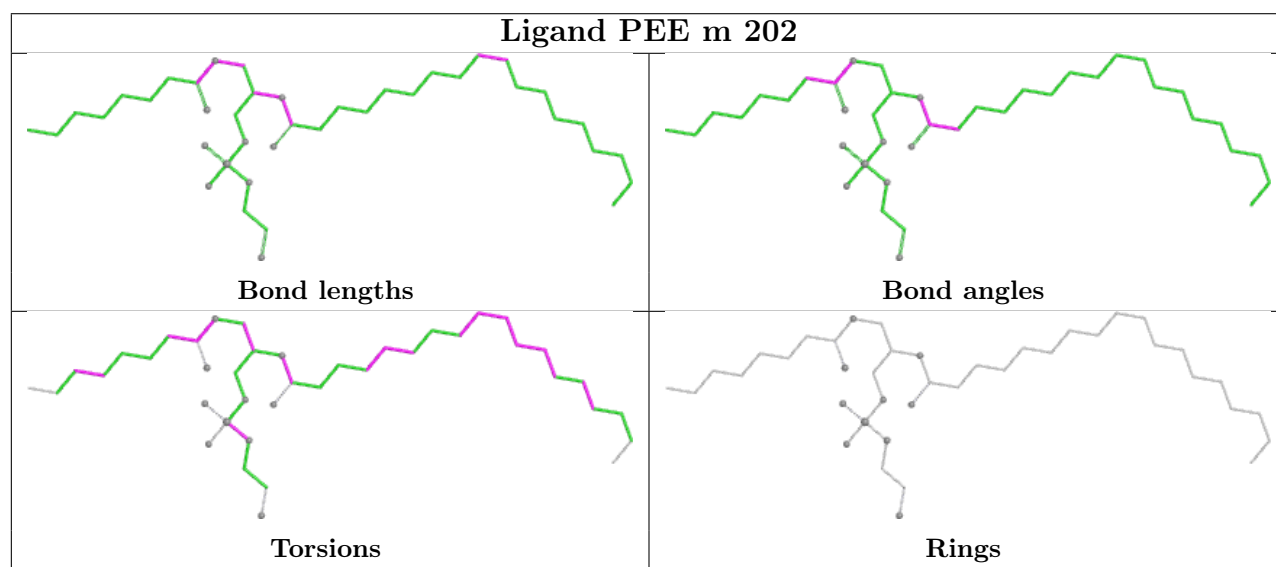
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 48  | m     | 202 | PEE  | 8       | 0            |
| 54  | r     | 714 | CDL  | 8       | 0            |
| 54  | a     | 201 | CDL  | 18      | 0            |
| 48  | U     | 101 | PEE  | 6       | 0            |
| 48  | l     | 720 | PEE  | 20      | 0            |
| 51  | J     | 401 | NDP  | 6       | 0            |
| 49  | e     | 201 | PLX  | 7       | 0            |
| 49  | V     | 205 | PLX  | 4       | 0            |
| 46  | A     | 502 | FMN  | 4       | 0            |
| 48  | l     | 719 | PEE  | 8       | 0            |
| 49  | n     | 101 | PLX  | 9       | 0            |
| 57  | w     | 401 | ADP  | 4       | 0            |
| 48  | V     | 207 | PEE  | 7       | 0            |
| 49  | i     | 705 | PLX  | 1       | 0            |
| 48  | V     | 202 | PEE  | 21      | 0            |
| 54  | N     | 202 | CDL  | 12      | 0            |
| 45  | A     | 501 | SF4  | 2       | 0            |
| 49  | C     | 312 | PLX  | 2       | 0            |
| 48  | l     | 718 | PEE  | 10      | 0            |

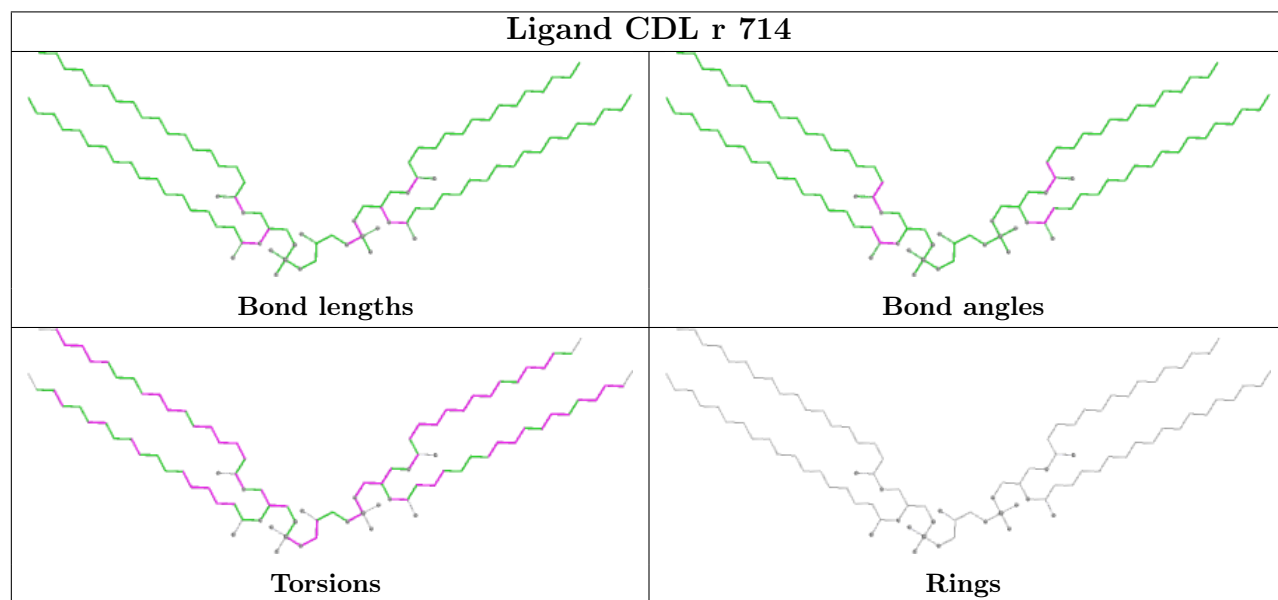
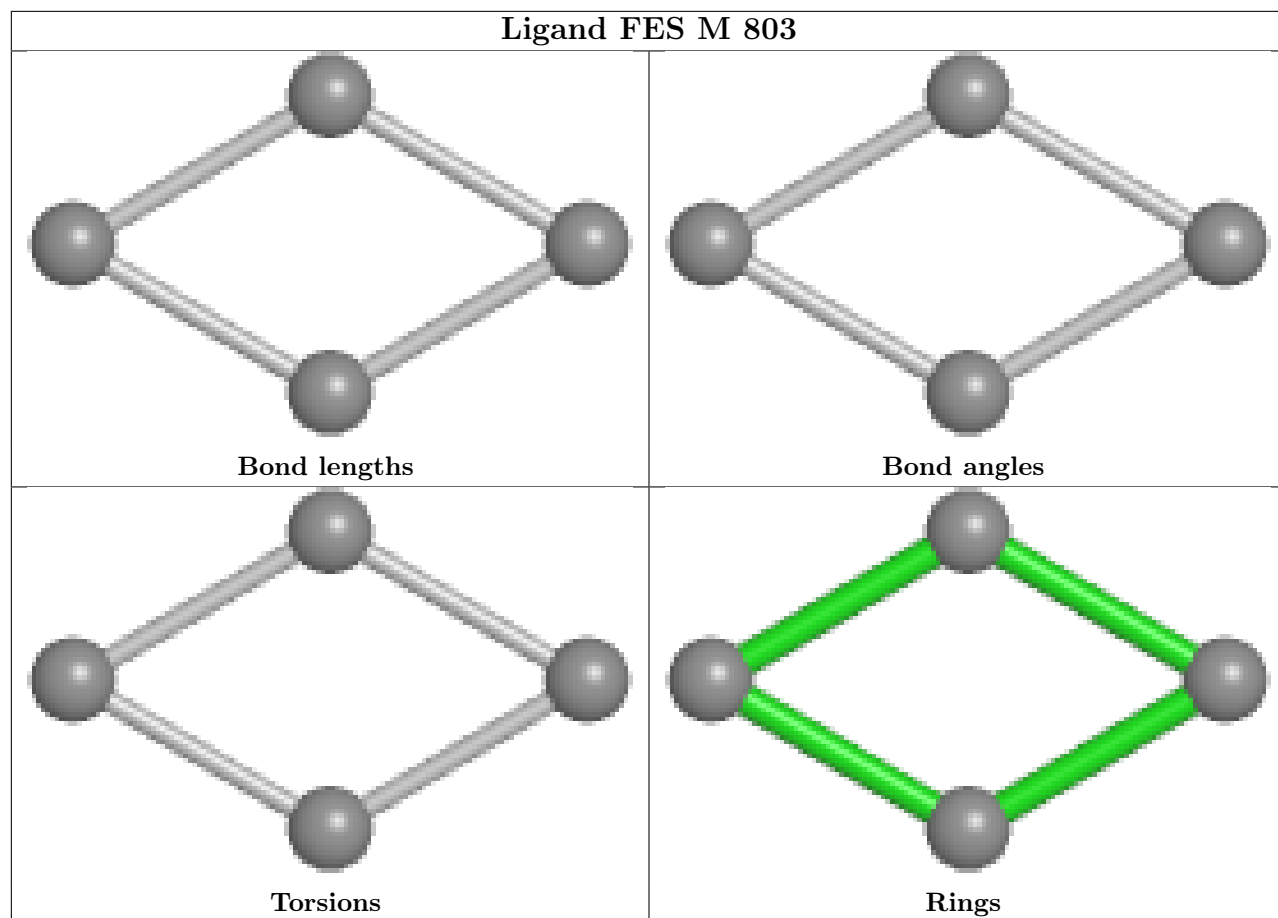
*Continued on next page...*

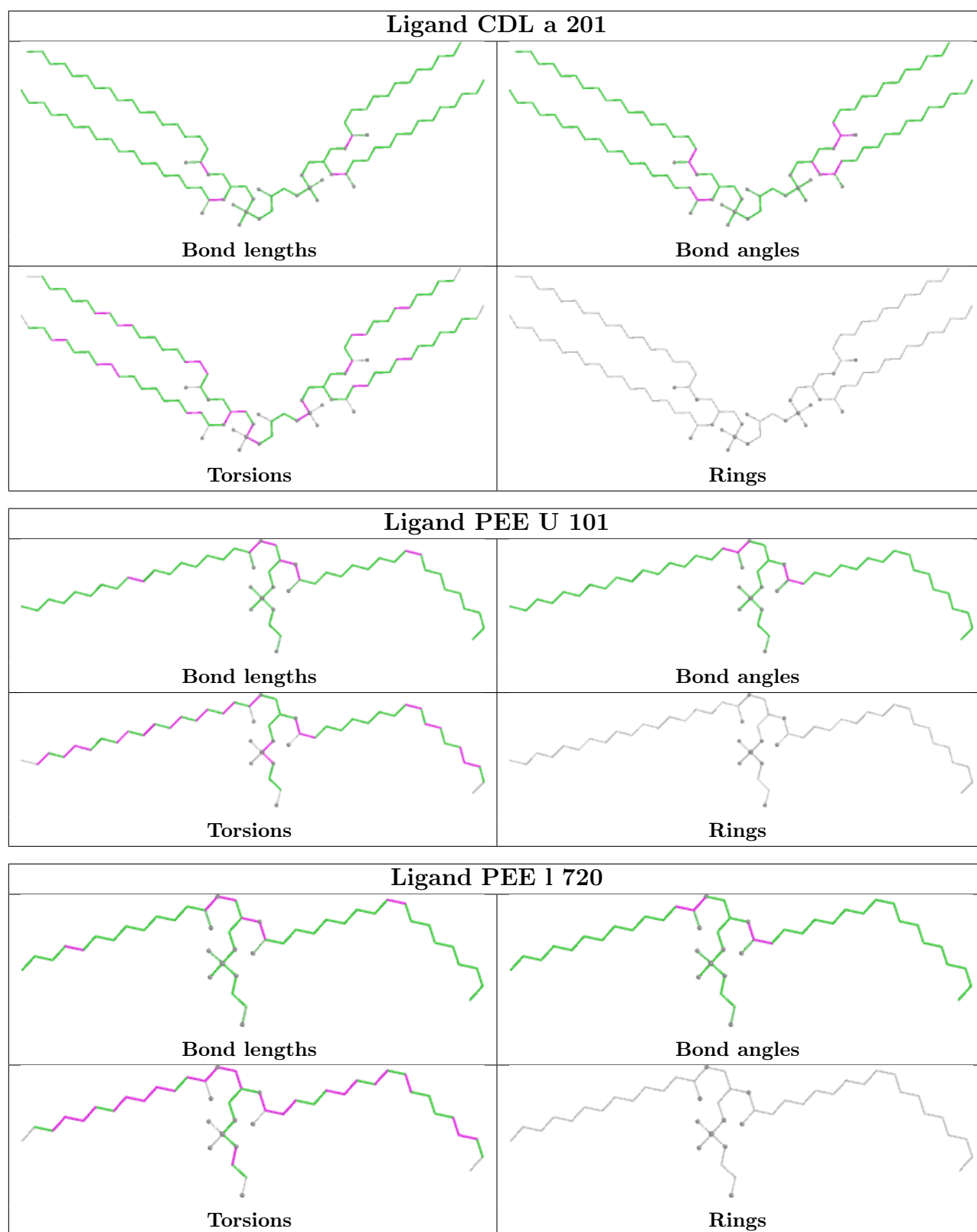
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 54  | n     | 102 | CDL  | 13      | 0            |
| 56  | s     | 403 | UQ   | 4       | 0            |
| 54  | l     | 712 | CDL  | 39      | 0            |
| 47  | A     | 503 | NAI  | 4       | 0            |
| 48  | s     | 401 | PEE  | 2       | 0            |
| 54  | i     | 401 | CDL  | 16      | 0            |
| 54  | l     | 713 | CDL  | 7       | 0            |
| 50  | X     | 201 | 8Q1  | 1       | 0            |
| 54  | V     | 203 | CDL  | 15      | 0            |
| 54  | V     | 201 | CDL  | 19      | 0            |
| 49  | j     | 203 | PLX  | 2       | 0            |
| 45  | M     | 802 | SF4  | 1       | 0            |
| 48  | C     | 311 | PEE  | 21      | 0            |

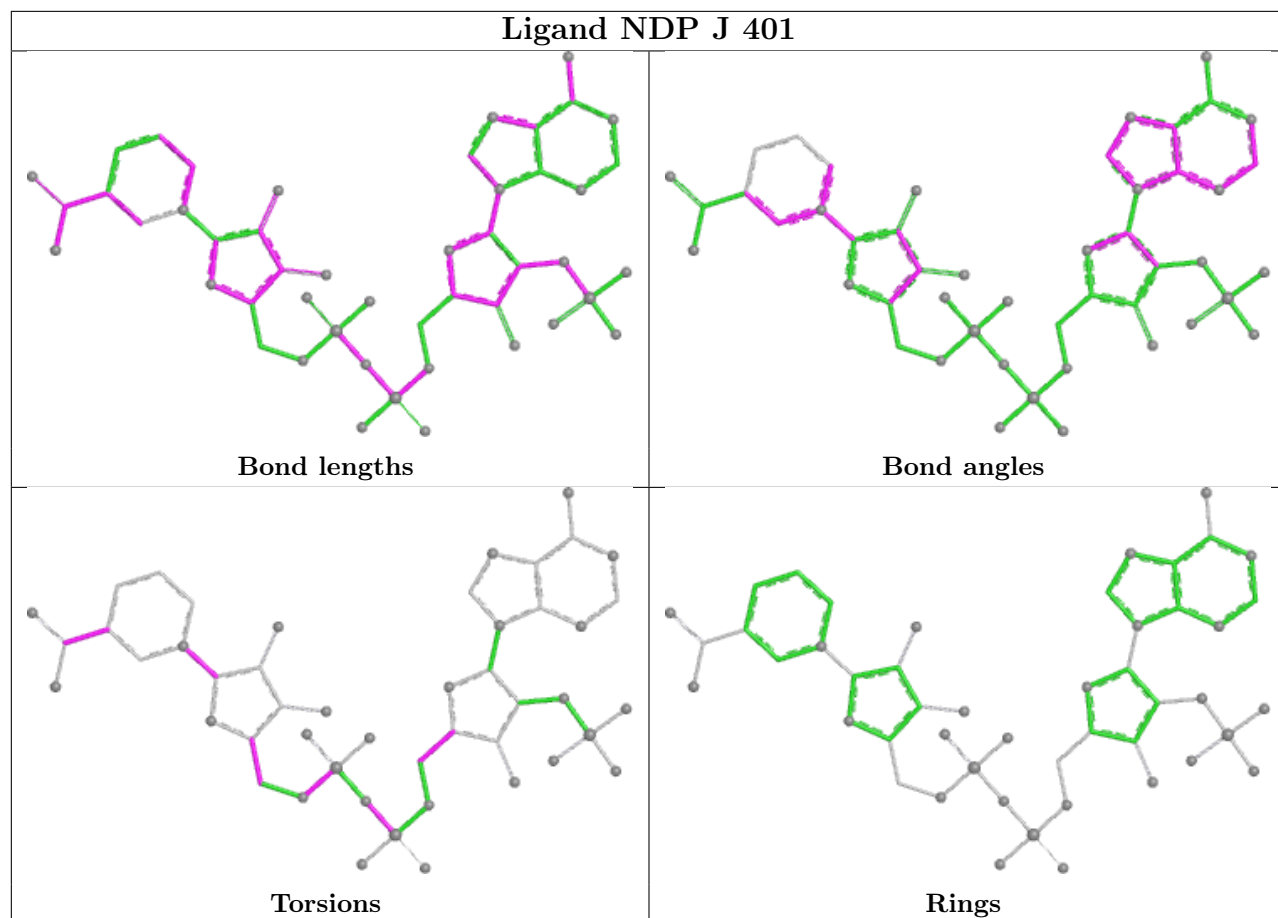
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



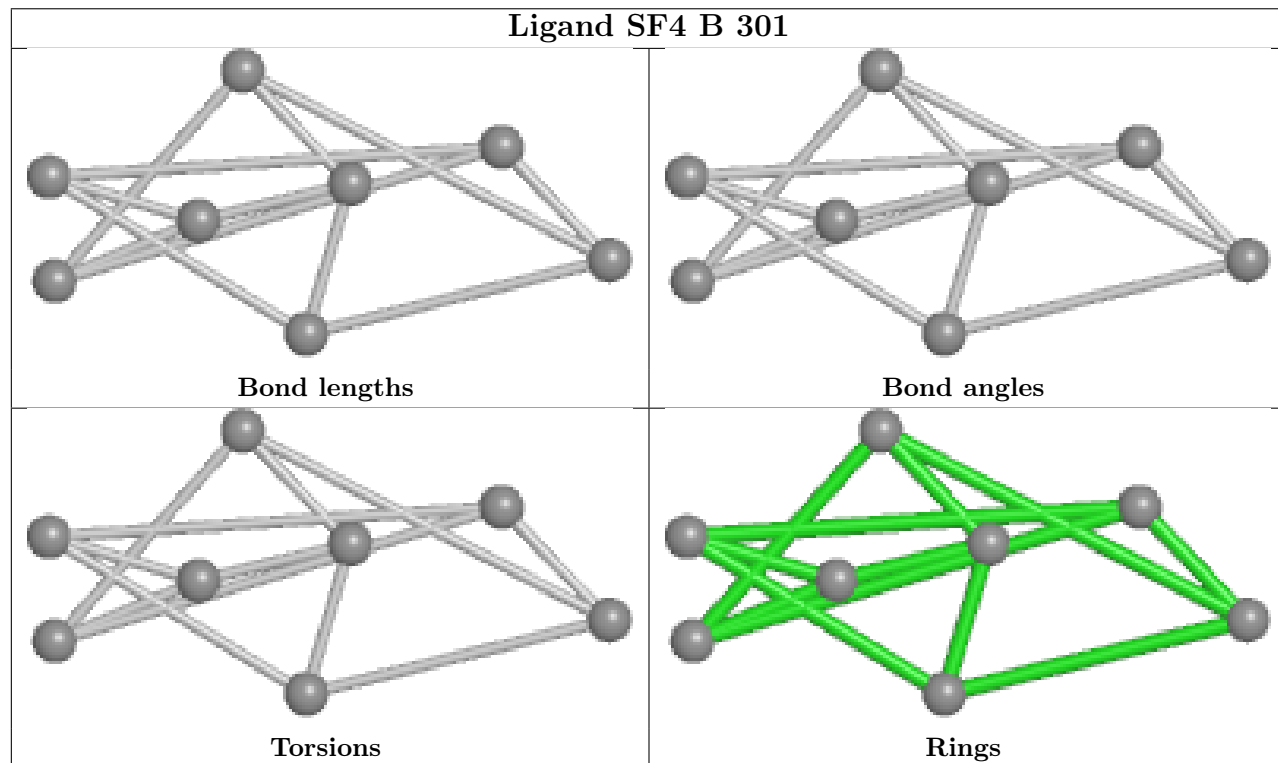




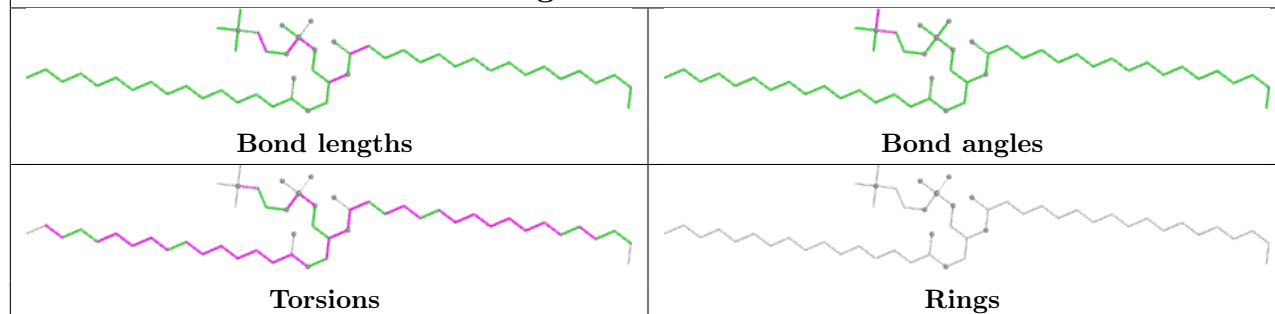
## Ligand NDP J 401



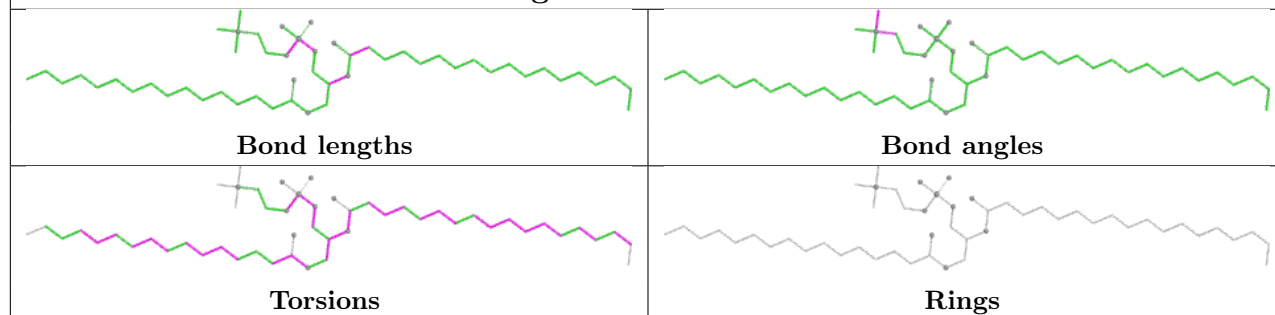
## Ligand SF4 B 301



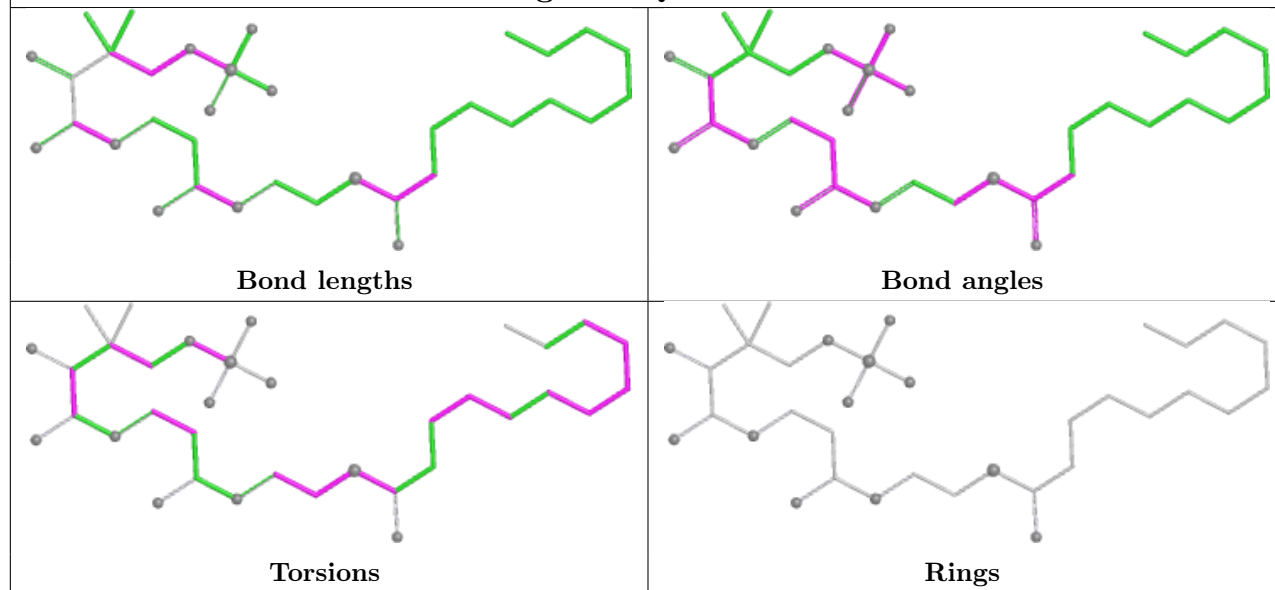
## Ligand PLX e 201

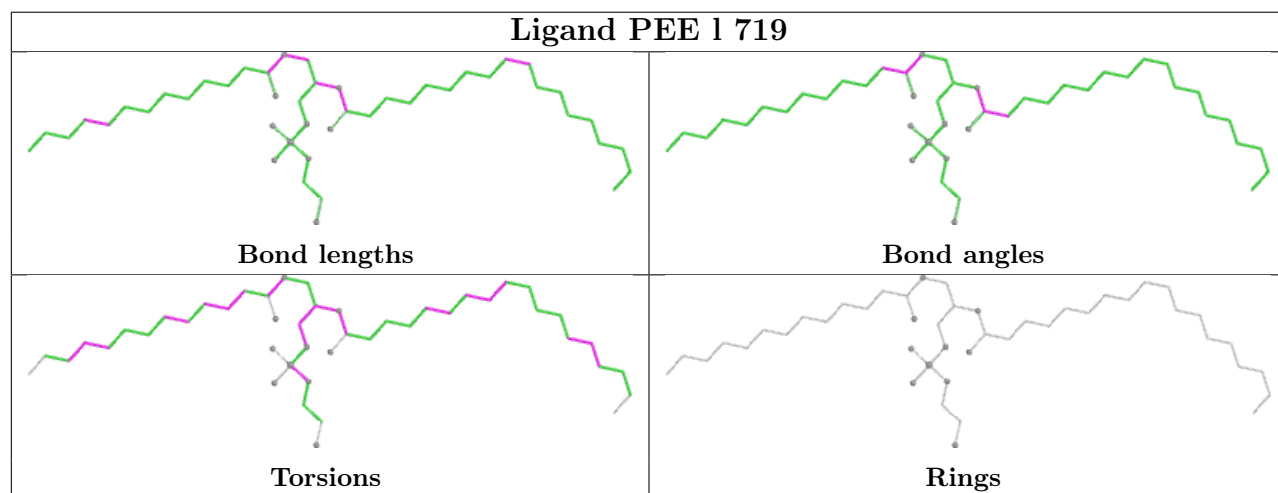
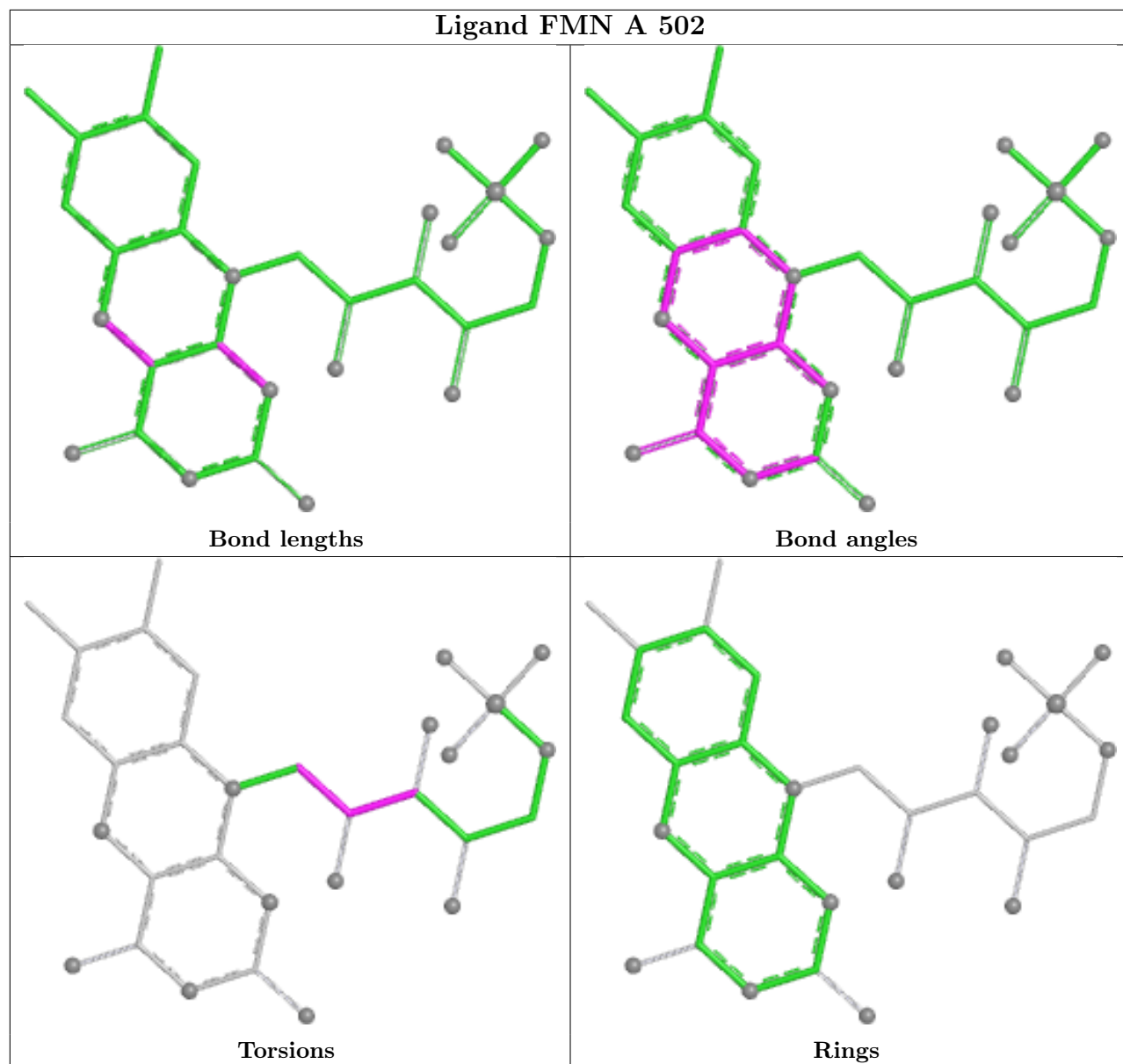


## Ligand PLX V 205

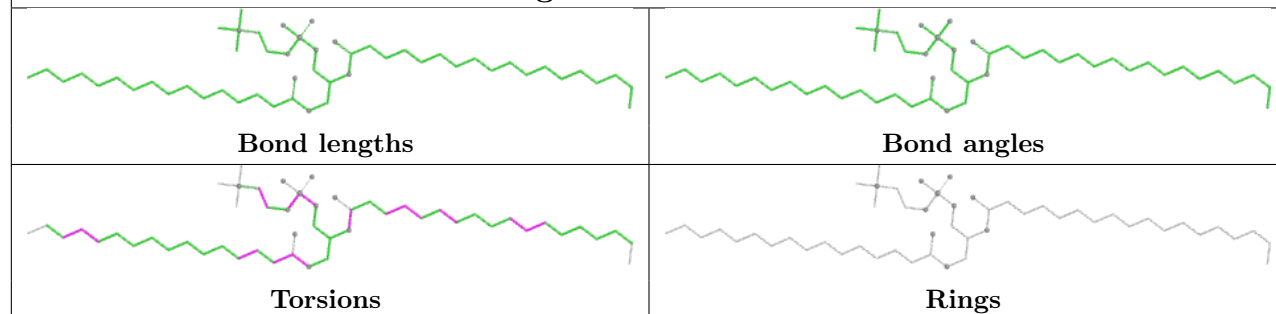


## Ligand 8Q1 G 201

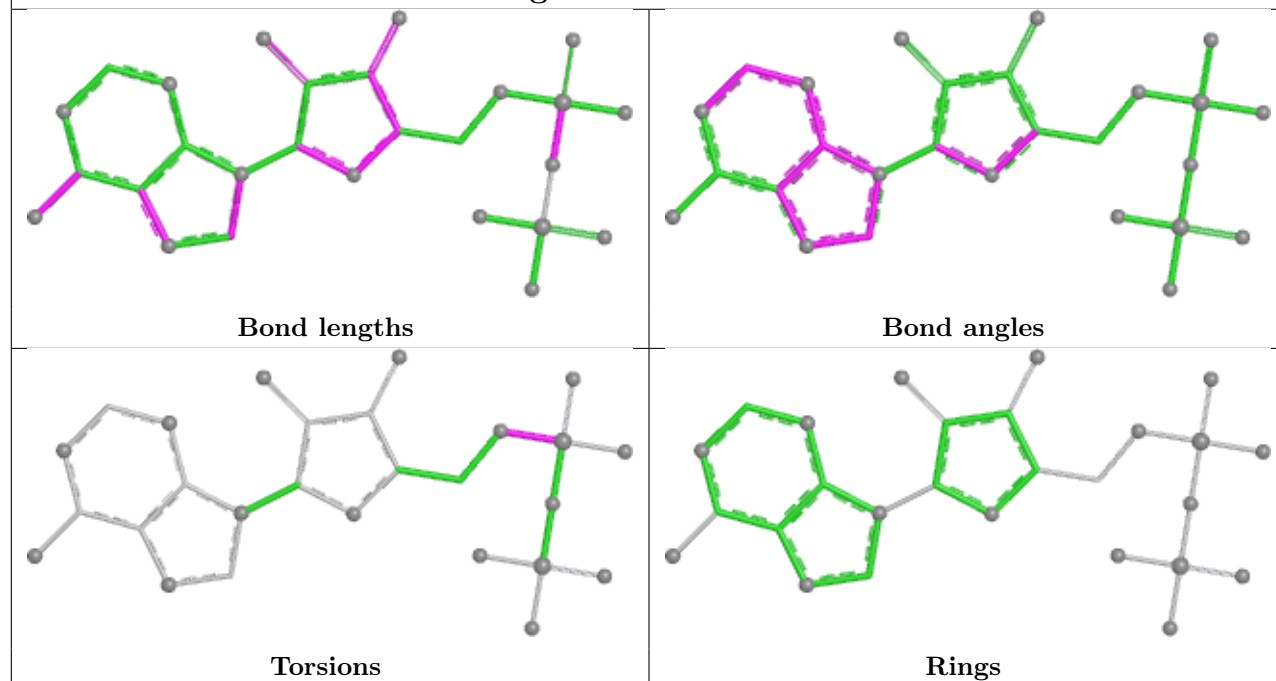




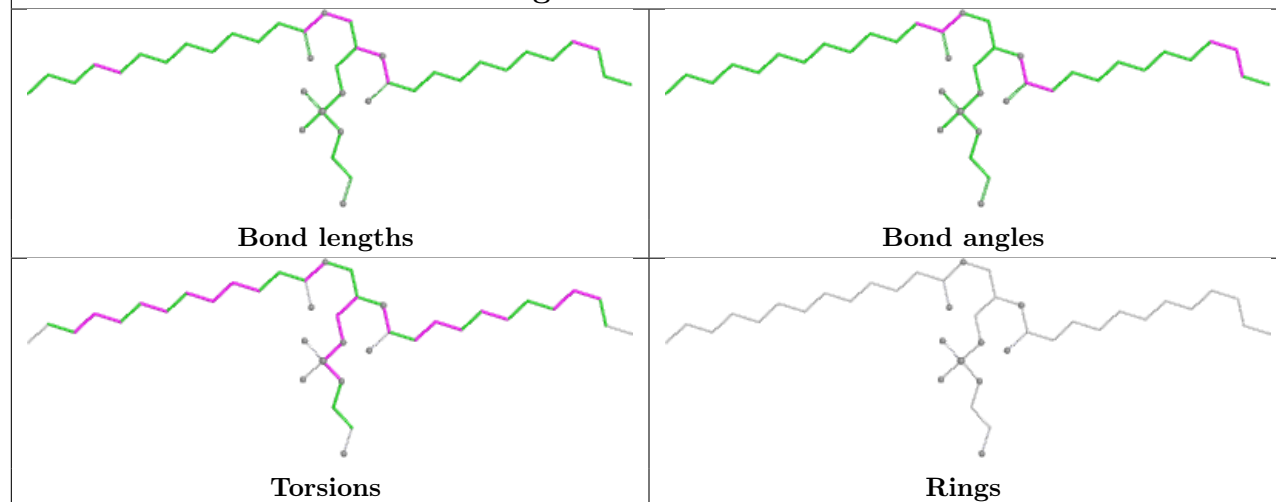
## Ligand PLX n 101

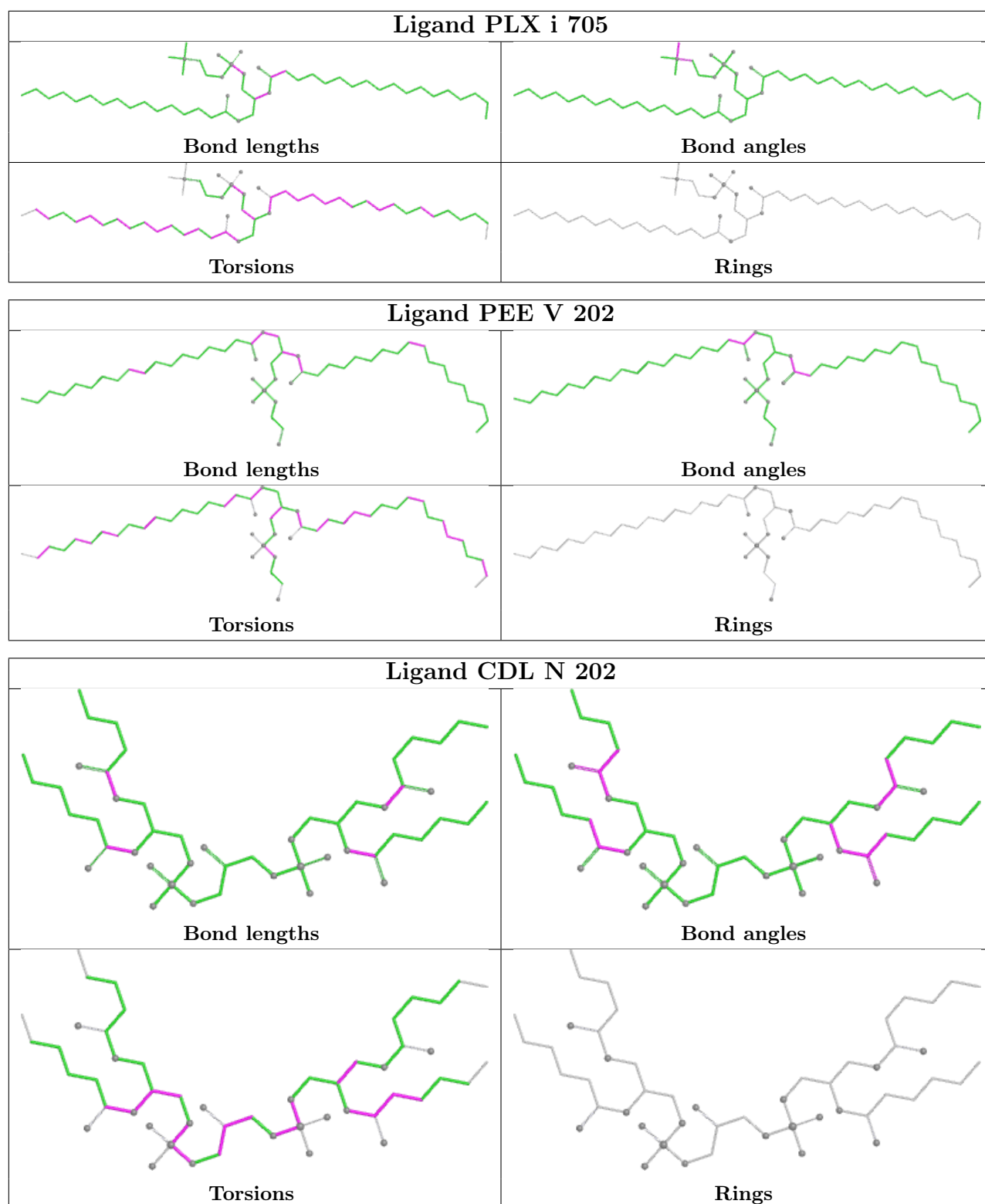


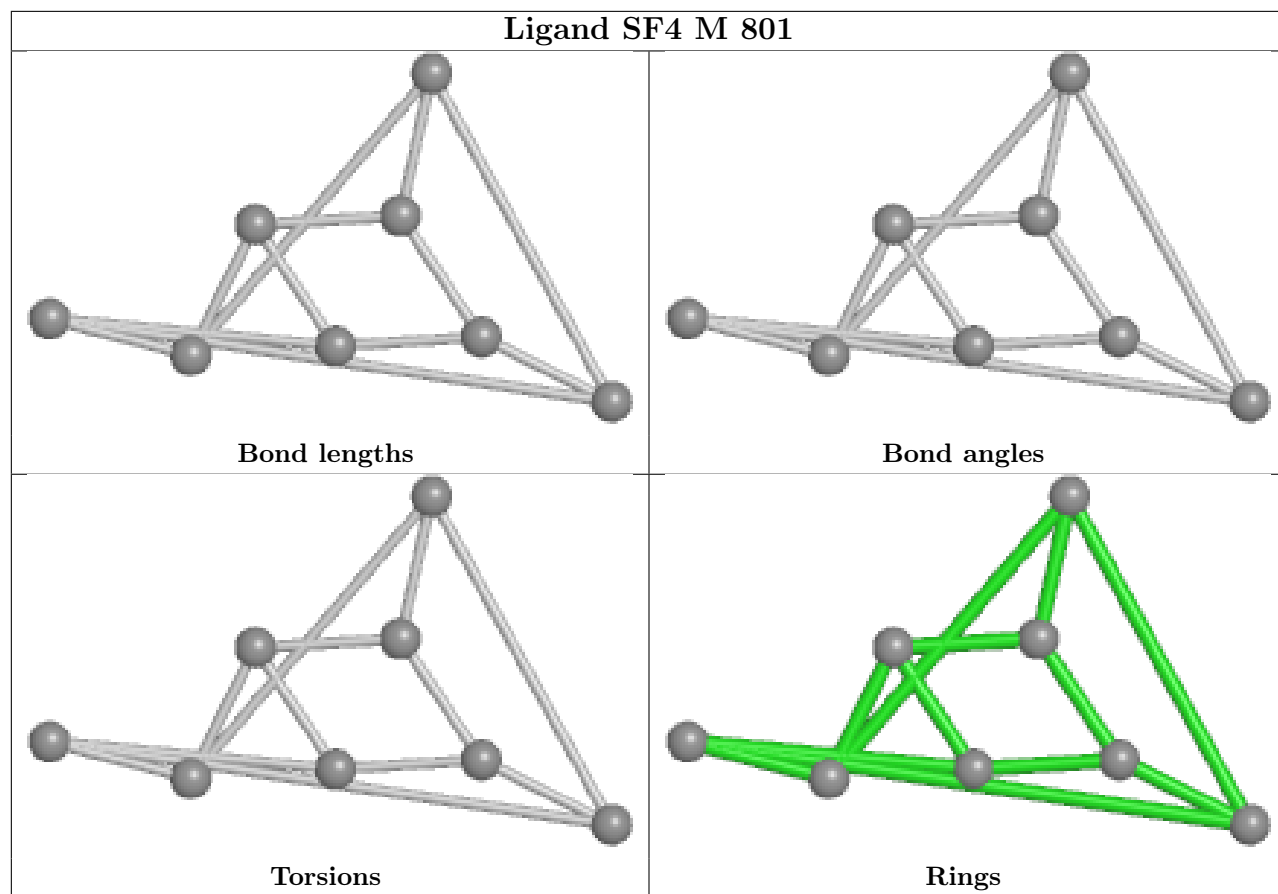
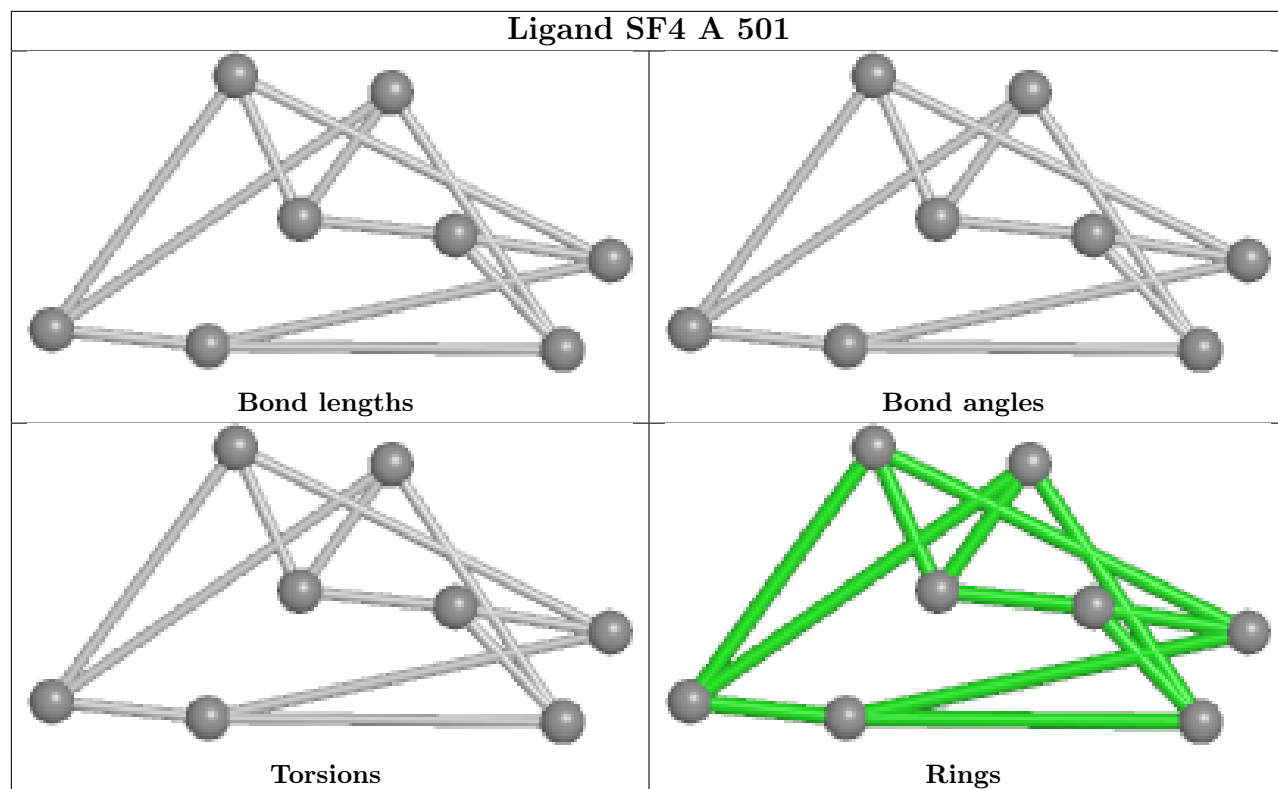
## Ligand ADP w 401

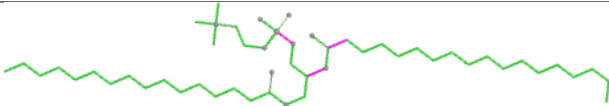
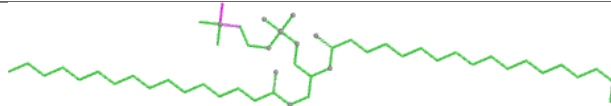
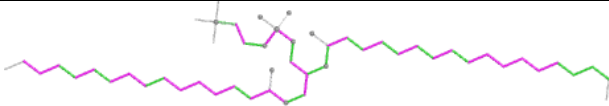
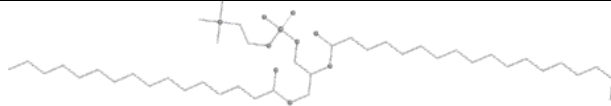


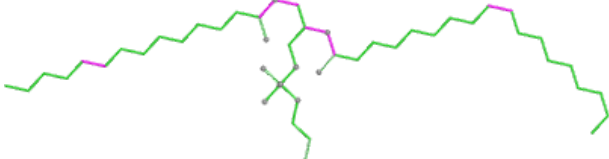
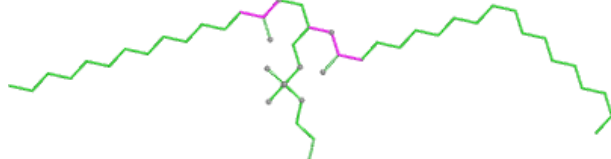
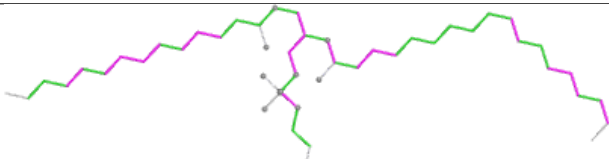
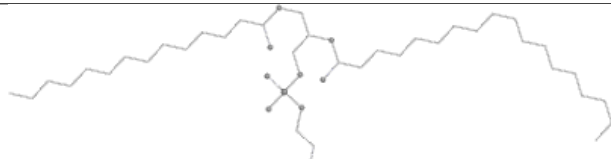
## Ligand PEE V 207

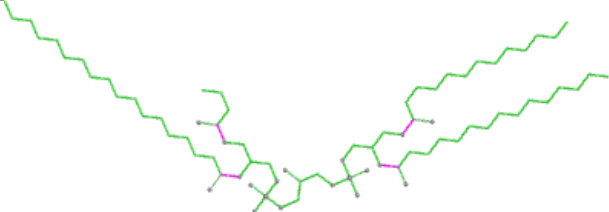
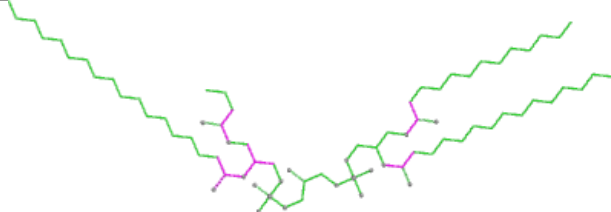
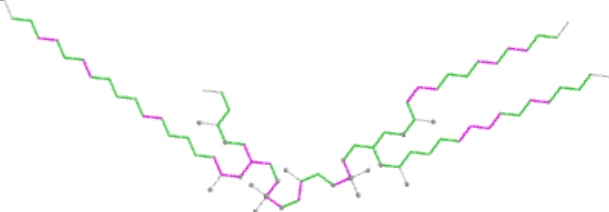
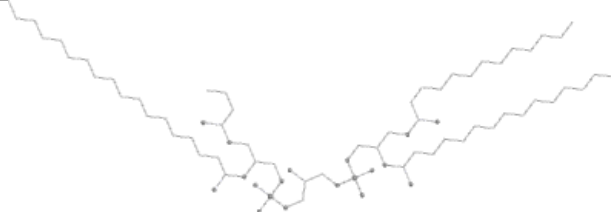


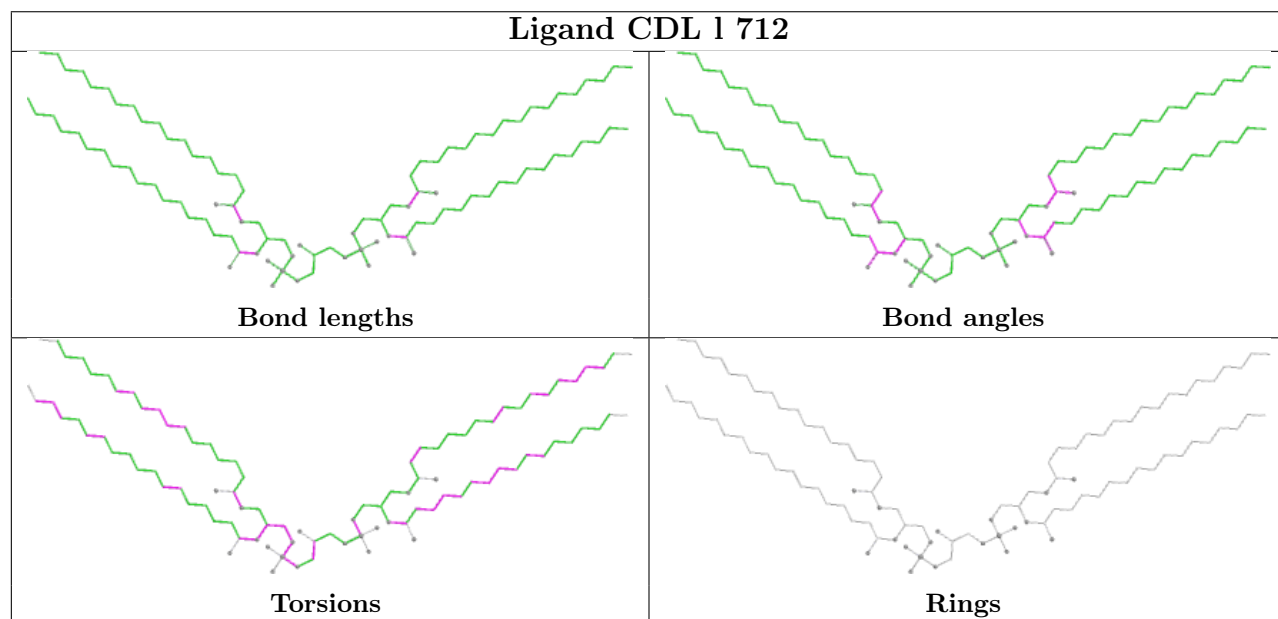
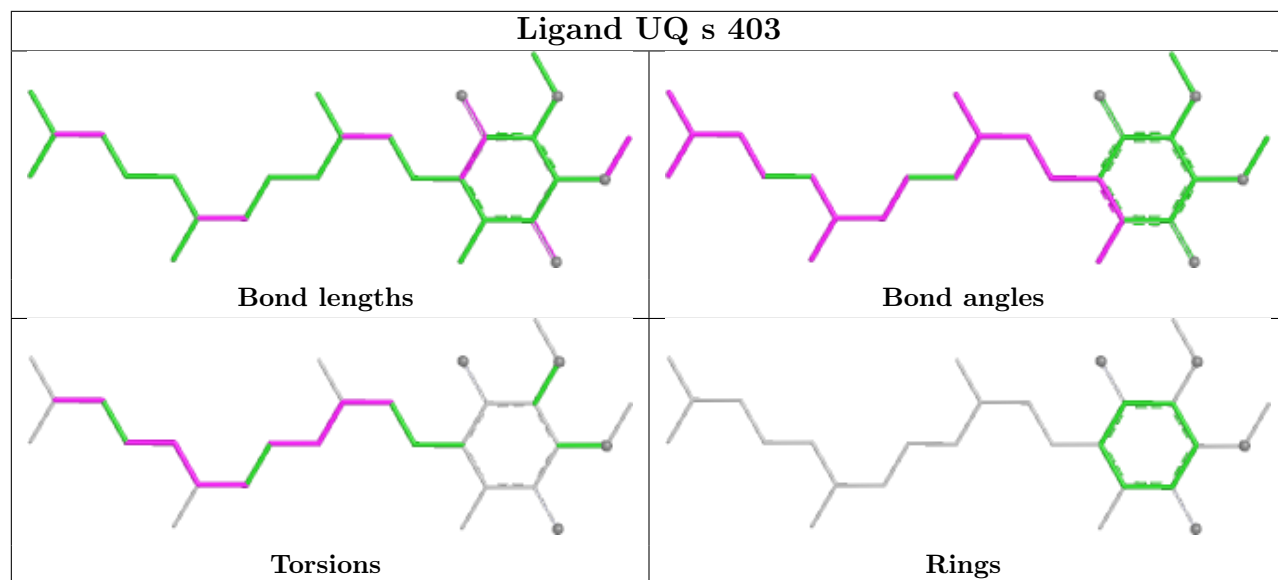


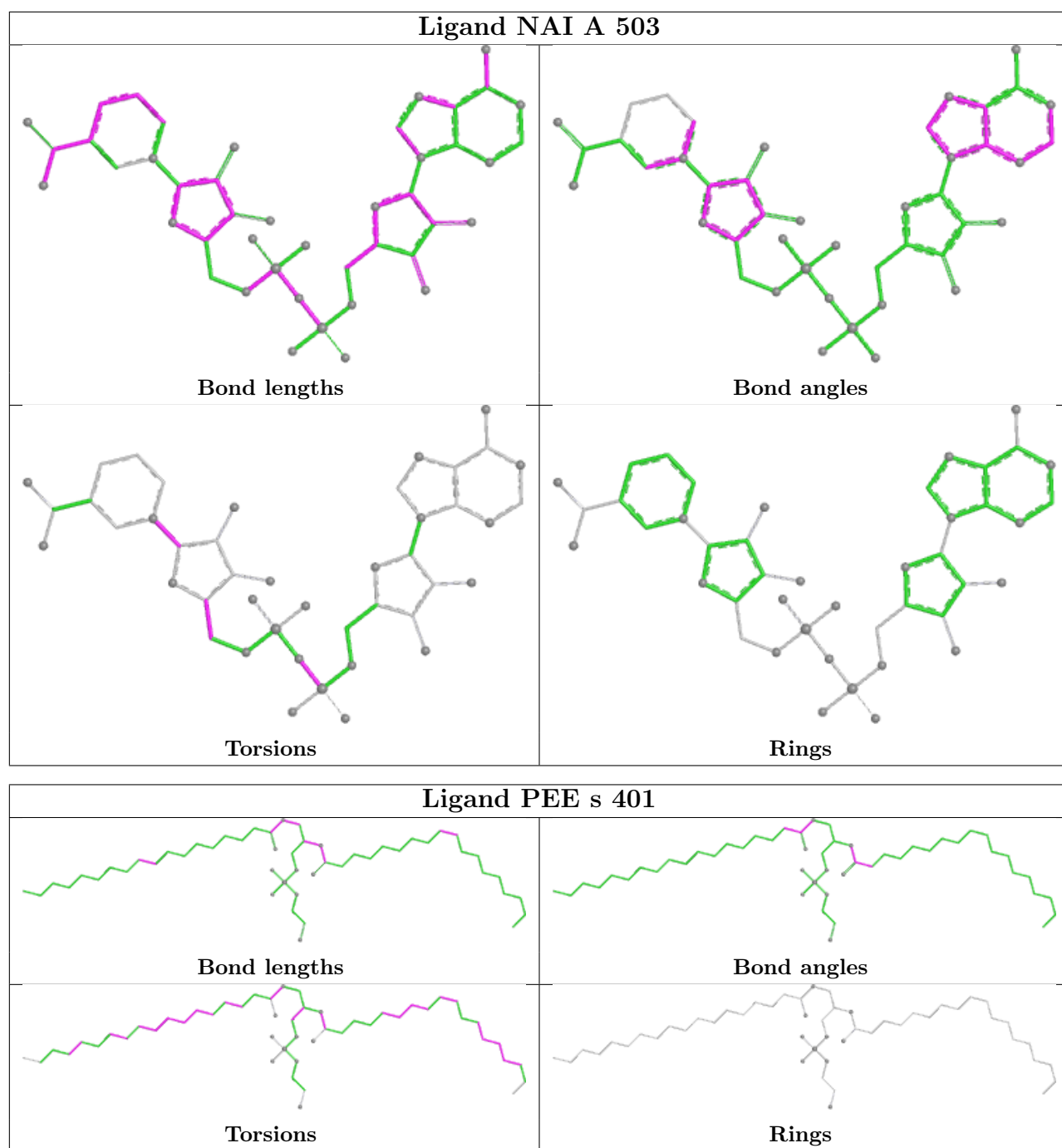


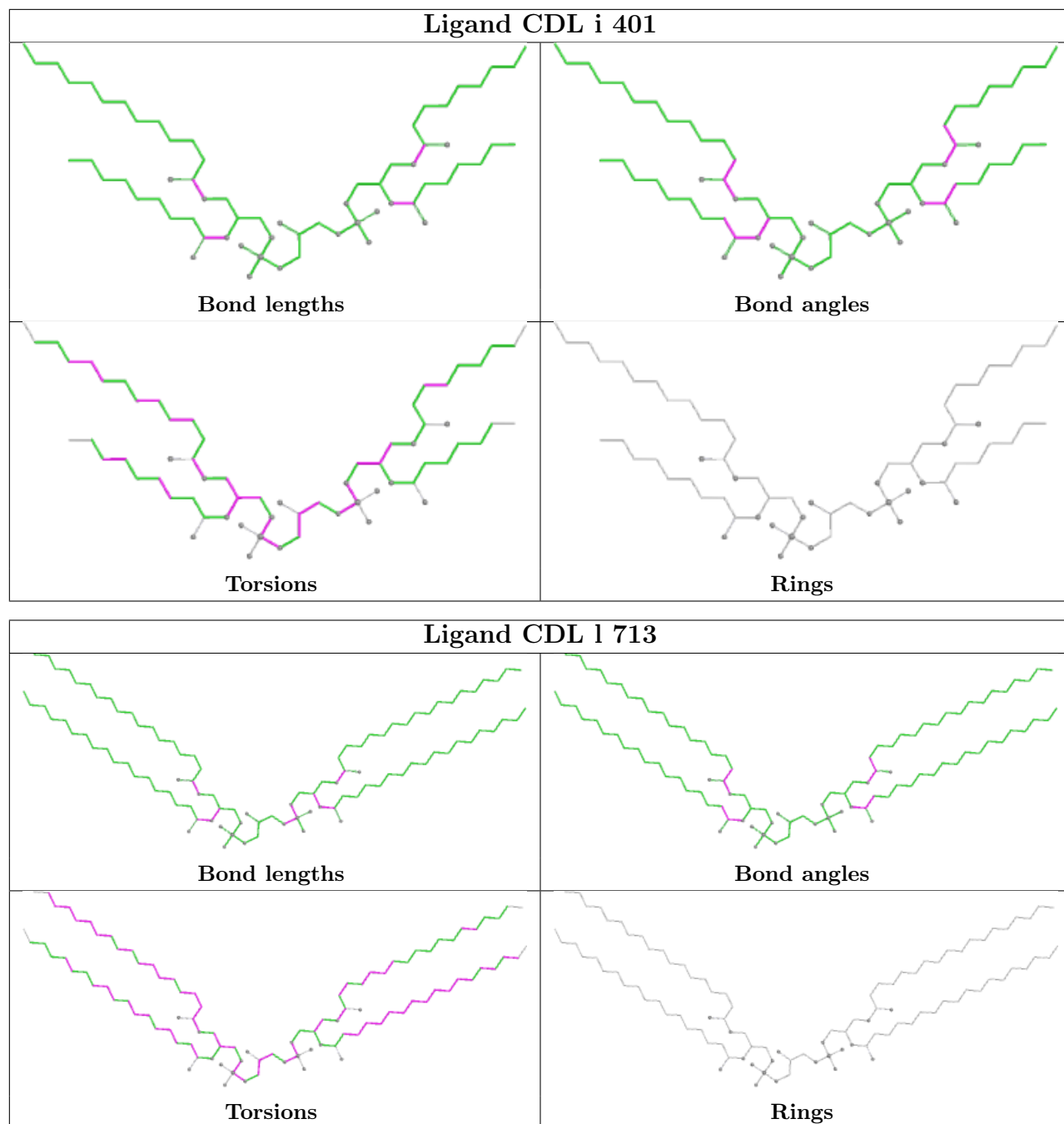
| Ligand PLX C 312                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

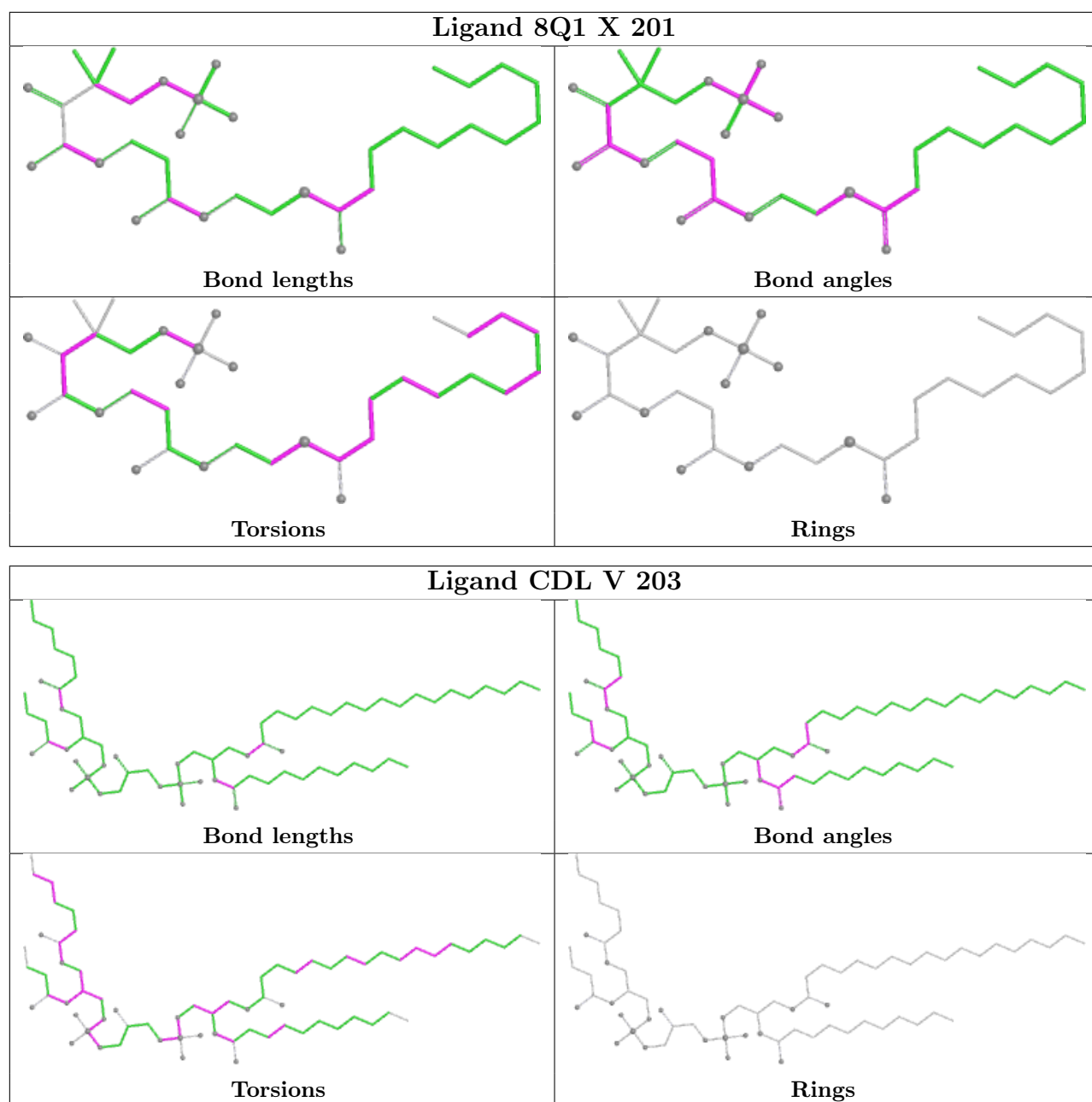
| Ligand PEE 1 718                                                                  |                                                                                    |
|-----------------------------------------------------------------------------------|------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

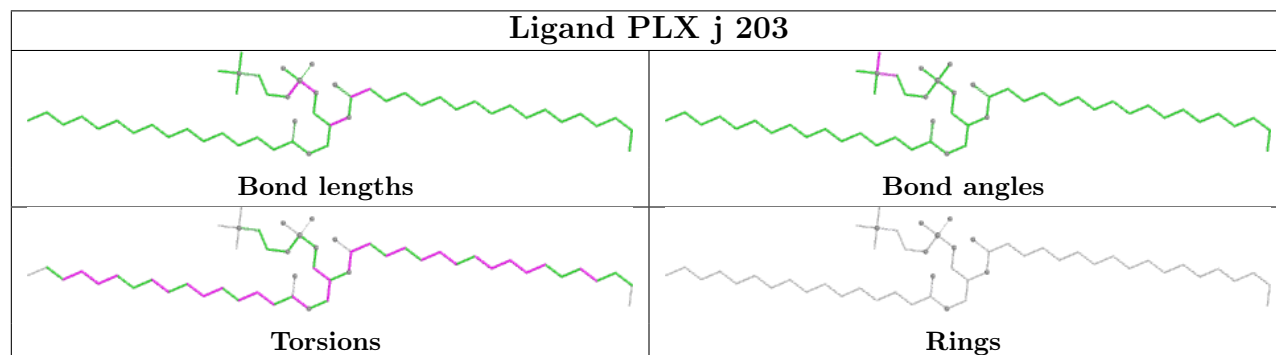
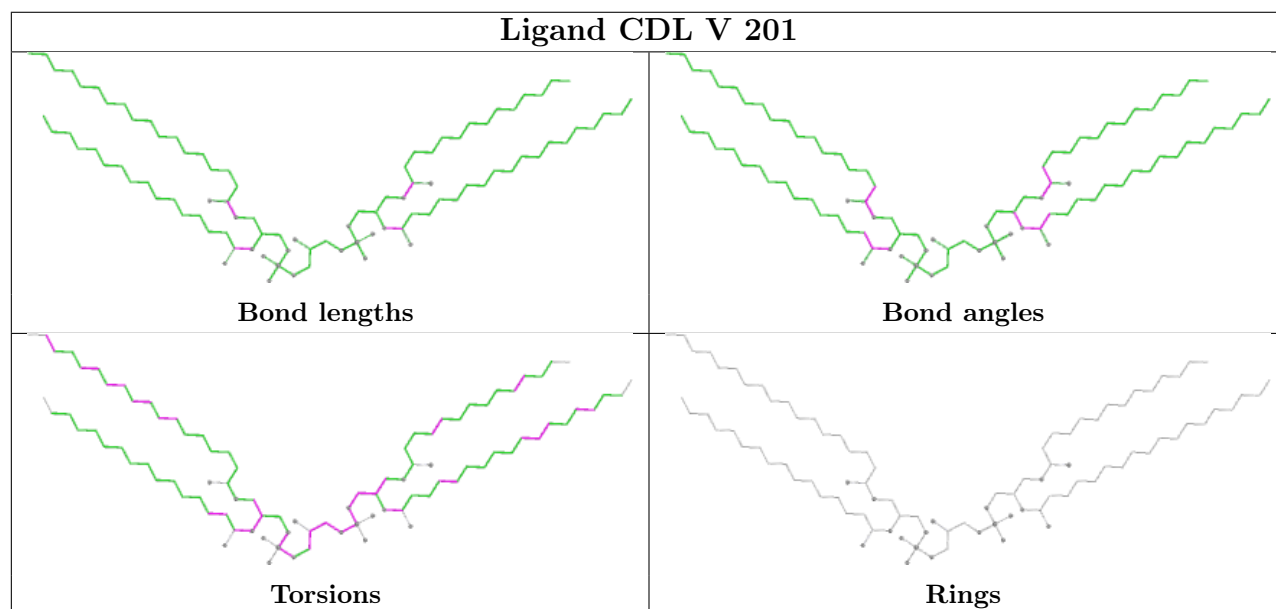
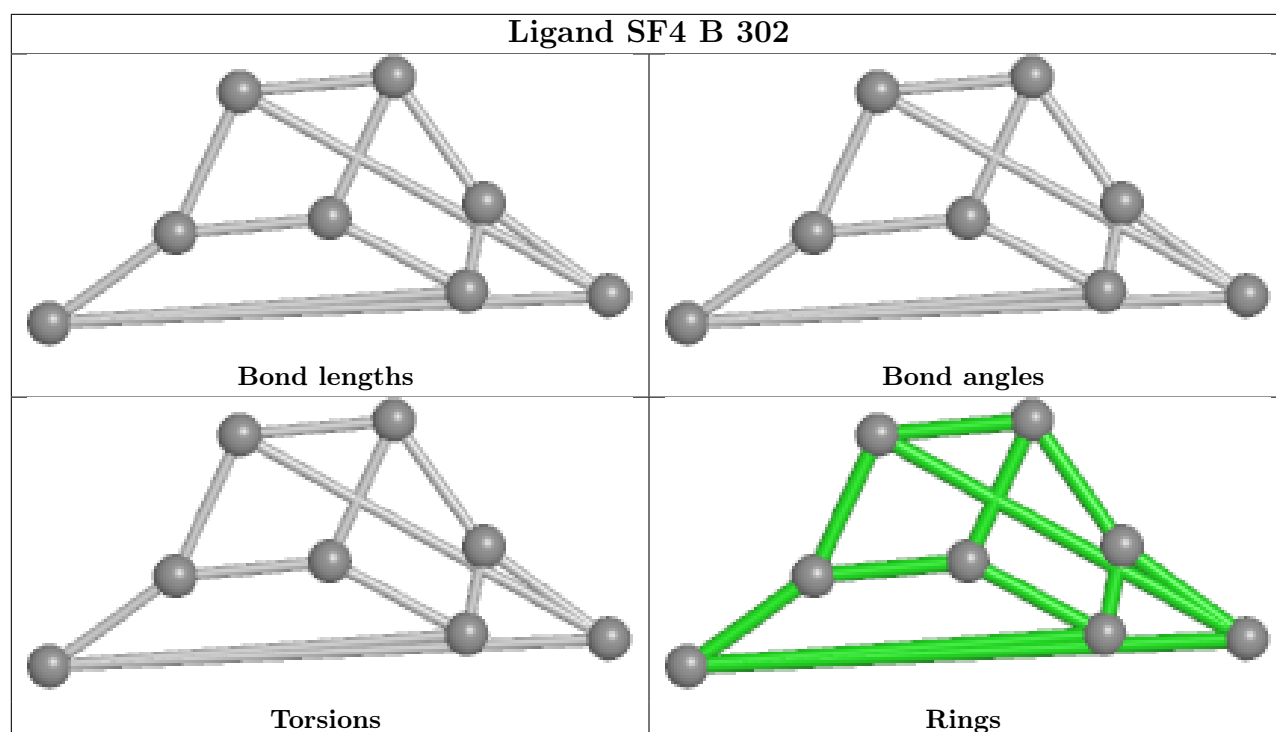
| Ligand CDL n 102                                                                    |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|  |  |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

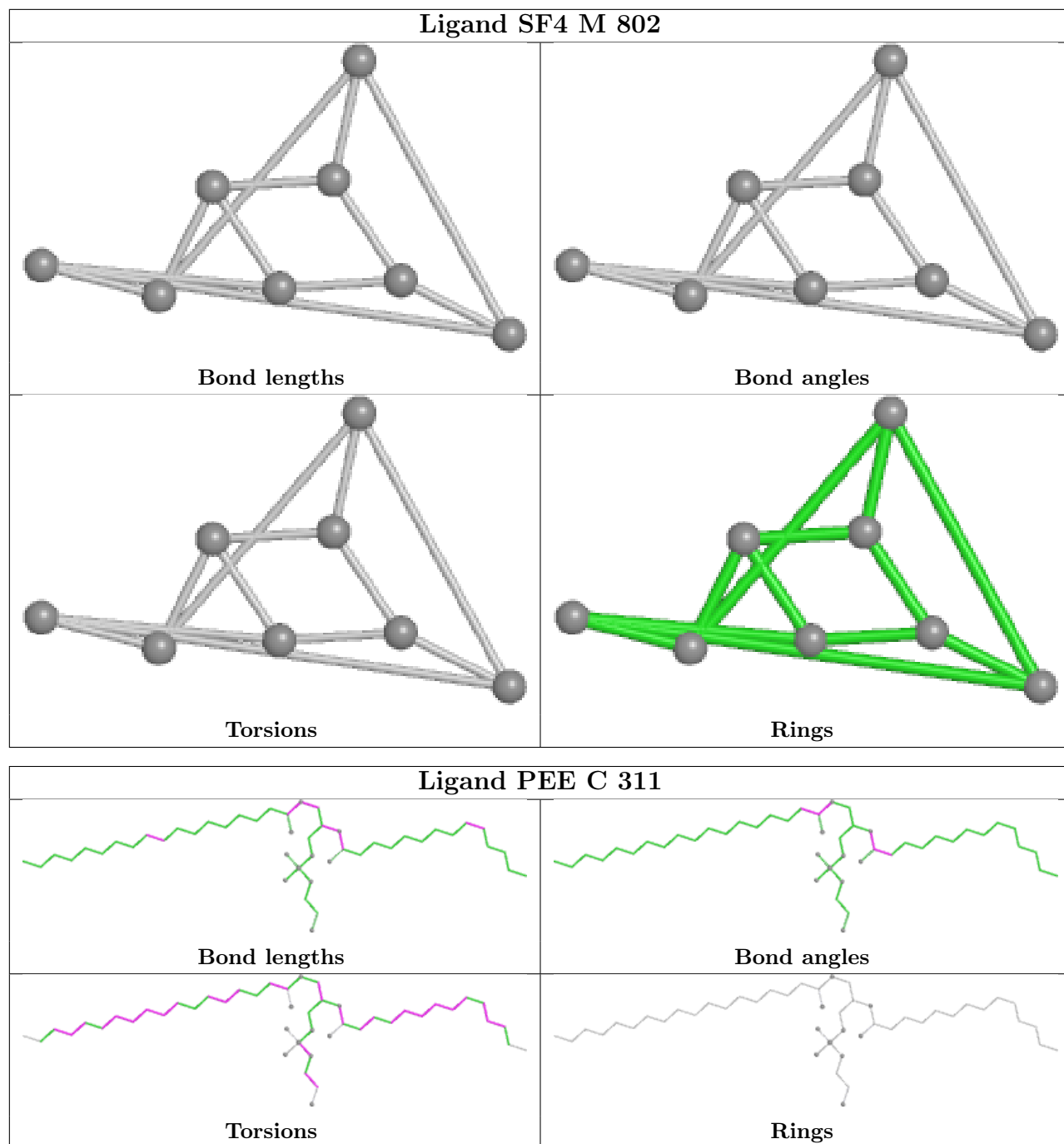


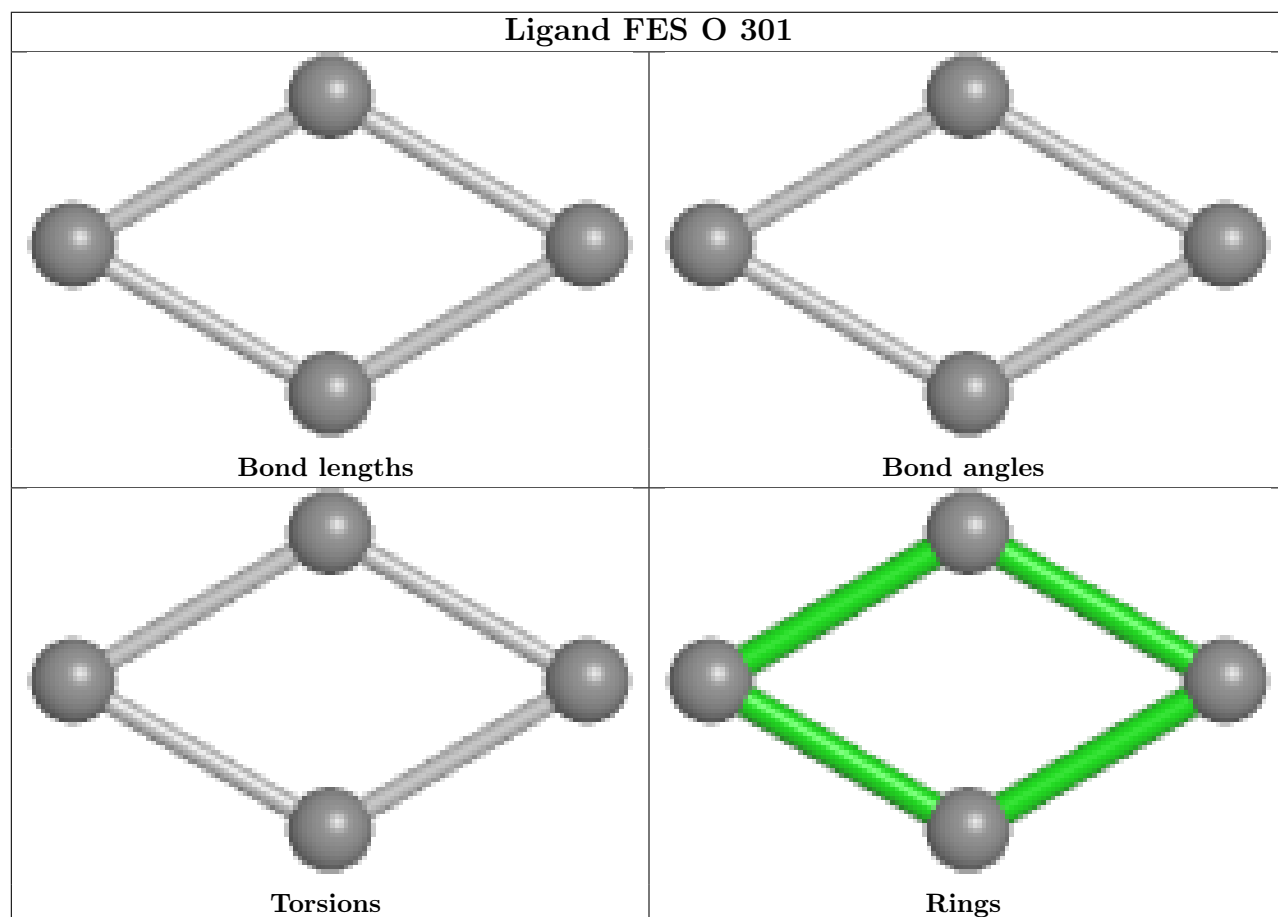
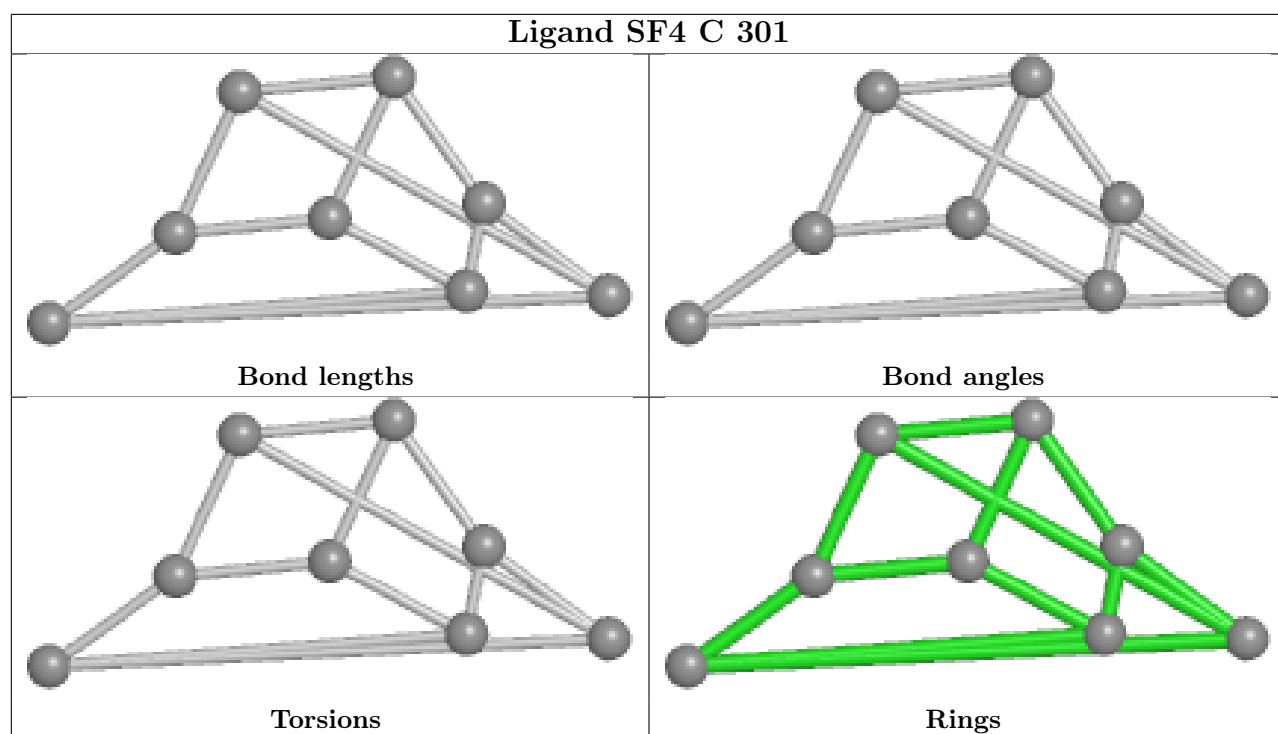












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

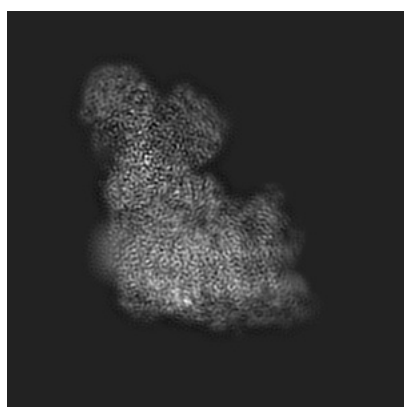
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31644. These allow visual inspection of the internal detail of the map and identification of artifacts.

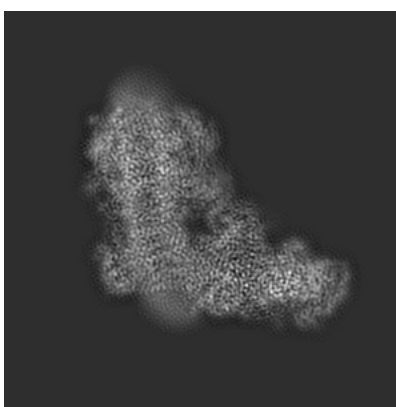
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

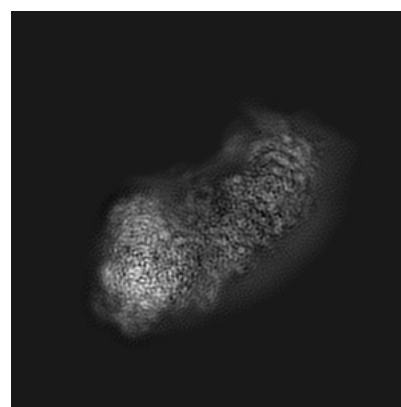
#### 6.1.1 Primary map



X



Y

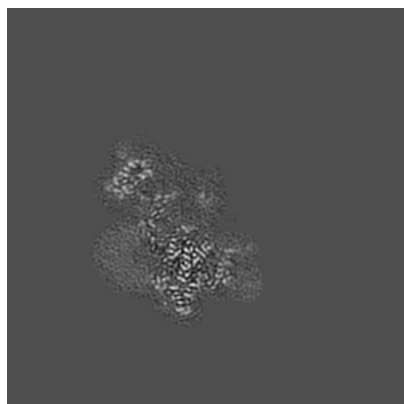


Z

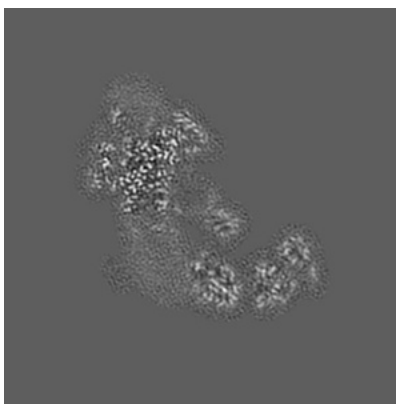
The images above show the map projected in three orthogonal directions.

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

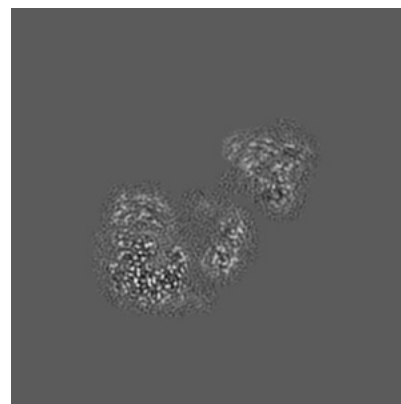
#### 6.2.1 Primary map



X Index: 155



Y Index: 155

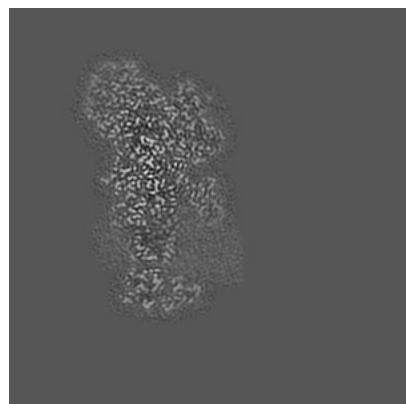


Z Index: 155

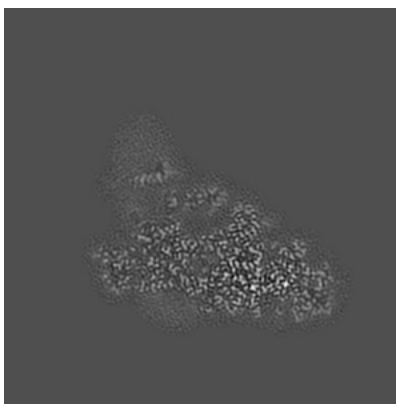
The images above show central slices of the map in three orthogonal directions.

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

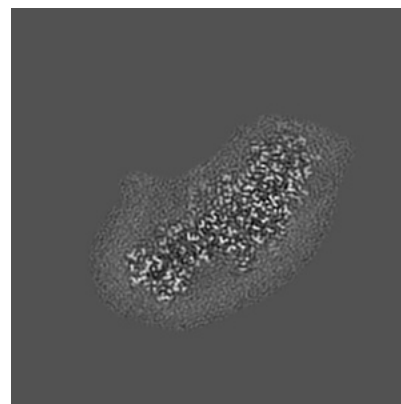
### 6.3.1 Primary map



X Index: 102



Y Index: 107

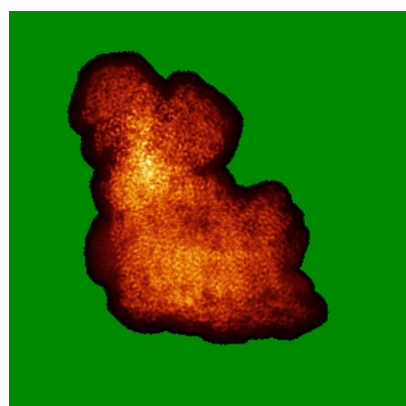


Z Index: 119

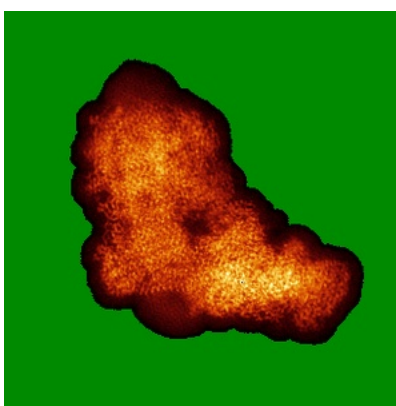
The images above show the largest variance slices of the map in three orthogonal directions.

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

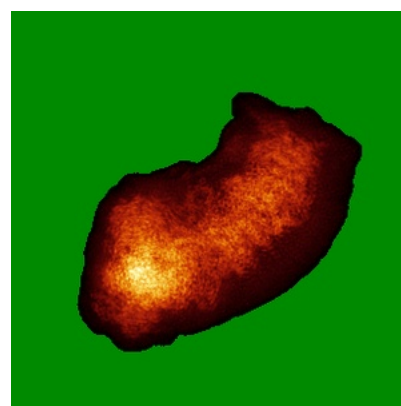
### 6.4.1 Primary map



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 0.0232. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

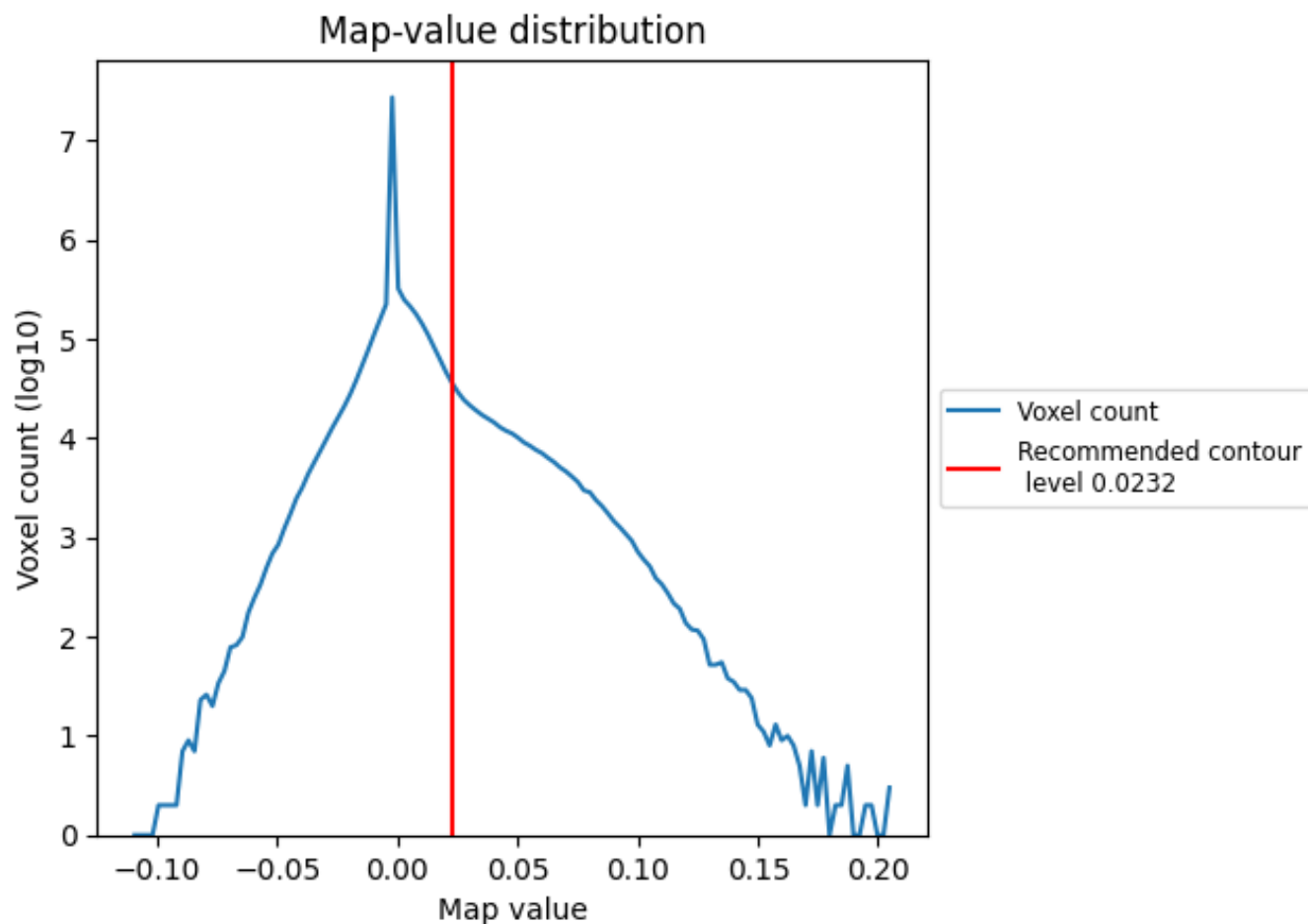
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

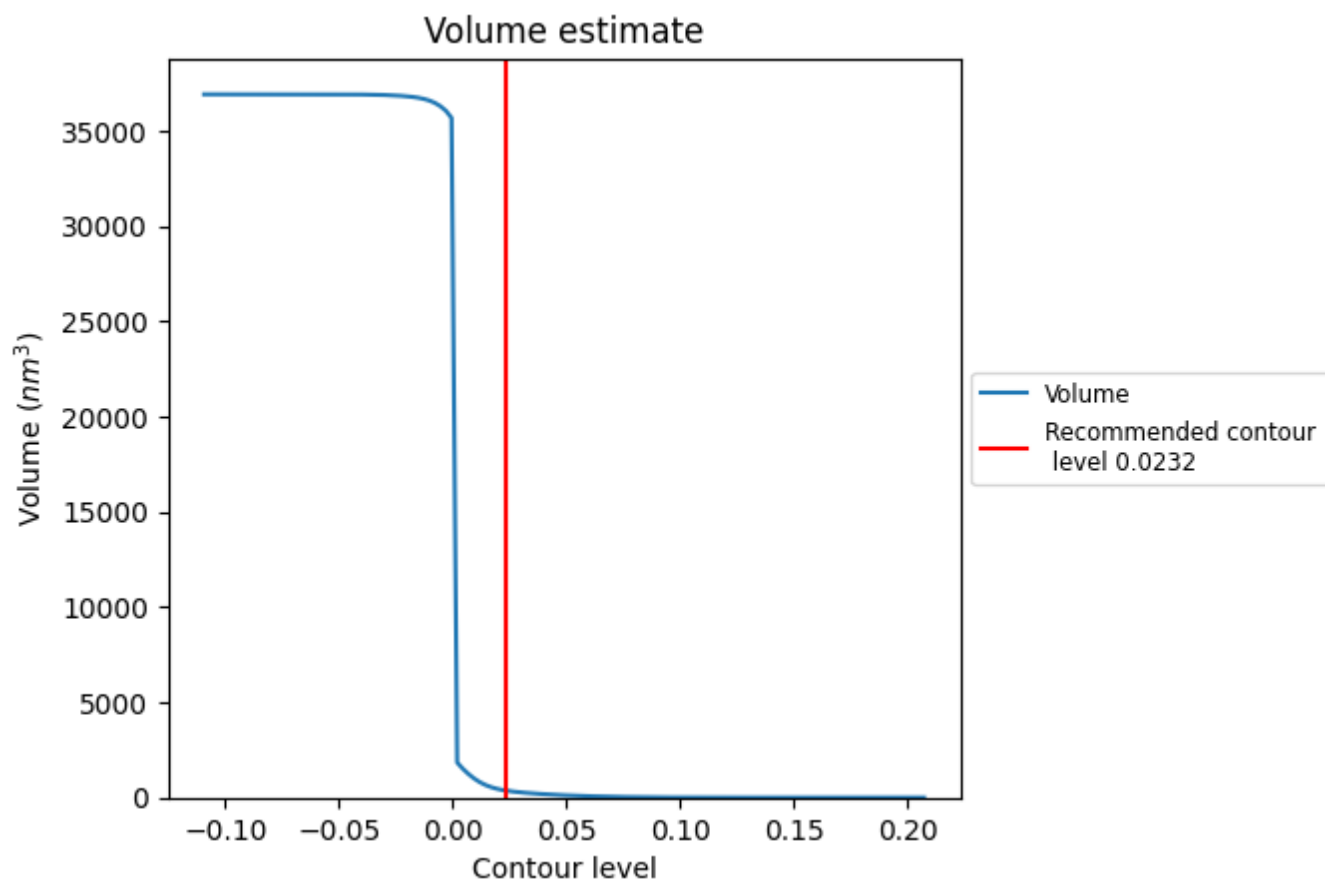
This section contains the results of statistical analysis of the map.

### 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.

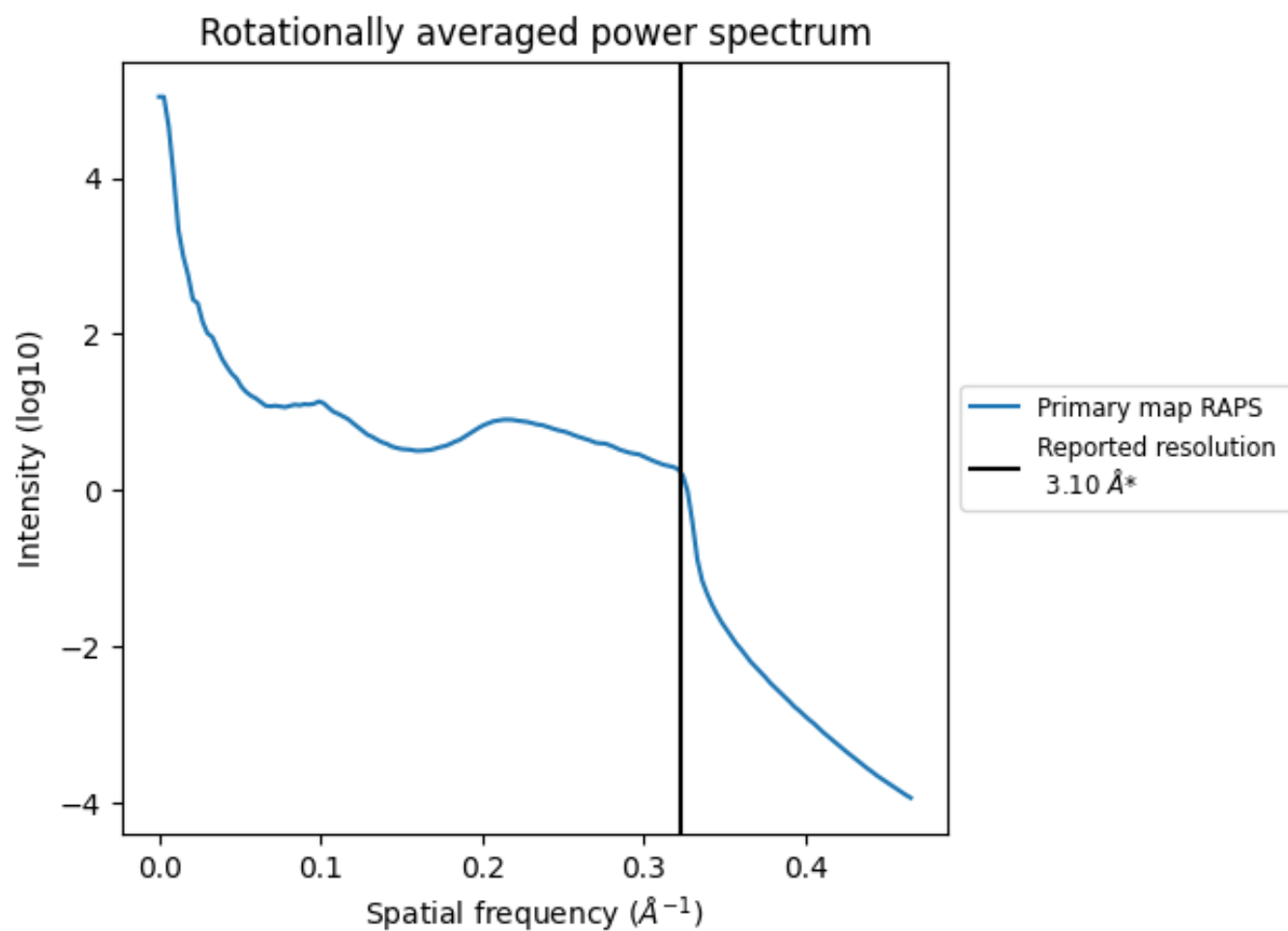
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm<sup>3</sup>; this corresponds to an approximate mass of 336 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 0.323 Å<sup>-1</sup>

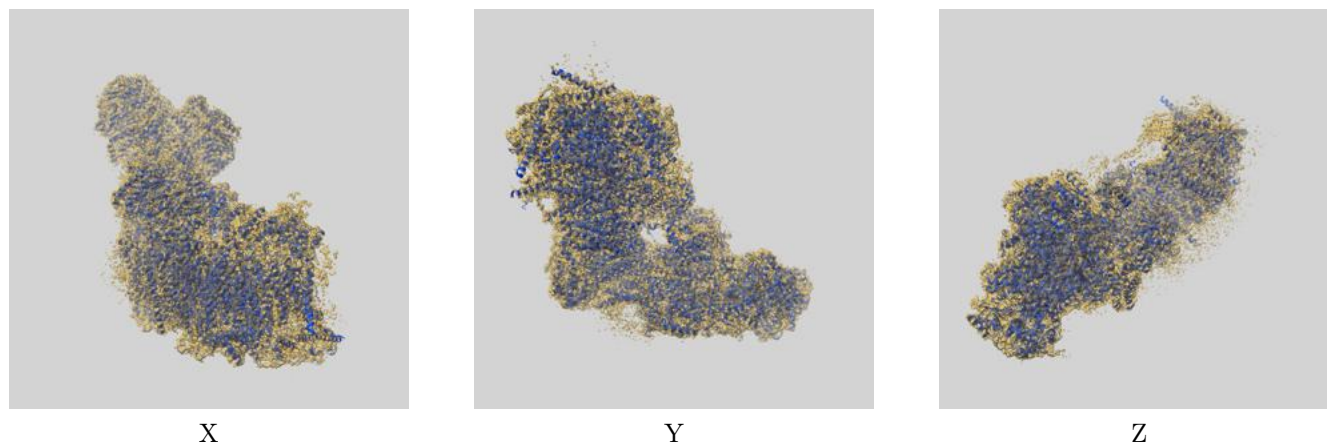
## 8 Fourier-Shell correlation ⓘ

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

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

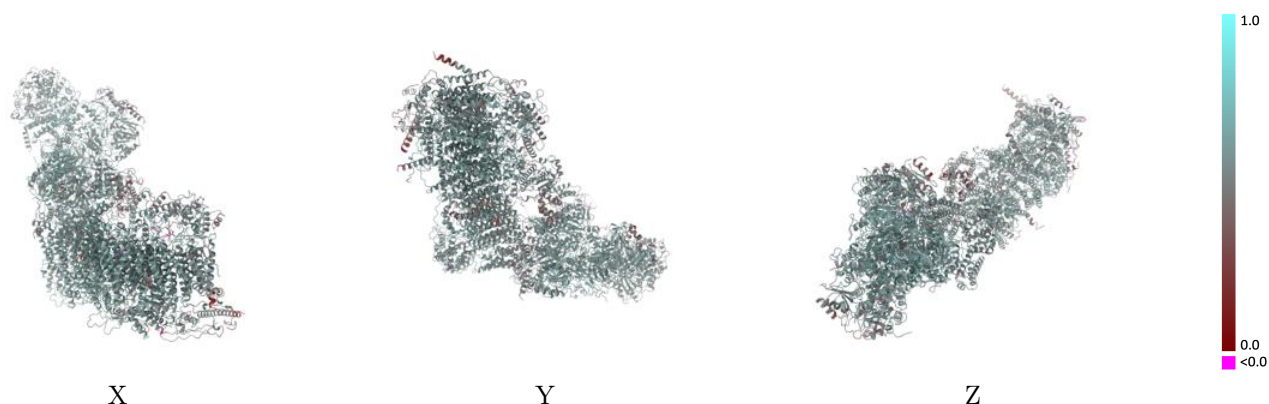
This section contains information regarding the fit between EMDB map EMD-31644 and PDB model 7V2F. Per-residue inclusion information can be found in section [3](#) on page [20](#).

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



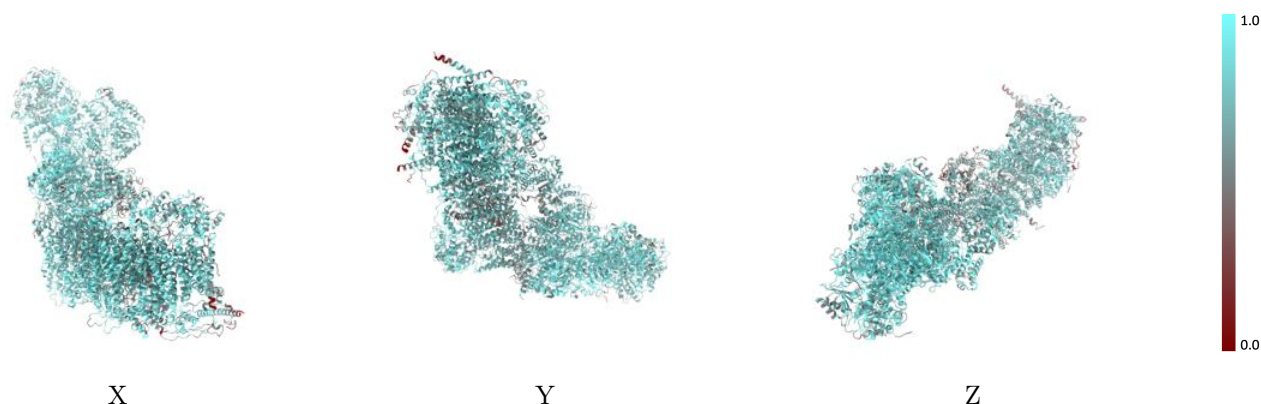
The images above show the 3D surface view of the map at the recommended contour level 0.0232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



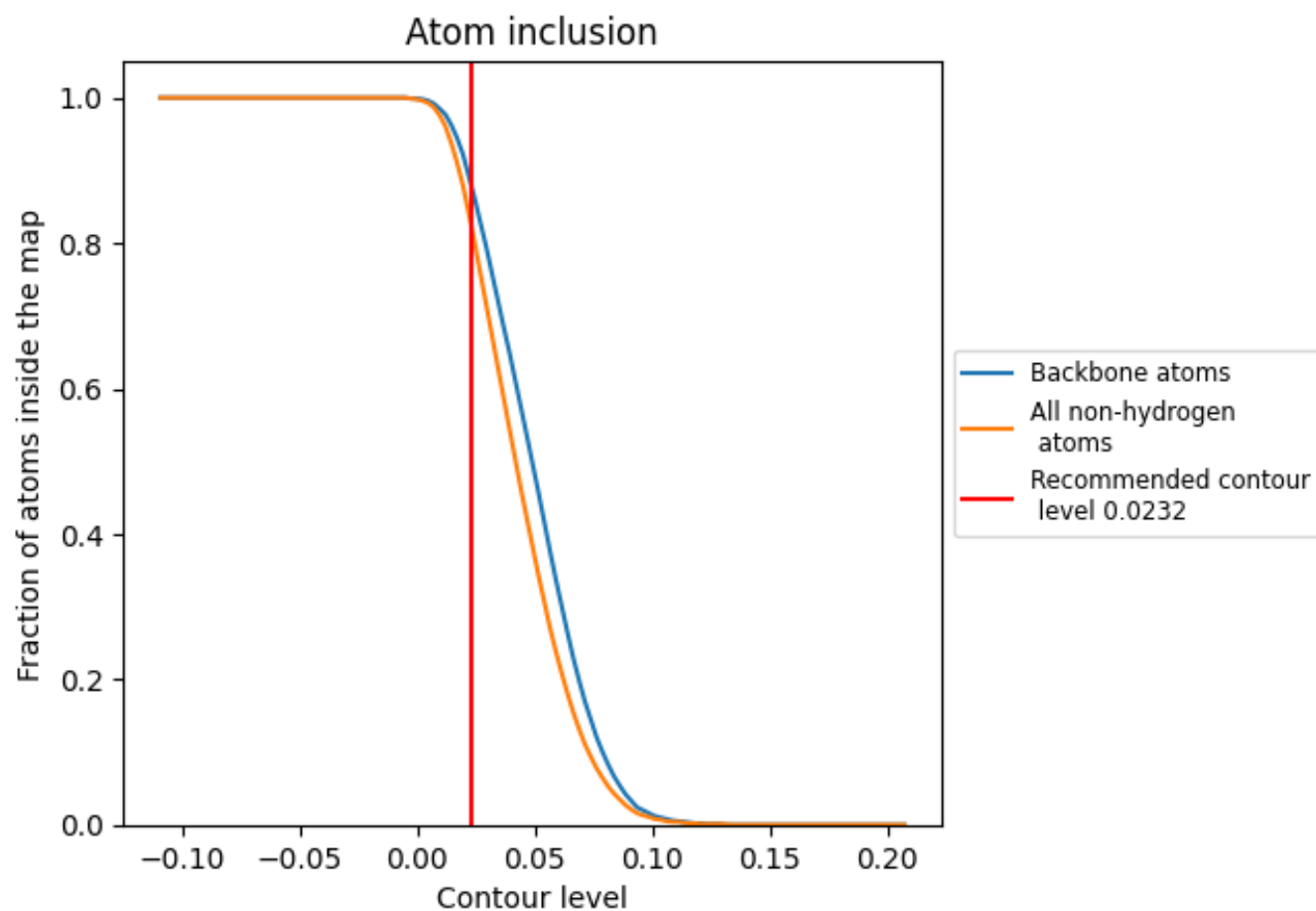
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0232).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.0232) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8200   |  0.5650   |
| A     |  0.8190   |  0.5520   |
| B     |  0.9540   |  0.6180   |
| C     |  0.8820   |  0.6000   |
| E     |  0.8100   |  0.5640   |
| F     |  0.7310   |  0.4900   |
| G     |  0.5360   |  0.4080   |
| H     |  0.8190   |  0.5530   |
| I     |  0.8330   |  0.5750   |
| J     |  0.7970   |  0.5490   |
| K     |  0.7760   |  0.5300   |
| L     |  0.8670   |  0.5890   |
| M     |  0.8710   |  0.5830   |
| N     |  0.8380   |  0.5810   |
| O     |  0.7580  |  0.5270  |
| P     |  0.9320 |  0.6130 |
| Q     |  0.9000 |  0.6110 |
| S     |  0.8910 |  0.5840 |
| T     |  0.8770 |  0.5930 |
| U     |  0.8310 |  0.5590 |
| V     |  0.5440 |  0.5000 |
| W     |  0.8580 |  0.5780 |
| X     |  0.7350 |  0.5190 |
| Y     |  0.6500 |  0.4970 |
| Z     |  0.6060 |  0.4530 |
| a     |  0.8230 |  0.5750 |
| b     |  0.7230 |  0.5090 |
| c     |  0.7890 |  0.5550 |
| d     |  0.7750 |  0.5420 |
| e     |  0.7530 |  0.5460 |
| f     |  0.7540 |  0.5390 |
| g     |  0.8720 |  0.5870 |
| h     |  0.8560 |  0.5750 |
| i     |  0.8850 |  0.6000 |
| j     |  0.7370 |  0.5440 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| k     |  0.7920 |  0.5650 |
| l     |  0.8090 |  0.5700 |
| m     |  0.7710 |  0.5510 |
| n     |  0.7090 |  0.5310 |
| o     |  0.7870 |  0.5530 |
| p     |  0.7980 |  0.5470 |
| r     |  0.8870 |  0.5990 |
| s     |  0.8580 |  0.5870 |
| u     |  0.8510 |  0.5750 |
| v     |  0.6940 |  0.4830 |
| w     |  0.8070 |  0.5520 |