



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:52 AM UTC

PDB ID : 7W4K / pdb\_00007w4k  
EMDB ID : EMD-32306  
Title : Deactive state CI from Q1-NADH dataset, Subclass 2  
Authors : Gu, J.; Yang, M.  
Deposited on : 2021-11-28  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

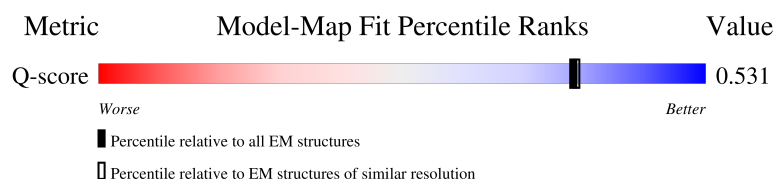
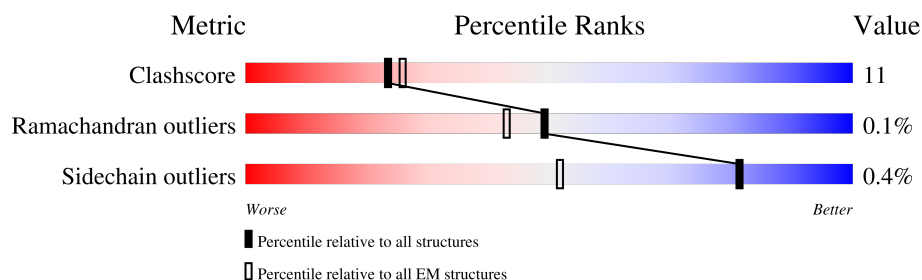
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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                       | 15020 ( 2.70 - 3.70 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | A     | 433    | <div> <div>13%</div> <div>70%</div> <div>29%</div> <div>.</div> </div> |
| 2   | B     | 176    | <div> <div>77%</div> <div>23%</div> </div>                             |
| 3   | C     | 156    | <div> <div>81%</div> <div>19%</div> <div>.</div> </div>                |
| 4   | E     | 115    | <div> <div>13%</div> <div>75%</div> <div>25%</div> </div>              |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | F     | 86     |                  |
| 6   | G     | 88     |                  |
| 6   | X     | 88     |                  |
| 7   | H     | 112    |                  |
| 8   | I     | 112    |                  |
| 9   | J     | 342    |                  |
| 10  | K     | 43     |                  |
| 11  | L     | 125    |                  |
| 12  | M     | 690    |                  |
| 13  | N     | 144    |                  |
| 14  | O     | 217    |                  |
| 15  | P     | 208    |                  |
| 16  | Q     | 430    |                  |
| 17  | S     | 70     |                  |
| 18  | T     | 96     |                  |
| 19  | U     | 83     |                  |
| 20  | V     | 140    |                  |
| 21  | W     | 142    |                  |
| 22  | Y     | 70     |                  |
| 23  | Z     | 84     |                  |
| 24  | a     | 140    |                  |
| 25  | b     | 126    |                  |
| 26  | c     | 156    |                  |
| 27  | d     | 175    |                  |
| 28  | e     | 107    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | f     | 49     |                  |
| 30  | g     | 122    |                  |
| 31  | h     | 105    |                  |
| 32  | i     | 347    |                  |
| 33  | j     | 115    |                  |
| 34  | k     | 98     |                  |
| 35  | l     | 603    |                  |
| 36  | m     | 175    |                  |
| 37  | n     | 56     |                  |
| 38  | o     | 128    |                  |
| 39  | p     | 178    |                  |
| 40  | r     | 459    |                  |
| 41  | s     | 318    |                  |
| 42  | u     | 171    |                  |
| 43  | v     | 124    |                  |
| 44  | w     | 320    |                  |

## 2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66374 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     |
|     |       |          | 3314  | 2094 | 590 | 610 | 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     |
|     |       |          | 672   | 425 | 122 | 123 | 2 |         |       |

- Molecule 6 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | G     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 690   | 446 | 102 | 137 | 5 |         |       |
| 6   | X     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 696   | 449 | 103 | 139 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 586 | 154 | 163 | 3 |         |       |

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

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

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | J     | 297      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2355  | 1512 | 421 | 414 | 8 |         |       |

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

| 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 Complex I-30kD.

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

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | Q     | 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   | 0       | 0     |
|     |       |          | 640   | 415 | 110 | 115 |         |       |

- 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     |
|     |       |          | 1015  | 648 | 171 | 190 | 6 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1173  | 755 | 203 | 206 | 9 |         |       |

- Molecule 22 is a protein called Complex I-AGGG.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 22  | Y     | 70       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 597   | 392 | 98 | 106 | 1 |         |       |

- Molecule 23 is a protein called Complex I-B12.

| 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 Complex I-SGDH.

| 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 Complex I-B17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | b     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 870   | 569 | 158 | 142 | 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     |
|     |       |          | 1311  | 851 | 213 | 239 | 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     |
|     |       |          | 2706  | 1780 | 420 | 460 | 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     |
|     |       |          | 4782  | 3172 | 740 | 819 | 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     |
|     |       |          | 948   | 636 | 138 | 166 | 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     |
|     |       |          | 466   | 305 | 84 | 76 | 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   | S | 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     |
|     |       |          | 1529  | 979 | 277 | 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 |         |       |

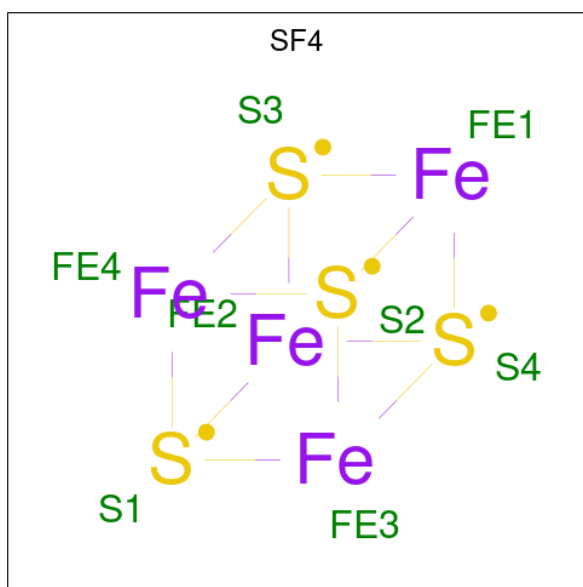
- Molecule 43 is a protein called Complex I-B18.

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

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

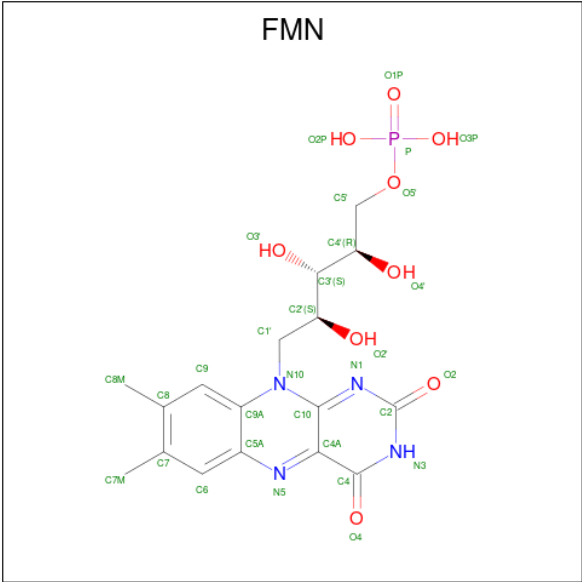
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44  | w     | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2579  | 1642 | 438 | 489 | 10 |         |       |

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



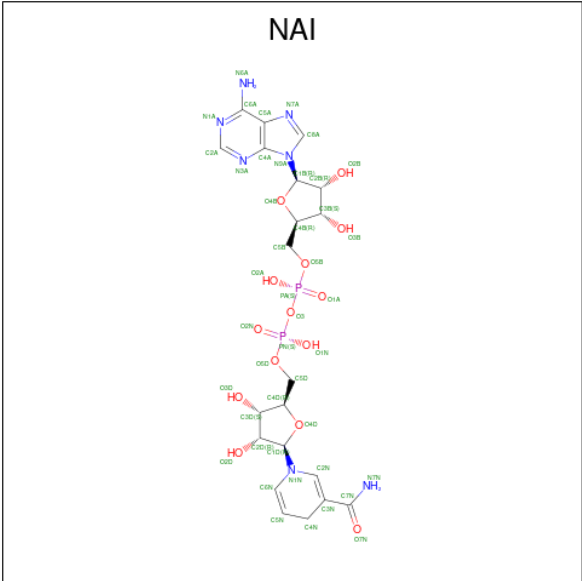
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 45  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 45  | B     | 1        | Total | Fe | S | 0       |
|     |       |          | 8  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

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



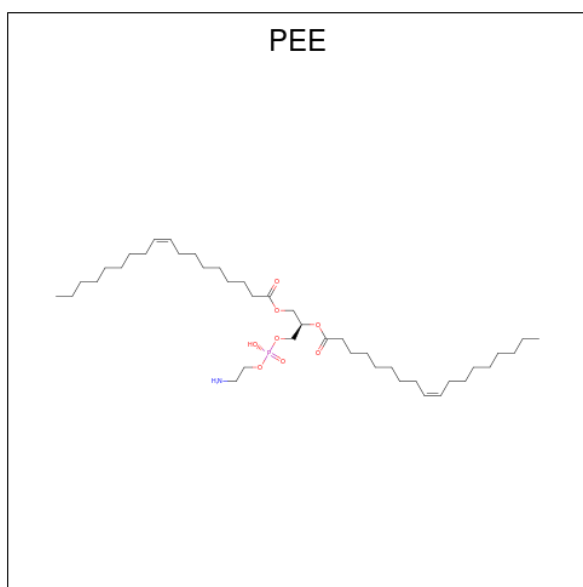
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 46  | A     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

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



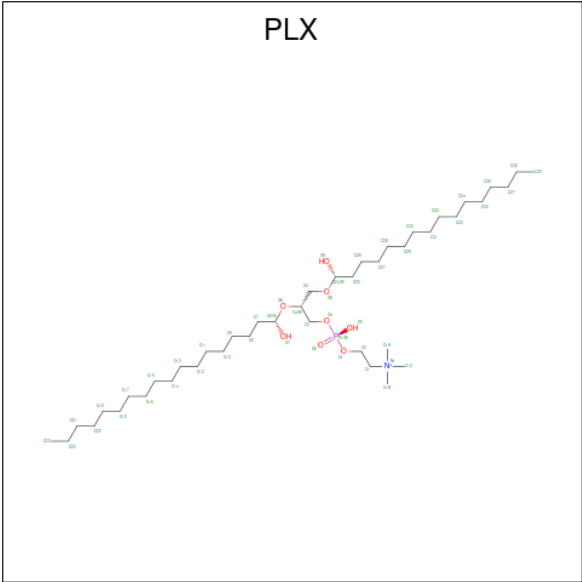
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 47  | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |

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



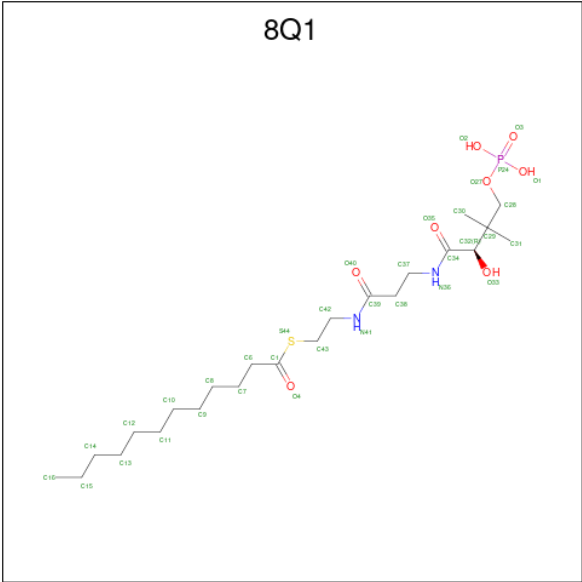
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 48  | Q     | 1        | Total | C  | N | O | P | 0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

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



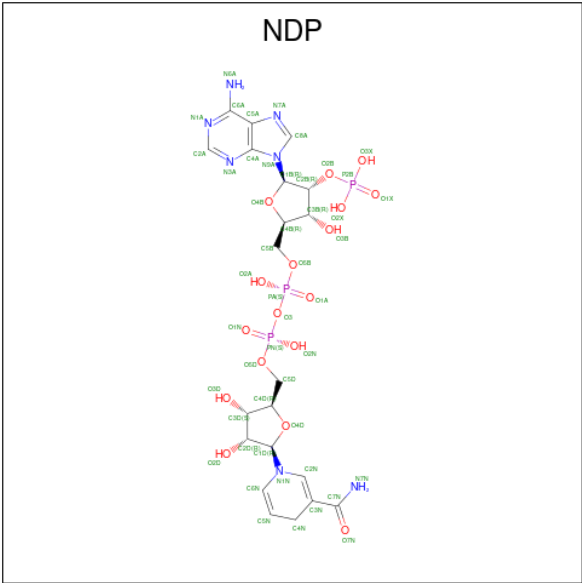
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 49  | C     | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 49  | a     | 1        | Total | C  | N | O | P | 0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

- Molecule 50 is 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 |         |

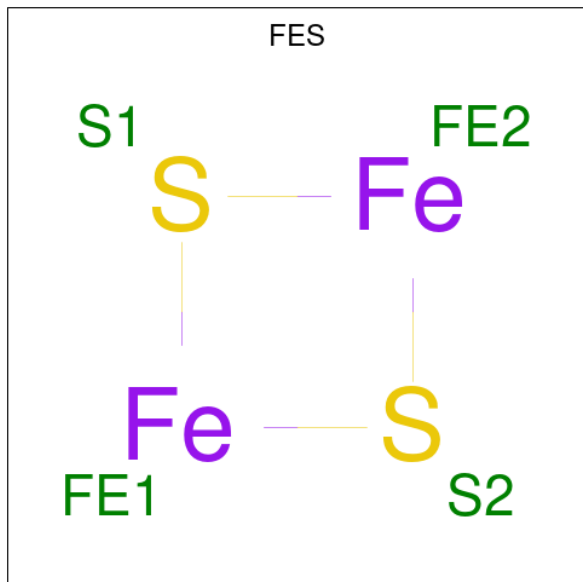
- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| 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 |         |

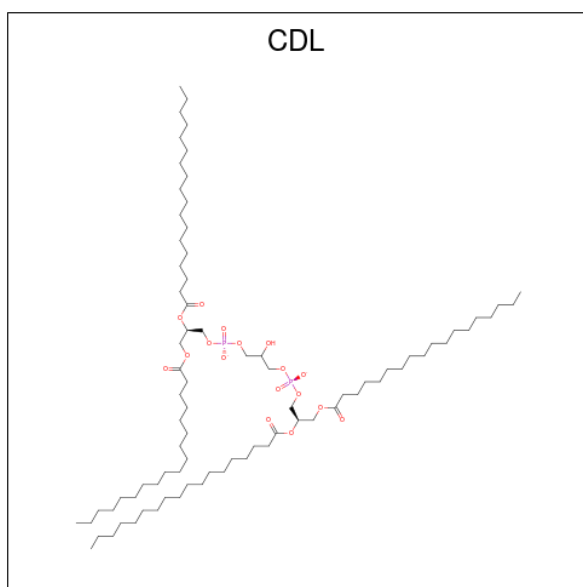
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula:  $\text{Mg}$ ) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ) (labeled as "Ligand of Interest" by depositor).

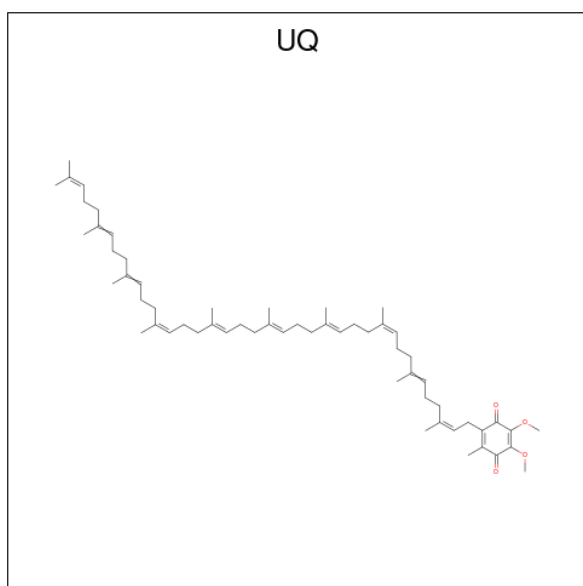
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 54  | T     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 55 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).



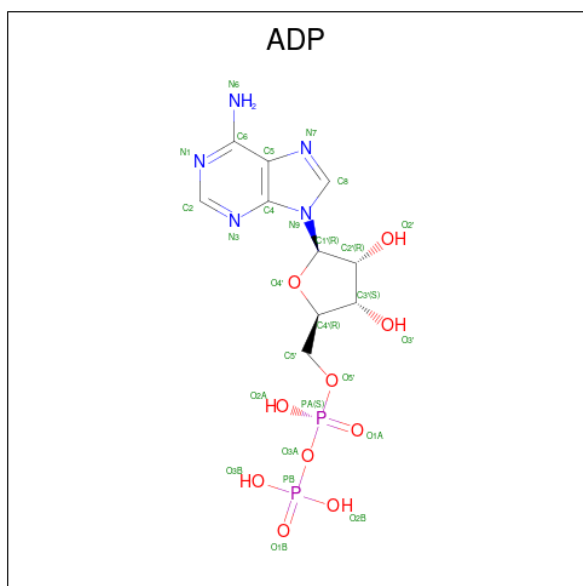
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
|     |       |          | Total | C  | O  | P |         |
| 55  | a     | 1        | 91    | 72 | 17 | 2 | 0       |
| 55  | i     | 1        | 100   | 81 | 17 | 2 | 0       |
| 55  | l     | 1        | 100   | 81 | 17 | 2 | 0       |

- 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).

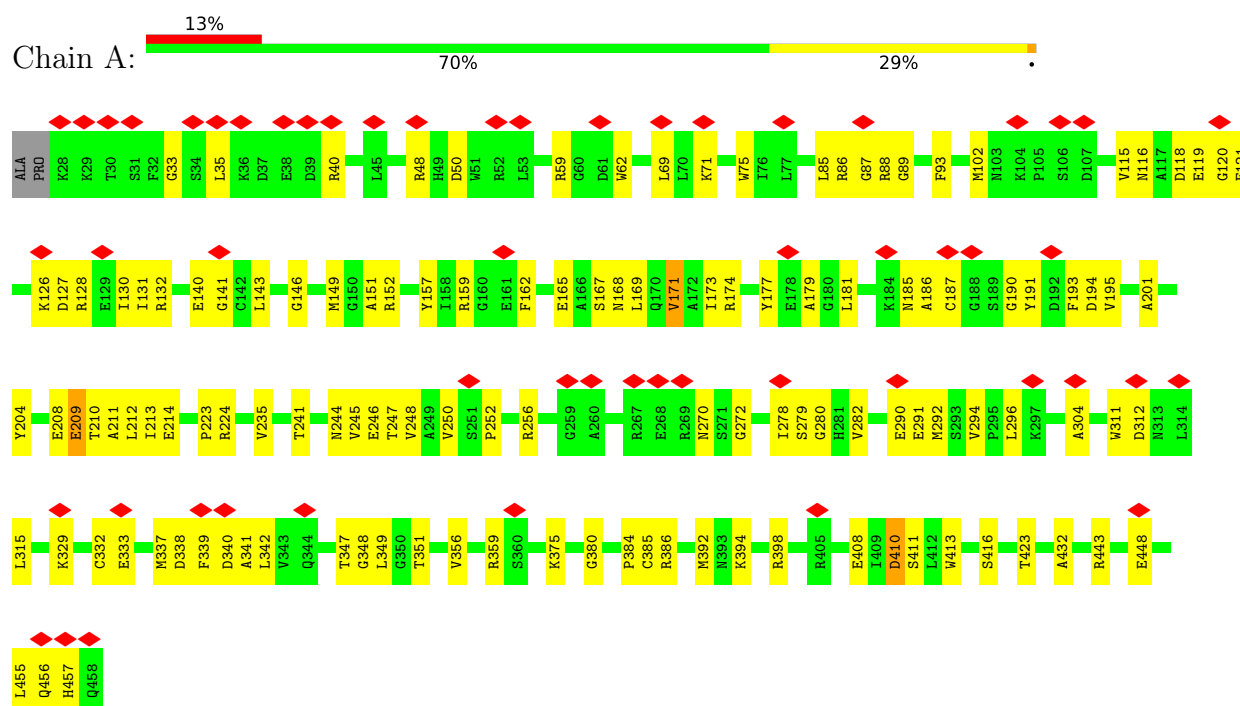


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 57  | w     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 27    | 10 | 5 | 10 | 2 |         |

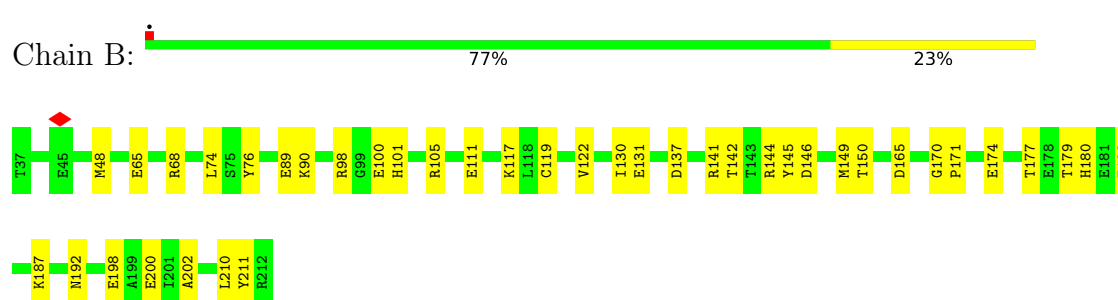
### 3 Residue-property plots

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.

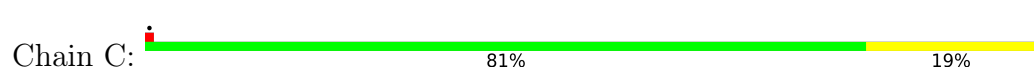
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

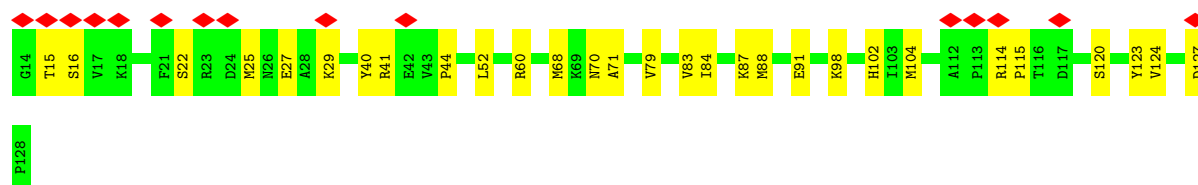
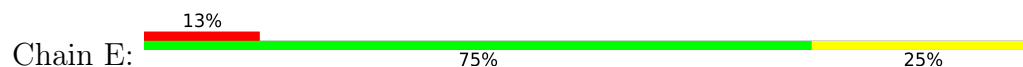


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

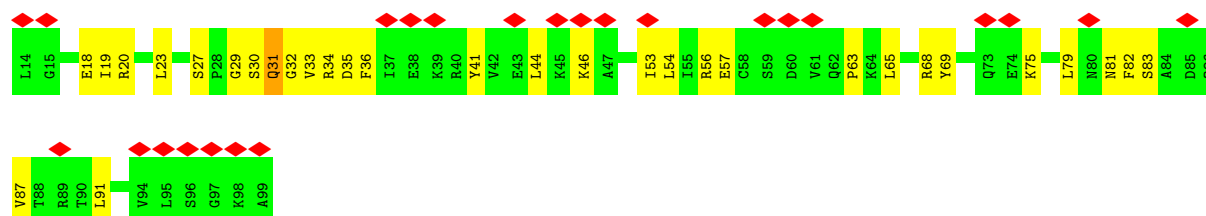




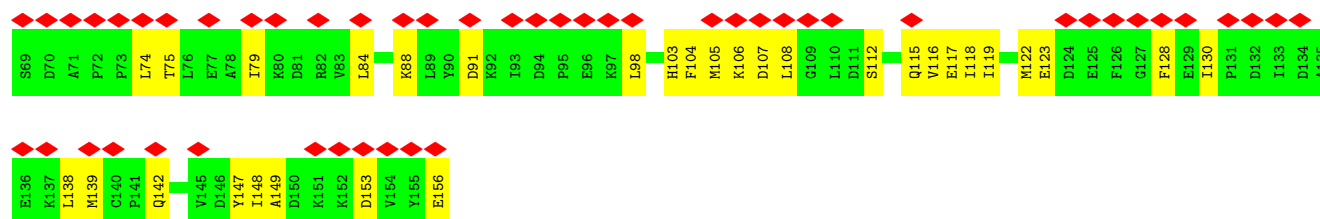
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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



- Molecule 6: Acyl carrier protein

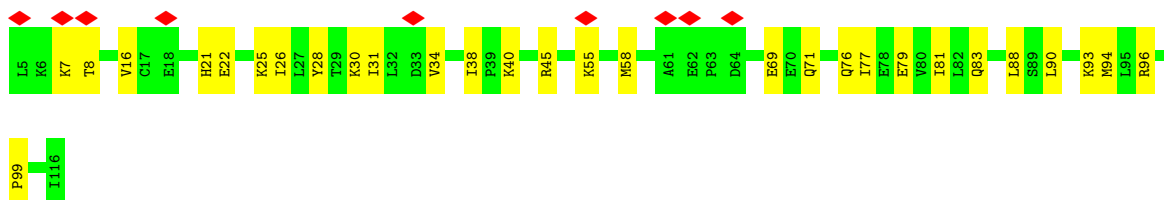


- Molecule 6: Acyl carrier protein



- Molecule 7: Complex I subunit B13

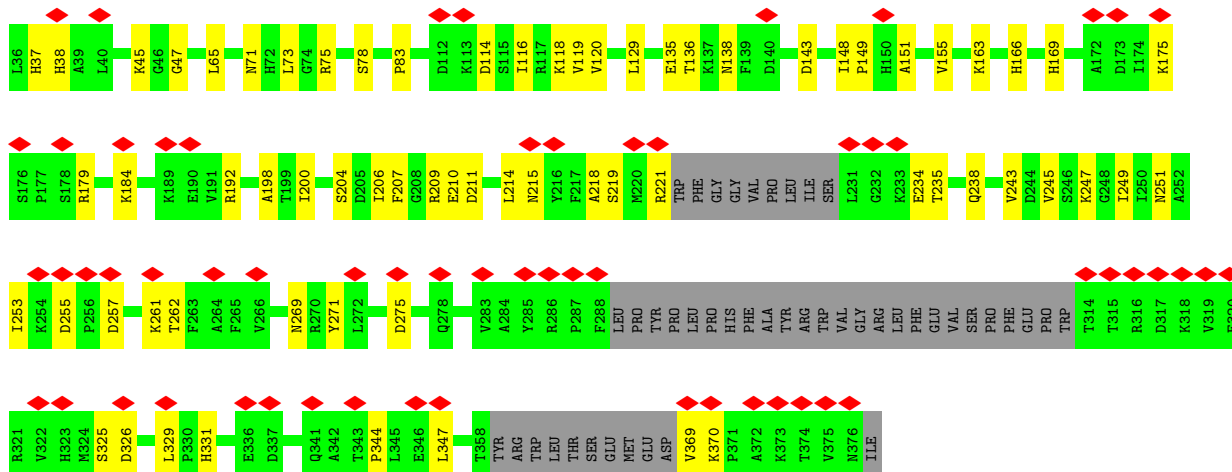




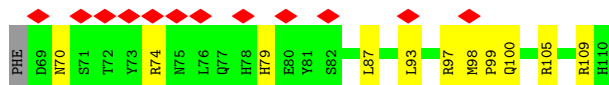
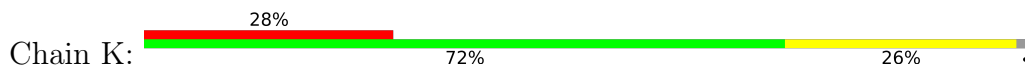
- Molecule 8: Complex I-B14.5a



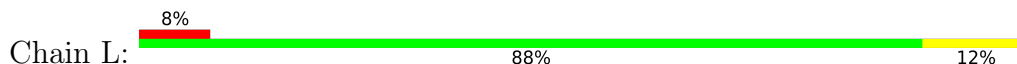
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



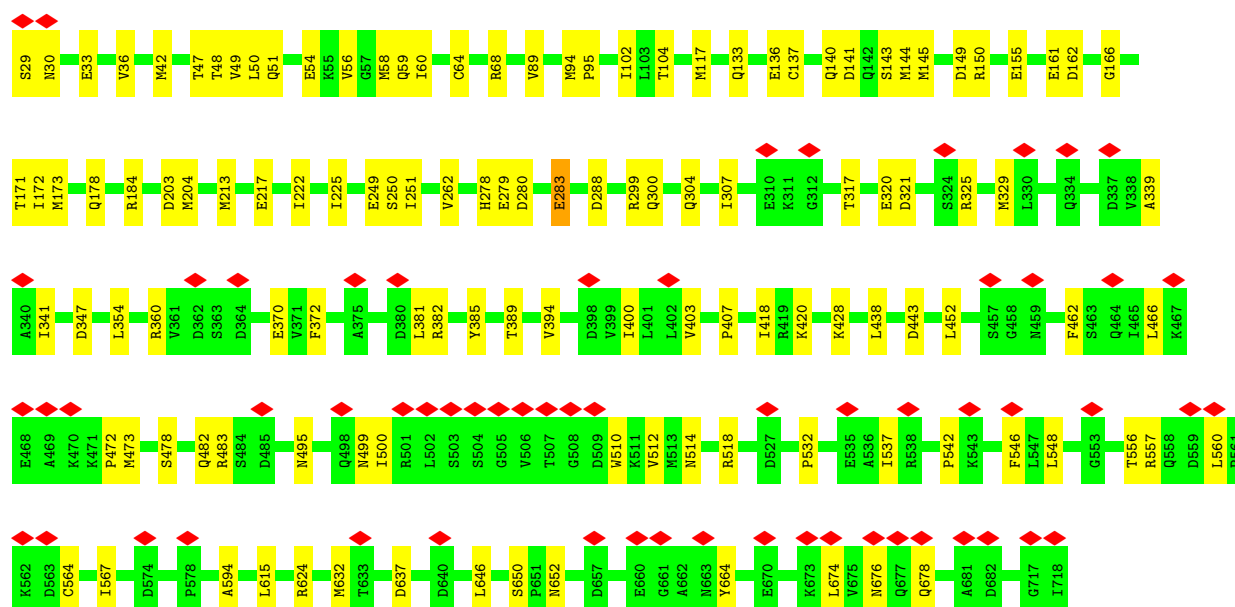
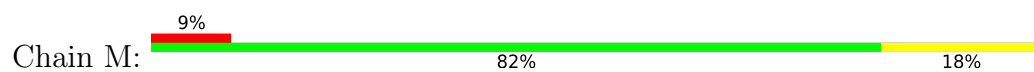
- Molecule 10: Complex I-9kD



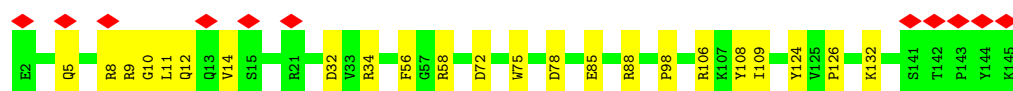
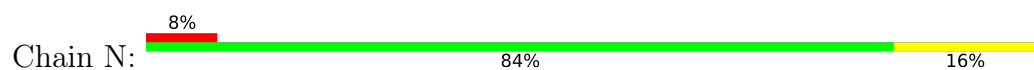
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



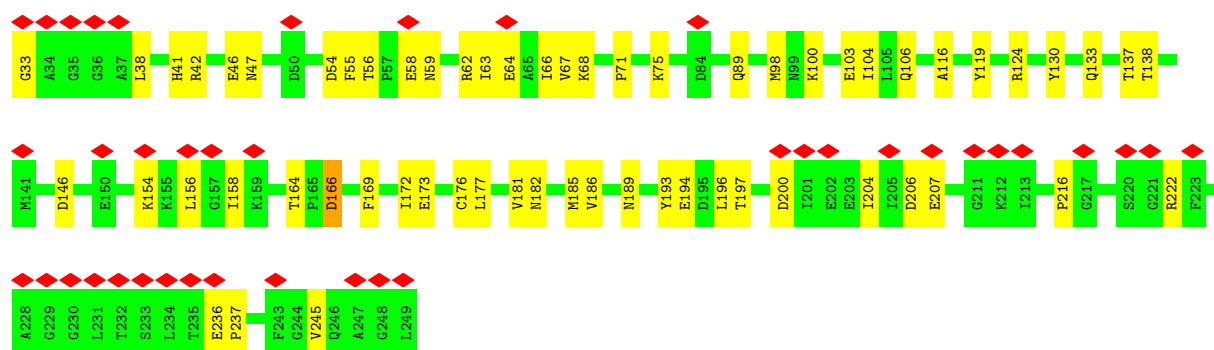
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



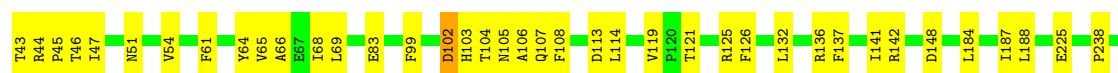
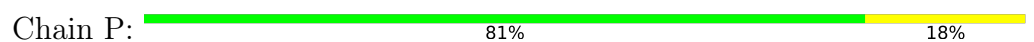
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



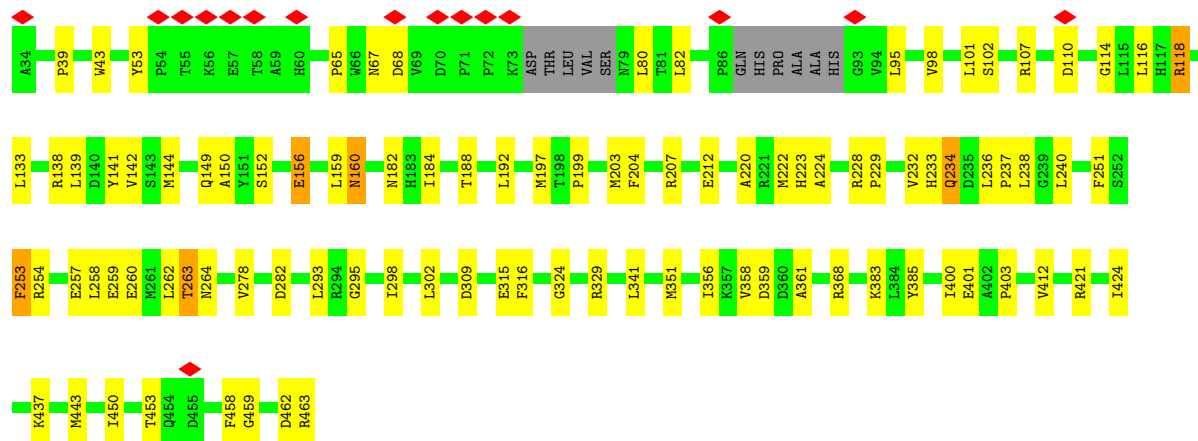
- Molecule 15: Complex I-30kD





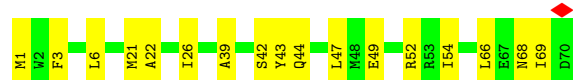
• Molecule 16: Complex I-49kD

Chain Q: 75% 21%



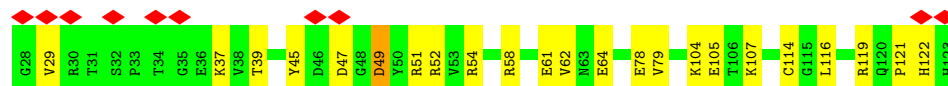
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 76% 24%



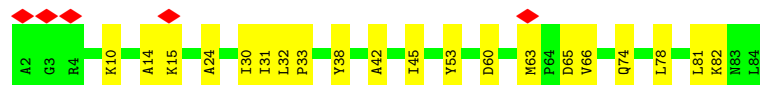
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T: 10% 76% 23%



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

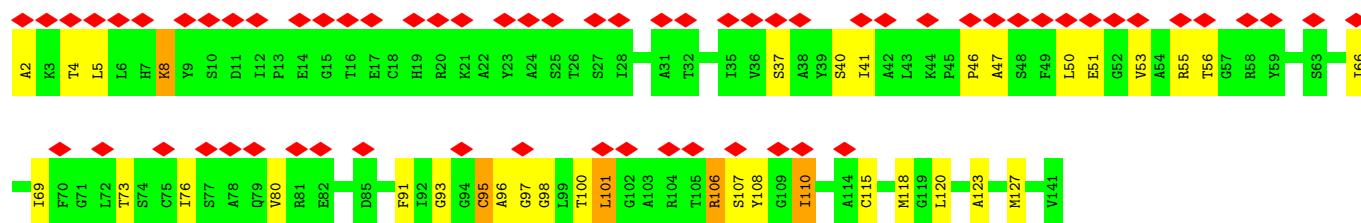
Chain U: 6% 76% 24%



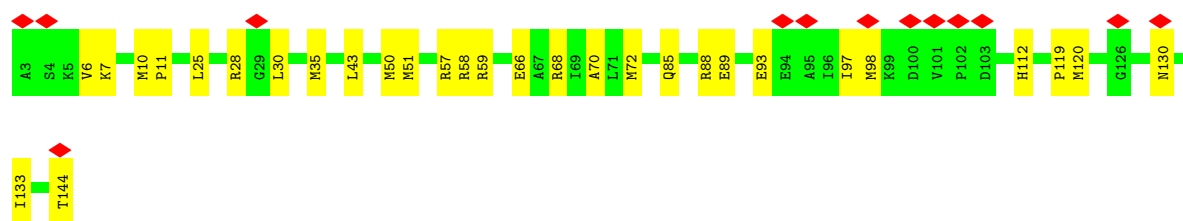
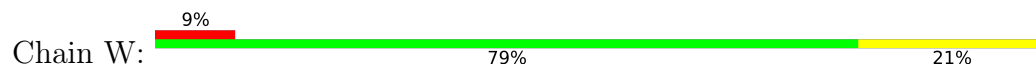
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 46% 74% 22%

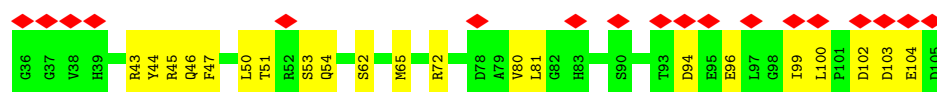




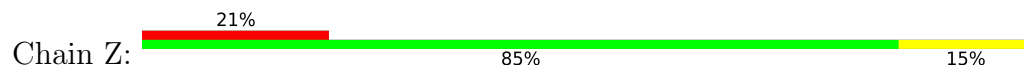
• Molecule 21: Complex I-B16.6



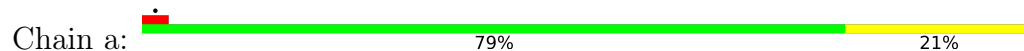
• Molecule 22: Complex I-AGGG



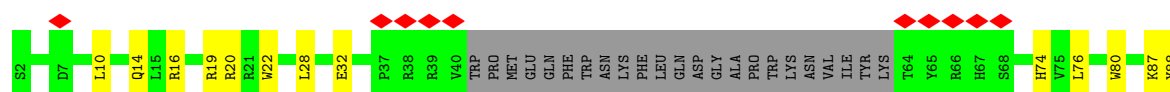
• Molecule 23: Complex I-B12

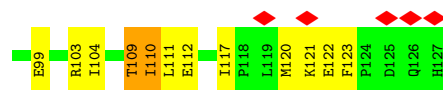


• Molecule 24: Complex I-SGDH

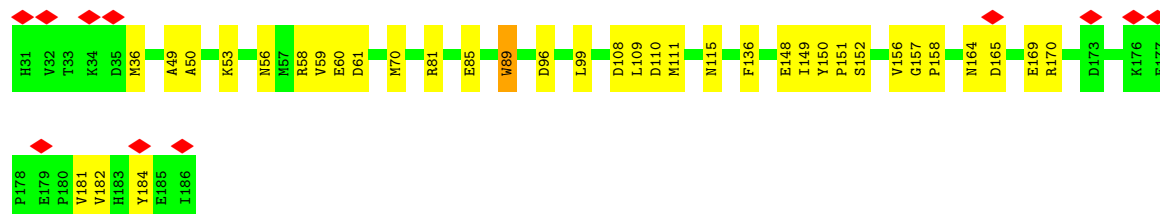
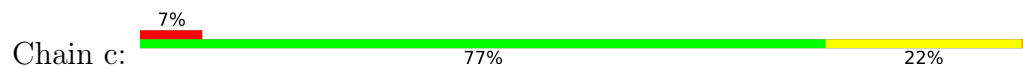


• Molecule 25: Complex I-B17

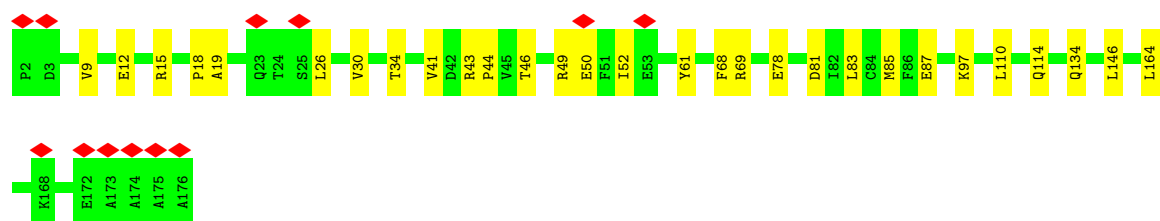
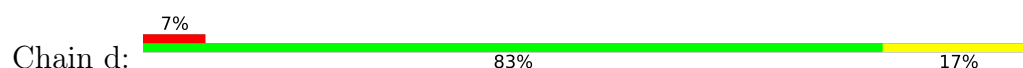




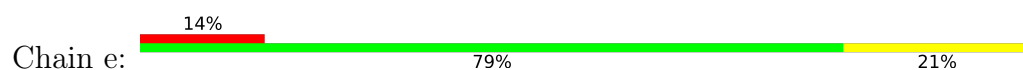
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



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



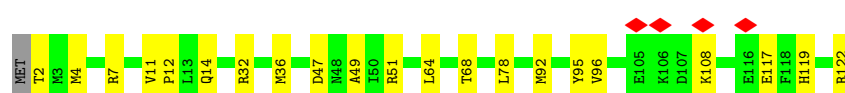
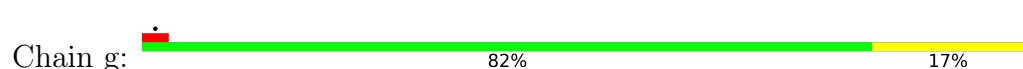
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



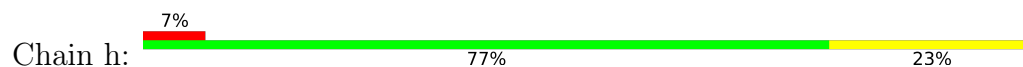
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



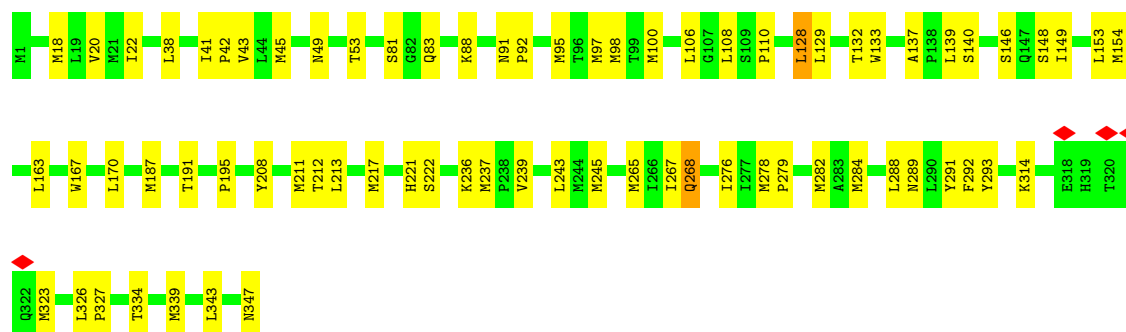
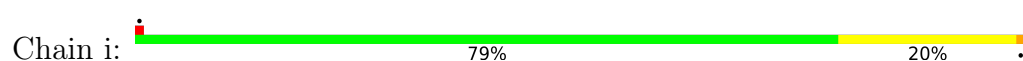
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



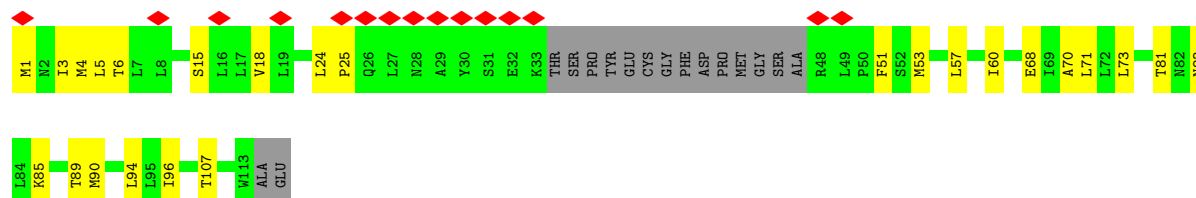
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



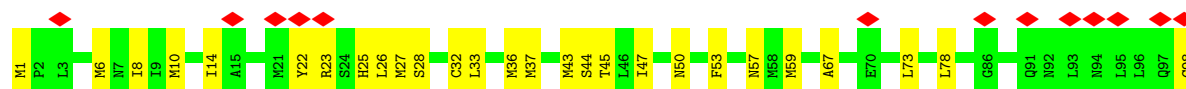
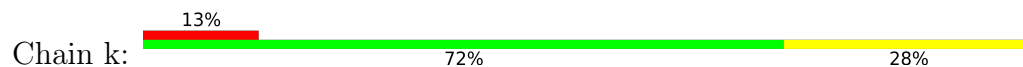
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



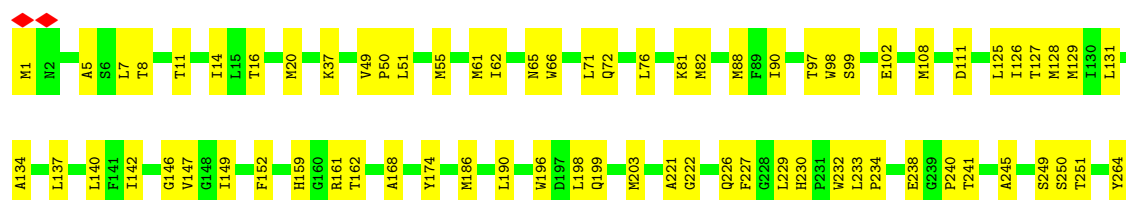
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

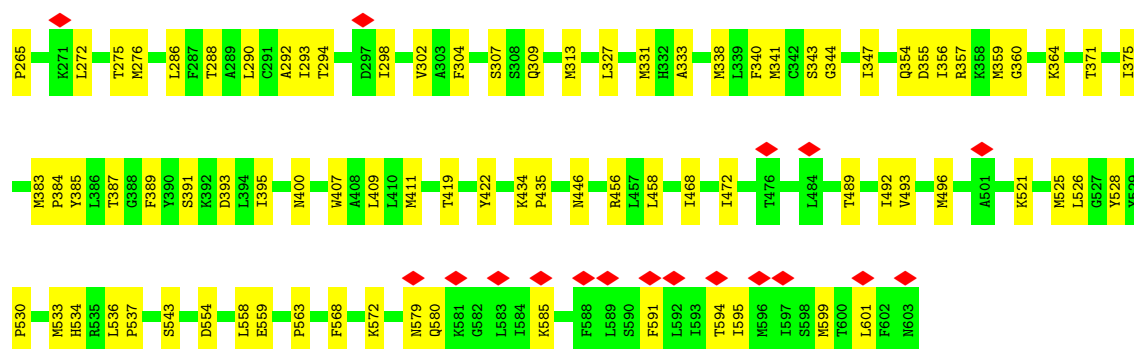


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

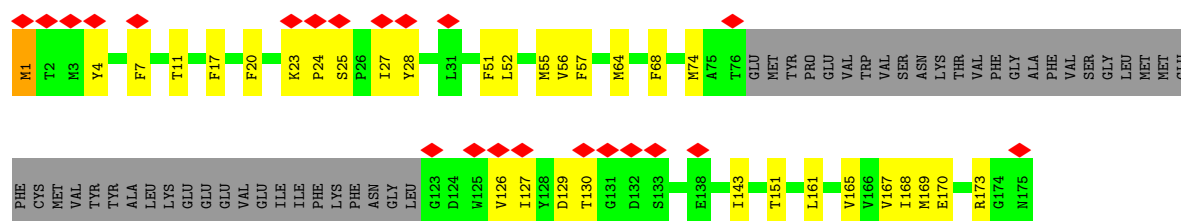


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

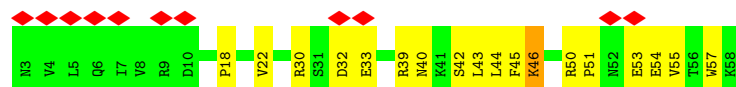




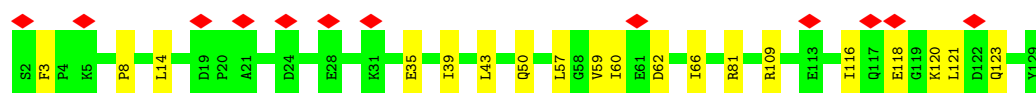
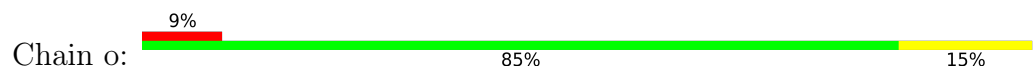
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



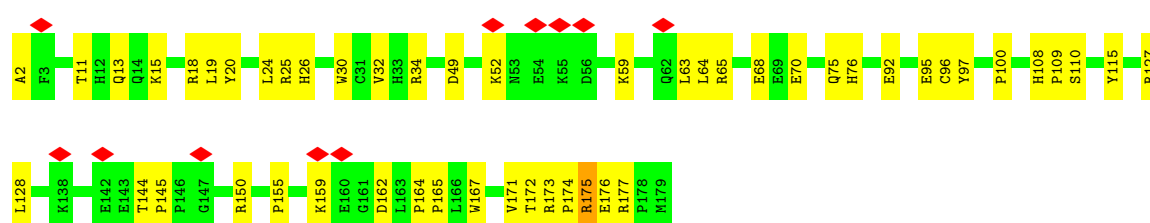
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

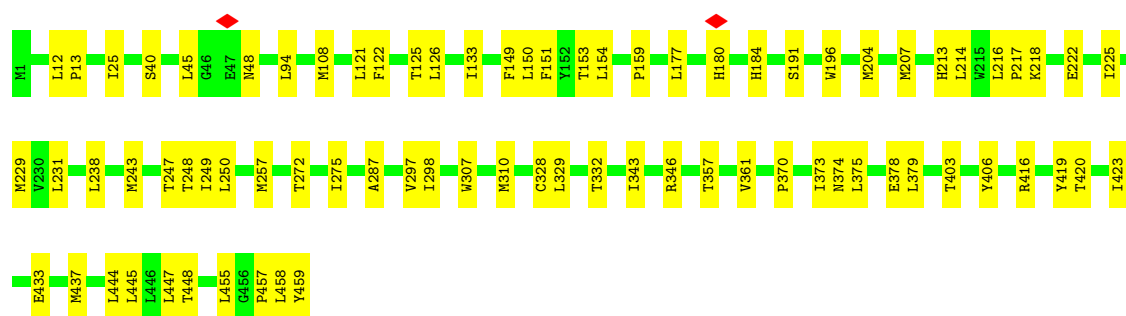


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



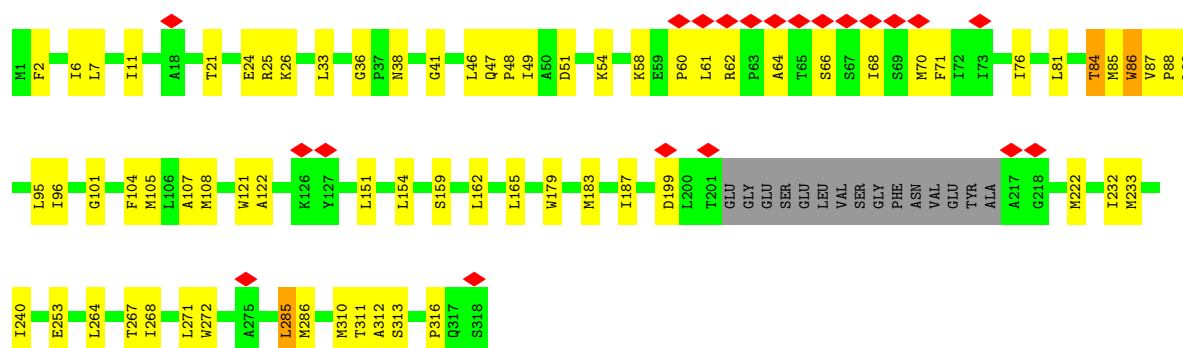
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:  83% 17%



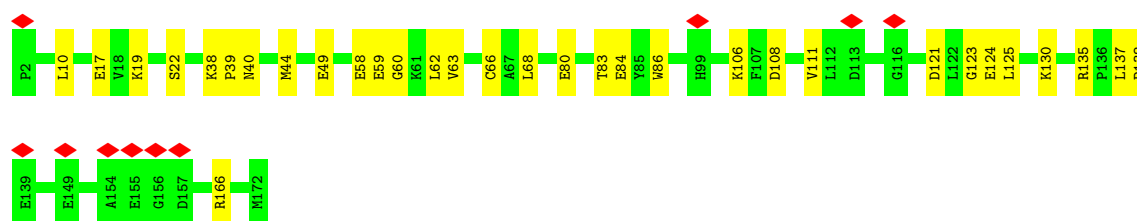
• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s:  7% 73% 21% 5%



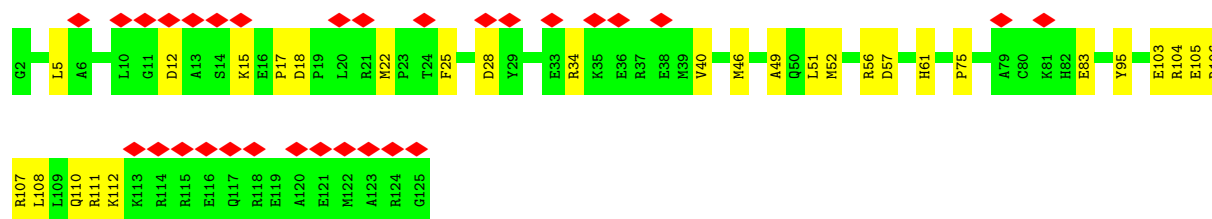
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u:  6% 81% 19%

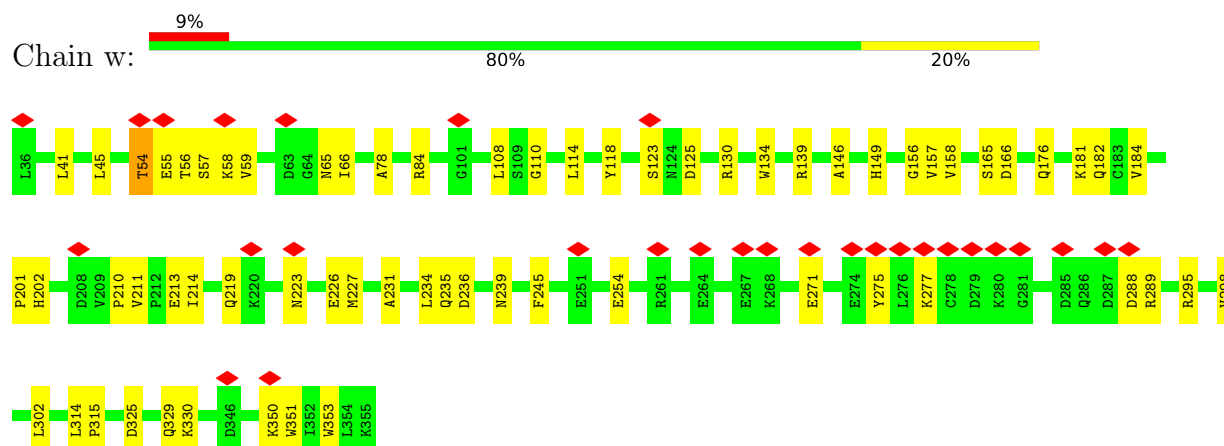


• Molecule 43: Complex I-B18

Chain v:  24% 77% 23%



- 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             | 23715                                   | 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                    | 0.230                                   | Depositor |
| Minimum map value                    | -0.103                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.0282                                  | Depositor |
| Map size ( $\text{\AA}$ )            | 333.7616, 333.7616, 333.7616            | wwPDB     |
| Map dimensions                       | 304, 304, 304                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.0979, 1.0979, 1.0979                  | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.18         | 0/3389        | 0.40        | 2/4579 (0.0%) |
| 2   | B     | 0.16         | 0/1443        | 0.29        | 0/1952        |
| 3   | C     | 0.19         | 0/1279        | 0.49        | 2/1730 (0.1%) |
| 4   | E     | 0.13         | 0/995         | 0.30        | 0/1340        |
| 5   | F     | 0.18         | 0/683         | 0.48        | 2/922 (0.2%)  |
| 6   | G     | 0.17         | 0/702         | 0.31        | 0/952         |
| 6   | X     | 0.13         | 0/708         | 0.35        | 0/959         |
| 7   | H     | 0.21         | 0/925         | 0.45        | 0/1253        |
| 8   | I     | 0.14         | 0/798         | 0.35        | 0/1079        |
| 9   | J     | 0.12         | 0/2407        | 0.30        | 0/3249        |
| 10  | K     | 0.09         | 0/365         | 0.22        | 0/493         |
| 11  | L     | 0.15         | 0/1039        | 0.28        | 0/1403        |
| 12  | M     | 0.13         | 0/5384        | 0.30        | 0/7295        |
| 13  | N     | 0.12         | 0/1245        | 0.30        | 0/1694        |
| 14  | O     | 0.13         | 0/1711        | 0.32        | 0/2328        |
| 15  | P     | 0.20         | 0/1789        | 0.41        | 1/2436 (0.0%) |
| 16  | Q     | 0.22         | 0/3451        | 0.48        | 5/4672 (0.1%) |
| 17  | S     | 0.17         | 0/582         | 0.38        | 0/783         |
| 18  | T     | 0.12         | 0/755         | 0.29        | 0/1018        |
| 19  | U     | 0.17         | 0/661         | 0.48        | 2/909 (0.2%)  |
| 20  | V     | 0.28         | 1/1036 (0.1%) | 0.48        | 0/1404        |
| 21  | W     | 0.16         | 0/1204        | 0.31        | 0/1624        |
| 22  | Y     | 0.22         | 0/623         | 0.49        | 0/853         |
| 23  | Z     | 0.13         | 0/695         | 0.28        | 0/939         |
| 24  | a     | 0.16         | 0/1199        | 0.35        | 0/1623        |
| 25  | b     | 0.21         | 0/897         | 0.56        | 3/1221 (0.2%) |
| 26  | c     | 0.19         | 0/1367        | 0.39        | 1/1870 (0.1%) |
| 27  | d     | 0.15         | 0/1494        | 0.32        | 0/2015        |
| 28  | e     | 0.16         | 0/916         | 0.38        | 0/1246        |
| 29  | f     | 0.19         | 0/350         | 0.44        | 0/473         |
| 30  | g     | 0.16         | 0/1031        | 0.31        | 0/1394        |
| 31  | h     | 0.14         | 0/889         | 0.29        | 0/1190        |



| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 32  | i     | 0.18         | 0/2769         | 0.37        | 0/3763          |
| 33  | j     | 0.19         | 0/819          | 0.38        | 0/1117          |
| 34  | k     | 0.19         | 0/759          | 0.33        | 0/1029          |
| 35  | l     | 0.17         | 0/4911         | 0.38        | 0/6679          |
| 36  | m     | 0.19         | 0/970          | 0.40        | 0/1316          |
| 37  | n     | 0.19         | 0/478          | 0.49        | 0/647           |
| 38  | o     | 0.15         | 0/1092         | 0.37        | 0/1481          |
| 39  | p     | 0.18         | 0/1584         | 0.41        | 0/2147          |
| 40  | r     | 0.17         | 0/3723         | 0.34        | 0/5078          |
| 41  | s     | 0.20         | 0/2464         | 0.45        | 1/3369 (0.0%)   |
| 42  | u     | 0.14         | 0/1436         | 0.35        | 0/1938          |
| 43  | v     | 0.15         | 0/1052         | 0.35        | 0/1411          |
| 44  | w     | 0.13         | 0/2639         | 0.31        | 0/3576          |
| All | All   | 0.17         | 1/66708 (0.0%) | 0.37        | 19/90449 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | V     | 8   | LYS  | CE-NZ | -5.03 | 1.34        | 1.49     |

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | Q     | 233 | HIS  | N-CA-C | 10.07 | 122.26      | 111.28   |
| 3   | C     | 124 | MET  | CA-C-N | 8.20  | 128.14      | 119.85   |
| 3   | C     | 124 | MET  | C-N-CA | 8.20  | 128.14      | 119.85   |
| 15  | P     | 102 | ASP  | N-CA-C | 7.99  | 120.07      | 111.36   |
| 25  | b     | 111 | LEU  | N-CA-C | 7.81  | 119.79      | 111.28   |
| 25  | b     | 109 | THR  | N-CA-C | 7.60  | 119.64      | 111.36   |
| 16  | Q     | 234 | GLN  | N-CA-C | 7.39  | 124.39      | 114.12   |
| 41  | s     | 86  | TRP  | N-CA-C | 7.01  | 119.78      | 111.71   |
| 1   | A     | 250 | VAL  | N-CA-C | 6.76  | 117.54      | 110.72   |
| 26  | c     | 89  | TRP  | N-CA-C | 6.60  | 119.47      | 111.82   |
| 16  | Q     | 262 | LEU  | N-CA-C | 6.30  | 121.63      | 113.88   |
| 25  | b     | 112 | GLU  | N-CA-C | 5.72  | 117.19      | 111.07   |
| 1   | A     | 209 | GLU  | N-CA-C | 5.62  | 117.08      | 111.07   |
| 19  | U     | 63  | MET  | CA-C-N | 5.47  | 125.12      | 119.05   |
| 19  | U     | 63  | MET  | C-N-CA | 5.47  | 125.12      | 119.05   |
| 16  | Q     | 238 | LEU  | N-CA-C | 5.29  | 117.05      | 111.28   |
| 16  | Q     | 142 | VAL  | N-CA-C | -5.18 | 107.78      | 112.96   |
| 5   | F     | 27  | SER  | CA-C-N | 5.10  | 124.41      | 118.85   |
| 5   | F     | 27  | SER  | C-N-CA | 5.10  | 124.41      | 118.85   |

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     | 3314  | 0        | 3273     | 120     | 0            |
| 2   | B     | 1412  | 0        | 1363     | 41      | 0            |
| 3   | C     | 1248  | 0        | 1254     | 29      | 0            |
| 4   | E     | 971   | 0        | 975      | 22      | 0            |
| 5   | F     | 672   | 0        | 674      | 31      | 0            |
| 6   | G     | 690   | 0        | 669      | 33      | 0            |
| 6   | X     | 696   | 0        | 680      | 34      | 0            |
| 7   | H     | 906   | 0        | 946      | 32      | 0            |
| 8   | I     | 780   | 0        | 808      | 15      | 0            |
| 9   | J     | 2355  | 0        | 2398     | 44      | 0            |
| 10  | K     | 355   | 0        | 329      | 12      | 0            |
| 11  | L     | 1016  | 0        | 1016     | 16      | 0            |
| 12  | M     | 5296  | 0        | 5326     | 86      | 0            |
| 13  | N     | 1204  | 0        | 1162     | 20      | 0            |
| 14  | O     | 1671  | 0        | 1673     | 53      | 0            |
| 15  | P     | 1738  | 0        | 1693     | 41      | 0            |
| 16  | Q     | 3377  | 0        | 3318     | 75      | 0            |
| 17  | S     | 567   | 0        | 565      | 15      | 0            |
| 18  | T     | 741   | 0        | 702      | 20      | 0            |
| 19  | U     | 640   | 0        | 635      | 20      | 0            |
| 20  | V     | 1015  | 0        | 1018     | 39      | 0            |
| 21  | W     | 1173  | 0        | 1166     | 39      | 0            |
| 22  | Y     | 597   | 0        | 537      | 21      | 0            |
| 23  | Z     | 674   | 0        | 643      | 14      | 0            |
| 24  | a     | 1165  | 0        | 1174     | 34      | 0            |
| 25  | b     | 870   | 0        | 888      | 30      | 0            |
| 26  | c     | 1311  | 0        | 1204     | 31      | 0            |
| 27  | d     | 1461  | 0        | 1429     | 33      | 0            |
| 28  | e     | 890   | 0        | 837      | 19      | 0            |
| 29  | f     | 342   | 0        | 341      | 14      | 0            |
| 30  | g     | 1000  | 0        | 994      | 21      | 0            |
| 31  | h     | 867   | 0        | 871      | 24      | 0            |
| 32  | i     | 2706  | 0        | 2870     | 67      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | j     | 800   | 0        | 855      | 24      | 0            |
| 34  | k     | 748   | 0        | 799      | 26      | 0            |
| 35  | l     | 4782  | 0        | 4929     | 135     | 0            |
| 36  | m     | 948   | 0        | 960      | 41      | 0            |
| 37  | n     | 466   | 0        | 467      | 26      | 0            |
| 38  | o     | 1062  | 0        | 1072     | 14      | 0            |
| 39  | p     | 1529  | 0        | 1465     | 45      | 0            |
| 40  | r     | 3631  | 0        | 3839     | 60      | 0            |
| 41  | s     | 2394  | 0        | 2508     | 77      | 0            |
| 42  | u     | 1398  | 0        | 1378     | 25      | 0            |
| 43  | v     | 1028  | 0        | 980      | 31      | 0            |
| 44  | w     | 2579  | 0        | 2529     | 56      | 0            |
| 45  | A     | 8     | 0        | 0        | 1       | 0            |
| 45  | B     | 16    | 0        | 0        | 0       | 0            |
| 45  | C     | 8     | 0        | 0        | 1       | 0            |
| 45  | M     | 16    | 0        | 0        | 0       | 0            |
| 46  | A     | 31    | 0        | 19       | 6       | 0            |
| 47  | A     | 44    | 0        | 27       | 5       | 0            |
| 48  | C     | 47    | 0        | 71       | 0       | 0            |
| 48  | Q     | 98    | 0        | 153      | 8       | 0            |
| 48  | U     | 51    | 0        | 82       | 3       | 0            |
| 48  | l     | 92    | 0        | 138      | 5       | 0            |
| 48  | m     | 41    | 0        | 59       | 3       | 0            |
| 48  | r     | 51    | 0        | 82       | 6       | 0            |
| 49  | C     | 52    | 0        | 88       | 2       | 0            |
| 49  | a     | 52    | 0        | 88       | 3       | 0            |
| 49  | i     | 52    | 0        | 88       | 3       | 0            |
| 49  | j     | 52    | 0        | 88       | 3       | 0            |
| 49  | r     | 104   | 0        | 176      | 4       | 0            |
| 50  | G     | 35    | 0        | 0        | 8       | 0            |
| 50  | X     | 35    | 0        | 0        | 4       | 0            |
| 51  | J     | 48    | 0        | 24       | 1       | 0            |
| 52  | M     | 4     | 0        | 0        | 0       | 0            |
| 52  | O     | 4     | 0        | 0        | 0       | 0            |
| 53  | M     | 1     | 0        | 0        | 0       | 0            |
| 54  | T     | 1     | 0        | 0        | 0       | 0            |
| 55  | a     | 91    | 0        | 132      | 6       | 0            |
| 55  | i     | 100   | 0        | 156      | 8       | 0            |
| 55  | l     | 100   | 0        | 156      | 4       | 0            |
| 56  | s     | 28    | 0        | 31       | 5       | 0            |
| 57  | w     | 27    | 0        | 11       | 2       | 0            |
| All | All   | 66374 | 0        | 66881    | 1459    | 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 11.

All (1459) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:112:SER:CB    | 50:G:201:8Q1:O1   | 1.70                     | 1.38              |
| 6:X:112:SER:CB    | 50:X:201:8Q1:O1   | 1.70                     | 1.37              |
| 20:V:4:THR:HG22   | 20:V:8:LYS:NZ     | 1.53                     | 1.22              |
| 47:A:503:NAI:C1B  | 47:A:503:NAI:O4B  | 1.63                     | 1.19              |
| 24:a:106:VAL:HG13 | 37:n:50:ARG:NH2   | 1.56                     | 1.19              |
| 51:J:401:NDP:O4D  | 51:J:401:NDP:C4D  | 1.68                     | 1.18              |
| 41:s:87:VAL:CG2   | 41:s:88:PRO:HD3   | 1.75                     | 1.17              |
| 20:V:66:ILE:HD11  | 20:V:101:LEU:CD2  | 1.77                     | 1.15              |
| 20:V:66:ILE:CD1   | 20:V:101:LEU:HD22 | 1.81                     | 1.10              |
| 1:A:157:TYR:CG    | 1:A:212:LEU:HD11  | 1.87                     | 1.10              |
| 41:s:87:VAL:HG23  | 41:s:88:PRO:HD3   | 1.12                     | 1.07              |
| 1:A:456:GLN:OE1   | 1:A:457:HIS:ND1   | 1.90                     | 1.04              |
| 1:A:278:ILE:HD12  | 1:A:304:ALA:CB    | 1.88                     | 1.03              |
| 27:d:78:GLU:OE1   | 30:g:108:LYS:HB3  | 1.58                     | 1.03              |
| 32:i:149:ILE:HD12 | 32:i:154:MET:HG3  | 1.41                     | 1.02              |
| 1:A:141:GLY:HA2   | 1:A:252:PRO:HG3   | 1.38                     | 1.02              |
| 1:A:278:ILE:HD12  | 1:A:304:ALA:HB2   | 0.98                     | 0.98              |
| 30:g:2:THR:HG21   | 30:g:4:MET:HE2    | 1.45                     | 0.98              |
| 1:A:278:ILE:CD1   | 1:A:304:ALA:HB2   | 1.93                     | 0.97              |
| 35:l:525:MET:HE2  | 35:l:528:TYR:HE1  | 1.27                     | 0.97              |
| 24:a:106:VAL:HG13 | 37:n:50:ARG:HH21  | 1.12                     | 0.96              |
| 7:H:94:MET:HE1    | 7:H:99:PRO:HG3    | 1.46                     | 0.96              |
| 16:Q:236:LEU:HD22 | 16:Q:240:LEU:HD23 | 1.45                     | 0.96              |
| 1:A:127:ASP:OD2   | 1:A:245:VAL:HB    | 1.64                     | 0.96              |
| 6:G:115:GLN:O     | 6:G:119:ILE:HG12  | 1.65                     | 0.95              |
| 44:w:350:LYS:HB3  | 44:w:351:TRP:HE3  | 1.30                     | 0.95              |
| 44:w:350:LYS:HB3  | 44:w:351:TRP:CE3  | 2.01                     | 0.95              |
| 16:Q:282:ASP:OD2  | 16:Q:437:LYS:HE2  | 1.68                     | 0.94              |
| 44:w:66:ILE:O     | 44:w:214:ILE:HD11 | 1.67                     | 0.94              |
| 6:G:112:SER:CB    | 50:G:201:8Q1:P24  | 2.57                     | 0.92              |
| 7:H:31:ILE:HD13   | 7:H:88:LEU:HA     | 1.49                     | 0.92              |
| 19:U:53:TYR:HB2   | 21:W:72:MET:HE1   | 1.52                     | 0.91              |
| 12:M:33:GLU:HB2   | 12:M:42:MET:HE1   | 1.51                     | 0.91              |
| 20:V:98:GLY:HA2   | 20:V:118:MET:SD   | 2.10                     | 0.91              |
| 20:V:4:THR:HG22   | 20:V:8:LYS:HZ1    | 1.25                     | 0.90              |
| 21:W:98:MET:HE3   | 31:h:79:ILE:HG12  | 1.49                     | 0.90              |
| 35:l:90:ILE:HG12  | 35:l:129:MET:HE2  | 1.50                     | 0.90              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:121:GLU:HB2   | 47:A:503:NAI:H42N | 1.54                     | 0.90              |
| 45:C:301:SF4:S4   | 16:Q:223:HIS:CD2  | 2.65                     | 0.89              |
| 41:s:87:VAL:HG23  | 41:s:88:PRO:CD    | 2.01                     | 0.89              |
| 41:s:46:LEU:HA    | 41:s:49:ILE:HD13  | 1.54                     | 0.89              |
| 25:b:109:THR:CG2  | 27:d:19:ALA:HB3   | 2.03                     | 0.89              |
| 27:d:164:LEU:HD12 | 28:e:149:LEU:HD23 | 1.56                     | 0.88              |
| 35:l:331:MET:HB3  | 35:l:387:THR:HG22 | 1.56                     | 0.87              |
| 22:Y:80:VAL:HG23  | 35:l:385:TYR:OH   | 1.75                     | 0.87              |
| 32:i:88:LYS:HD2   | 32:i:148:SER:OG   | 1.75                     | 0.87              |
| 5:F:36:PHE:HD2    | 5:F:87:VAL:HG23   | 1.38                     | 0.86              |
| 30:g:2:THR:CG2    | 30:g:4:MET:HE2    | 2.05                     | 0.86              |
| 41:s:285:LEU:HD12 | 41:s:286:MET:N    | 1.91                     | 0.86              |
| 6:G:112:SER:O     | 6:G:116:VAL:HG23  | 1.76                     | 0.86              |
| 2:B:130:ILE:HD11  | 2:B:145:TYR:HE1   | 1.40                     | 0.85              |
| 20:V:66:ILE:HD11  | 20:V:101:LEU:HD22 | 0.91                     | 0.85              |
| 34:k:10:MET:O     | 34:k:14:ILE:HG13  | 1.76                     | 0.85              |
| 1:A:168:ASN:O     | 1:A:171:VAL:HG13  | 1.77                     | 0.84              |
| 7:H:94:MET:HE1    | 7:H:99:PRO:CG     | 2.07                     | 0.83              |
| 20:V:4:THR:CG2    | 20:V:8:LYS:NZ     | 2.38                     | 0.83              |
| 5:F:20:ARG:HG2    | 5:F:54:LEU:HD13   | 1.60                     | 0.83              |
| 20:V:106:ARG:HA   | 20:V:106:ARG:NE   | 1.92                     | 0.83              |
| 15:P:51:ASN:ND2   | 15:P:54:VAL:HG23  | 1.93                     | 0.82              |
| 1:A:141:GLY:HA2   | 1:A:252:PRO:CG    | 2.10                     | 0.81              |
| 1:A:102:MET:HG2   | 1:A:149:MET:HB3   | 1.61                     | 0.81              |
| 35:l:525:MET:HE2  | 35:l:528:TYR:CE1  | 2.15                     | 0.81              |
| 41:s:49:ILE:HD12  | 41:s:49:ILE:H     | 1.44                     | 0.81              |
| 7:H:94:MET:CE     | 7:H:99:PRO:HG3    | 2.11                     | 0.81              |
| 24:a:87:THR:O     | 24:a:91:VAL:HG23  | 1.81                     | 0.81              |
| 1:A:181:LEU:O     | 1:A:186:ALA:HB1   | 1.80                     | 0.81              |
| 20:V:66:ILE:CD1   | 20:V:101:LEU:CD2  | 2.49                     | 0.80              |
| 32:i:132:THR:CG2  | 32:i:212:THR:CG2  | 2.60                     | 0.80              |
| 44:w:66:ILE:HD11  | 44:w:234:LEU:HD23 | 1.61                     | 0.79              |
| 15:P:46:THR:HG23  | 16:Q:358:VAL:CG2  | 2.11                     | 0.79              |
| 16:Q:282:ASP:OD2  | 16:Q:437:LYS:CE   | 2.29                     | 0.79              |
| 1:A:169:LEU:O     | 1:A:173:ILE:HG13  | 1.82                     | 0.79              |
| 37:n:42:SER:OG    | 37:n:45:PHE:HB2   | 1.82                     | 0.79              |
| 25:b:109:THR:HG21 | 27:d:19:ALA:HB3   | 1.65                     | 0.79              |
| 12:M:49:VAL:HG13  | 12:M:102:ILE:HD13 | 1.65                     | 0.78              |
| 1:A:167:SER:O     | 1:A:171:VAL:HG12  | 1.82                     | 0.78              |
| 15:P:51:ASN:HD22  | 15:P:54:VAL:CG2   | 1.97                     | 0.78              |
| 21:W:120:MET:CE   | 36:m:126:VAL:HG13 | 2.14                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:140:GLU:OE2   | 1:A:252:PRO:HB3   | 1.84                     | 0.77              |
| 6:X:112:SER:CB    | 50:X:201:8Q1:P24  | 2.73                     | 0.77              |
| 33:j:73:LEU:HD13  | 36:m:55:MET:HE1   | 1.65                     | 0.77              |
| 35:l:129:MET:HE3  | 35:l:129:MET:HA   | 1.64                     | 0.77              |
| 41:s:70:MET:HG3   | 41:s:121:TRP:HZ3  | 1.48                     | 0.77              |
| 6:X:132:ASP:HB3   | 39:p:18:ARG:HE    | 1.50                     | 0.77              |
| 36:m:173:ARG:HG2  | 36:m:173:ARG:HH11 | 1.50                     | 0.76              |
| 5:F:69:TYR:HE2    | 5:F:75:LYS:HG3    | 1.51                     | 0.76              |
| 34:k:1:MET:HE2    | 34:k:6:MET:HG2    | 1.67                     | 0.76              |
| 40:r:207:MET:HE3  | 40:r:298:ILE:HG13 | 1.66                     | 0.75              |
| 32:i:132:THR:CG2  | 32:i:212:THR:HG21 | 2.15                     | 0.75              |
| 33:j:70:ALA:HA    | 33:j:73:LEU:HD12  | 1.68                     | 0.75              |
| 30:g:64:LEU:O     | 30:g:68:THR:HG23  | 1.86                     | 0.75              |
| 44:w:54:THR:HG23  | 44:w:56:THR:HG22  | 1.69                     | 0.75              |
| 20:V:95:CYS:HB2   | 20:V:115:CYS:SG   | 2.27                     | 0.75              |
| 20:V:98:GLY:CA    | 20:V:118:MET:SD   | 2.75                     | 0.75              |
| 36:m:170:GLU:OE1  | 36:m:173:ARG:NH2  | 2.20                     | 0.74              |
| 40:r:370:PRO:HB3  | 40:r:375:LEU:HD22 | 1.66                     | 0.74              |
| 6:G:119:ILE:CG2   | 6:G:130:ILE:HD11  | 2.17                     | 0.74              |
| 34:k:33:LEU:HD23  | 34:k:36:MET:HE2   | 1.67                     | 0.74              |
| 49:a:202:PLX:H102 | 40:r:40:SER:HB3   | 1.69                     | 0.74              |
| 39:p:108:HIS:ND1  | 39:p:110:SER:OG   | 2.21                     | 0.74              |
| 14:O:55:PHE:HA    | 14:O:89:GLN:HE22  | 1.52                     | 0.74              |
| 26:c:115:ASN:OD1  | 35:l:162:THR:HG23 | 1.87                     | 0.74              |
| 35:l:383:MET:HG3  | 35:l:384:PRO:HD2  | 1.67                     | 0.74              |
| 44:w:211:VAL:HA   | 44:w:214:ILE:HG22 | 1.70                     | 0.74              |
| 32:i:213:LEU:O    | 32:i:217:MET:HG3  | 1.88                     | 0.73              |
| 29:f:40:ASP:O     | 29:f:44:VAL:HG23  | 1.88                     | 0.73              |
| 4:E:52:LEU:HG     | 4:E:104:MET:HE2   | 1.70                     | 0.73              |
| 39:p:174:PRO:O    | 39:p:175:ARG:HB2  | 1.88                     | 0.73              |
| 6:G:115:GLN:NE2   | 6:G:119:ILE:HD11  | 2.03                     | 0.73              |
| 3:C:79:MET:HE2    | 3:C:86:MET:HE2    | 1.70                     | 0.72              |
| 41:s:6:ILE:HD13   | 41:s:95:LEU:HD21  | 1.71                     | 0.72              |
| 1:A:244:ASN:ND2   | 46:A:502:FMN:O2   | 2.21                     | 0.72              |
| 6:X:93:ILE:HG22   | 6:X:110:LEU:HD21  | 1.70                     | 0.72              |
| 35:l:383:MET:CG   | 35:l:384:PRO:HD2  | 2.19                     | 0.72              |
| 1:A:315:LEU:HB2   | 1:A:359:ARG:HG3   | 1.70                     | 0.72              |
| 20:V:95:CYS:CB    | 20:V:115:CYS:SG   | 2.77                     | 0.72              |
| 44:w:325:ASP:O    | 44:w:329:GLN:HG2  | 1.89                     | 0.72              |
| 5:F:18:GLU:HG2    | 5:F:68:ARG:HE     | 1.55                     | 0.71              |
| 35:l:591:PHE:O    | 35:l:595:ILE:HG13 | 1.90                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:F:36:PHE:CD2    | 5:F:87:VAL:HG23   | 2.24                     | 0.71              |
| 15:P:105:ASN:O    | 15:P:137:PHE:CE2  | 2.43                     | 0.71              |
| 39:p:19:LEU:HD13  | 39:p:68:GLU:OE2   | 1.91                     | 0.71              |
| 1:A:141:GLY:CA    | 1:A:252:PRO:HG3   | 2.18                     | 0.71              |
| 2:B:171:PRO:HG3   | 2:B:200:GLU:HG2   | 1.73                     | 0.71              |
| 6:G:112:SER:N     | 50:G:201:8Q1:O1   | 2.22                     | 0.71              |
| 32:i:132:THR:HG22 | 32:i:212:THR:HG21 | 1.70                     | 0.71              |
| 25:b:104:ILE:HD12 | 25:b:110:ILE:HD11 | 1.72                     | 0.71              |
| 35:l:134:ALA:HB3  | 35:l:140:LEU:HD13 | 1.72                     | 0.71              |
| 6:G:112:SER:CA    | 50:G:201:8Q1:O1   | 2.39                     | 0.71              |
| 1:A:119:GLU:OE1   | 1:A:127:ASP:HB2   | 1.90                     | 0.71              |
| 16:Q:152:SER:O    | 16:Q:156:GLU:CG   | 2.38                     | 0.71              |
| 33:j:18:VAL:HG22  | 41:s:222:MET:HG3  | 1.72                     | 0.71              |
| 33:j:73:LEU:HD23  | 41:s:151:LEU:HD21 | 1.71                     | 0.71              |
| 1:A:168:ASN:O     | 1:A:171:VAL:CG1   | 2.39                     | 0.71              |
| 16:Q:236:LEU:HD22 | 16:Q:240:LEU:CD2  | 2.20                     | 0.71              |
| 44:w:210:PRO:HD2  | 44:w:213:GLU:OE1  | 1.90                     | 0.71              |
| 22:Y:100:LEU:HB2  | 43:v:111:ARG:HH12 | 1.56                     | 0.70              |
| 32:i:139:LEU:HD11 | 32:i:187:MET:HE1  | 1.71                     | 0.70              |
| 39:p:49:ASP:HB2   | 39:p:52:LYS:HD2   | 1.74                     | 0.70              |
| 1:A:62:TRP:CE3    | 1:A:181:LEU:HD12  | 2.27                     | 0.70              |
| 12:M:171:THR:HG23 | 12:M:173:MET:SD   | 2.32                     | 0.70              |
| 9:J:136:THR:HG22  | 9:J:138:ASN:H     | 1.56                     | 0.70              |
| 32:i:128:LEU:C    | 32:i:128:LEU:HD23 | 2.17                     | 0.70              |
| 41:s:87:VAL:HG12  | 41:s:95:LEU:HD23  | 1.73                     | 0.70              |
| 1:A:385:CYS:HB2   | 45:A:501:SF4:S4   | 2.31                     | 0.70              |
| 15:P:107:GLN:NE2  | 15:P:136:ARG:HG2  | 2.06                     | 0.70              |
| 1:A:211:ALA:HB2   | 1:A:223:PRO:HG3   | 1.73                     | 0.69              |
| 12:M:360:ARG:HH21 | 12:M:632:MET:HA   | 1.57                     | 0.69              |
| 11:L:109:ASN:ND2  | 11:L:111:LEU:O    | 2.24                     | 0.69              |
| 15:P:51:ASN:HD22  | 15:P:54:VAL:HG23  | 1.55                     | 0.69              |
| 18:T:54:ARG:O     | 18:T:58:ARG:NH2   | 2.23                     | 0.69              |
| 24:a:133:TYR:OH   | 27:d:87:GLU:HG3   | 1.92                     | 0.69              |
| 33:j:85:LYS:O     | 33:j:89:THR:HG23  | 1.92                     | 0.69              |
| 7:H:77:ILE:O      | 7:H:81:ILE:HG13   | 1.92                     | 0.69              |
| 1:A:33:GLY:HA2    | 1:A:294:VAL:HG12  | 1.73                     | 0.69              |
| 20:V:4:THR:CG2    | 20:V:8:LYS:HZ1    | 2.01                     | 0.69              |
| 34:k:23:ARG:HG2   | 36:m:23:LYS:HE2   | 1.75                     | 0.68              |
| 1:A:141:GLY:CA    | 1:A:252:PRO:CG    | 2.71                     | 0.68              |
| 33:j:25:PRO:HB2   | 41:s:60:PRO:HD3   | 1.75                     | 0.68              |
| 35:l:159:HIS:HB2  | 40:r:416:ARG:HG2  | 1.74                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:l:347:ILE:HD13 | 35:l:354:GLN:HG2  | 1.75                     | 0.68              |
| 1:A:342:LEU:HD22  | 1:A:347:THR:HG21  | 1.74                     | 0.68              |
| 19:U:66:VAL:CG1   | 42:u:130:LYS:HD3  | 2.24                     | 0.68              |
| 29:f:62:HIS:O     | 29:f:66:VAL:HG23  | 1.94                     | 0.68              |
| 12:M:161:GLU:OE1  | 14:O:42:ARG:NH2   | 2.27                     | 0.68              |
| 41:s:70:MET:HG3   | 41:s:121:TRP:CZ3  | 2.28                     | 0.68              |
| 9:J:218:ALA:O     | 9:J:221:ARG:NH1   | 2.25                     | 0.68              |
| 29:f:39:PRO:HG2   | 44:w:351:TRP:CD1  | 2.28                     | 0.68              |
| 12:M:500:ILE:HD11 | 12:M:512:VAL:HG11 | 1.76                     | 0.67              |
| 28:e:72:ASP:OD1   | 39:p:108:HIS:NE2  | 2.26                     | 0.67              |
| 43:v:51:LEU:O     | 43:v:52:MET:HG2   | 1.93                     | 0.67              |
| 44:w:66:ILE:HD11  | 44:w:234:LEU:CD2  | 2.23                     | 0.67              |
| 17:S:54:ILE:O     | 42:u:19:LYS:NZ    | 2.28                     | 0.67              |
| 44:w:146:ALA:HB1  | 44:w:157:VAL:HG21 | 1.77                     | 0.67              |
| 40:r:374:ASN:O    | 40:r:378:GLU:HG2  | 1.94                     | 0.67              |
| 5:F:23:LEU:HD12   | 5:F:34:ARG:HG2    | 1.76                     | 0.67              |
| 5:F:30:SER:O      | 5:F:33:VAL:N      | 2.28                     | 0.67              |
| 14:O:156:LEU:HD11 | 14:O:169:PHE:HD2  | 1.58                     | 0.67              |
| 5:F:36:PHE:HD2    | 5:F:87:VAL:CG2    | 2.08                     | 0.67              |
| 16:Q:152:SER:O    | 16:Q:156:GLU:HG2  | 1.94                     | 0.67              |
| 21:W:120:MET:HE3  | 36:m:126:VAL:HG13 | 1.77                     | 0.67              |
| 35:l:161:ARG:NH1  | 35:l:238:GLU:OE1  | 2.28                     | 0.67              |
| 15:P:51:ASN:ND2   | 15:P:54:VAL:CG2   | 2.57                     | 0.66              |
| 34:k:32:CYS:O     | 34:k:36:MET:HG3   | 1.96                     | 0.66              |
| 42:u:49:GLU:OE1   | 42:u:135:ARG:NH2  | 2.28                     | 0.66              |
| 1:A:132:ARG:HB3   | 1:A:165:GLU:HG3   | 1.77                     | 0.66              |
| 2:B:111:GLU:O     | 2:B:141:ARG:NH1   | 2.29                     | 0.66              |
| 7:H:93:LYS:HA     | 7:H:96:ARG:NH1    | 2.11                     | 0.66              |
| 18:T:78:GLU:OE2   | 18:T:119:ARG:NH1  | 2.26                     | 0.66              |
| 32:i:45:MET:HE3   | 32:i:53:THR:HG22  | 1.77                     | 0.66              |
| 9:J:83:PRO:HG3    | 9:J:119:VAL:HG11  | 1.78                     | 0.66              |
| 40:r:207:MET:HE3  | 40:r:298:ILE:CG1  | 2.26                     | 0.66              |
| 43:v:25:PHE:HZ    | 43:v:112:LYS:HD2  | 1.59                     | 0.66              |
| 18:T:47:ASP:HA    | 18:T:52:ARG:HH12  | 1.60                     | 0.66              |
| 22:Y:54:GLN:OE1   | 35:l:446:ASN:ND2  | 2.29                     | 0.66              |
| 29:f:39:PRO:HG3   | 44:w:351:TRP:HB3  | 1.78                     | 0.66              |
| 2:B:177:THR:HG22  | 2:B:179:THR:H     | 1.60                     | 0.66              |
| 32:i:88:LYS:HD2   | 32:i:148:SER:HG   | 1.61                     | 0.66              |
| 19:U:30:ILE:HD11  | 33:j:96:ILE:HD11  | 1.78                     | 0.65              |
| 21:W:93:GLU:OE2   | 31:h:95:PRO:HG2   | 1.96                     | 0.65              |
| 35:l:526:LEU:HD12 | 35:l:530:PRO:HG2  | 1.77                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:50:ASP:O      | 1:A:59:ARG:NH2    | 2.28                     | 0.65              |
| 1:A:157:TYR:CG    | 1:A:212:LEU:CD1   | 2.75                     | 0.65              |
| 12:M:428:LYS:NZ   | 12:M:443:ASP:OD2  | 2.28                     | 0.65              |
| 24:a:160:MET:HE2  | 30:g:95:TYR:CD1   | 2.31                     | 0.65              |
| 20:V:101:LEU:HD12 | 20:V:101:LEU:O    | 1.95                     | 0.65              |
| 30:g:47:ASP:OD1   | 30:g:51:ARG:NH1   | 2.30                     | 0.65              |
| 32:i:108:LEU:HD11 | 32:i:191:THR:HG21 | 1.79                     | 0.65              |
| 34:k:37:MET:HE1   | 36:m:64:MET:HE1   | 1.77                     | 0.65              |
| 1:A:152:ARG:NH2   | 10:K:99:PRO:O     | 2.29                     | 0.65              |
| 11:L:88:GLN:NE2   | 12:M:141:ASP:OD2  | 2.29                     | 0.65              |
| 20:V:47:ALA:HB3   | 20:V:51:GLU:OE1   | 1.97                     | 0.65              |
| 6:X:134:ASP:OD1   | 39:p:2:ALA:N      | 2.30                     | 0.65              |
| 35:l:391:SER:O    | 35:l:395:ILE:HG12 | 1.97                     | 0.65              |
| 1:A:157:TYR:CD2   | 1:A:212:LEU:HD11  | 2.31                     | 0.65              |
| 12:M:149:ASP:HB2  | 16:Q:361:ALA:HB3  | 1.78                     | 0.65              |
| 15:P:44:ARG:HE    | 15:P:45:PRO:HD3   | 1.61                     | 0.65              |
| 16:Q:149:GLN:NE2  | 16:Q:309:ASP:OD2  | 2.29                     | 0.64              |
| 32:i:149:ILE:HD11 | 32:i:195:PRO:HG3  | 1.79                     | 0.64              |
| 35:l:227:PHE:O    | 35:l:230:HIS:ND1  | 2.30                     | 0.64              |
| 48:r:501:PEE:H71  | 48:r:501:PEE:H32  | 1.78                     | 0.64              |
| 4:E:71:ALA:HA     | 50:G:201:8Q1:O40  | 1.98                     | 0.64              |
| 32:i:132:THR:HG21 | 32:i:212:THR:HG23 | 1.79                     | 0.64              |
| 33:j:4:MET:HE2    | 48:m:201:PEE:H19  | 1.78                     | 0.64              |
| 15:P:187:ILE:HG23 | 15:P:188:LEU:HG   | 1.77                     | 0.64              |
| 20:V:4:THR:HG22   | 20:V:8:LYS:HZ2    | 1.60                     | 0.64              |
| 9:J:169:HIS:H     | 9:J:184:LYS:HD3   | 1.61                     | 0.64              |
| 8:I:25:GLN:HB3    | 16:Q:254:ARG:NH1  | 2.13                     | 0.64              |
| 1:A:174:ARG:HD2   | 1:A:174:ARG:C     | 2.22                     | 0.64              |
| 20:V:106:ARG:HA   | 20:V:106:ARG:HE   | 1.63                     | 0.64              |
| 16:Q:302:LEU:HB2  | 16:Q:401:GLU:HB2  | 1.80                     | 0.64              |
| 19:U:53:TYR:HB2   | 21:W:72:MET:CE    | 2.26                     | 0.64              |
| 1:A:75:TRP:CD1    | 1:A:75:TRP:C      | 2.76                     | 0.63              |
| 36:m:57:PHE:HD2   | 41:s:107:ALA:HB1  | 1.62                     | 0.63              |
| 42:u:137:LEU:HD12 | 42:u:138:PRO:HD2  | 1.79                     | 0.63              |
| 44:w:176:GLN:NE2  | 44:w:236:ASP:OD2  | 2.30                     | 0.63              |
| 2:B:192:ASN:ND2   | 18:T:61:GLU:OE1   | 2.31                     | 0.63              |
| 7:H:30:LYS:O      | 7:H:34:VAL:HG23   | 1.99                     | 0.63              |
| 21:W:97:ILE:HG22  | 21:W:98:MET:HE2   | 1.80                     | 0.63              |
| 6:X:120:MET:HE1   | 39:p:24:LEU:HD13  | 1.80                     | 0.63              |
| 55:i:402:CDL:H742 | 55:i:402:CDL:H271 | 1.79                     | 0.63              |
| 16:Q:68:ASP:O     | 32:i:49:ASN:ND2   | 2.31                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 34:k:98:CYS:HB2   | 35:l:580:GLN:HB2  | 1.80                     | 0.63              |
| 43:v:25:PHE:HD2   | 43:v:108:LEU:HD23 | 1.62                     | 0.63              |
| 44:w:139:ARG:NH1  | 44:w:166:ASP:OD2  | 2.31                     | 0.63              |
| 14:O:63:ILE:O     | 14:O:67:VAL:HG23  | 1.99                     | 0.63              |
| 35:l:375:ILE:HD12 | 35:l:458:LEU:HD11 | 1.81                     | 0.63              |
| 43:v:12:ASP:HB3   | 43:v:15:LYS:HB2   | 1.81                     | 0.63              |
| 7:H:76:GLN:O      | 7:H:79:GLU:HG2    | 1.99                     | 0.63              |
| 21:W:85:GLN:OE1   | 31:h:105:ARG:NH1  | 2.28                     | 0.63              |
| 12:M:178:GLN:HG2  | 12:M:204:MET:HE2  | 1.81                     | 0.63              |
| 41:s:285:LEU:HD12 | 41:s:285:LEU:C    | 2.23                     | 0.63              |
| 2:B:177:THR:HG21  | 2:B:182:GLU:HB2   | 1.81                     | 0.62              |
| 25:b:123:PHE:HB3  | 43:v:40:VAL:HG21  | 1.80                     | 0.62              |
| 14:O:64:GLU:OE1   | 14:O:68:LYS:HE3   | 1.99                     | 0.62              |
| 9:J:192:ARG:NH2   | 9:J:262:THR:OG1   | 2.32                     | 0.62              |
| 5:F:30:SER:O      | 5:F:32:GLY:N      | 2.33                     | 0.62              |
| 18:T:104:LYS:HD2  | 18:T:107:LYS:HE2  | 1.82                     | 0.62              |
| 21:W:98:MET:HE1   | 31:h:79:ILE:HA    | 1.79                     | 0.62              |
| 41:s:87:VAL:CG2   | 41:s:88:PRO:CD    | 2.66                     | 0.62              |
| 55:a:201:CDL:H322 | 48:l:703:PEE:H62  | 1.80                     | 0.62              |
| 25:b:22:TRP:CD2   | 39:p:172:THR:HG22 | 2.34                     | 0.62              |
| 21:W:97:ILE:CG2   | 21:W:98:MET:HE2   | 2.29                     | 0.62              |
| 27:d:110:LEU:HD11 | 35:l:203:MET:HE2  | 1.82                     | 0.62              |
| 12:M:347:ASP:HB3  | 12:M:594:ALA:HB1  | 1.82                     | 0.62              |
| 24:a:120:TRP:O    | 24:a:124:THR:HG22 | 2.00                     | 0.62              |
| 23:Z:84:ALA:O     | 23:Z:88:LEU:HG    | 1.99                     | 0.62              |
| 1:A:256:ARG:HG2   | 14:O:245:VAL:HG12 | 1.81                     | 0.61              |
| 28:e:85:TRP:O     | 28:e:89:VAL:HG13  | 2.00                     | 0.61              |
| 35:l:108:MET:CE   | 35:l:240:PRO:HB3  | 2.30                     | 0.61              |
| 3:C:66:THR:HG21   | 3:C:76:MET:HG3    | 1.83                     | 0.61              |
| 14:O:38:LEU:O     | 14:O:124:ARG:NH2  | 2.32                     | 0.61              |
| 31:h:97:HIS:HA    | 31:h:102:GLU:HB3  | 1.81                     | 0.61              |
| 34:k:50:ASN:ND2   | 36:m:127:ILE:HD12 | 2.15                     | 0.61              |
| 35:l:331:MET:CB   | 35:l:387:THR:HG22 | 2.28                     | 0.61              |
| 44:w:125:ASP:O    | 44:w:130:ARG:NH2  | 2.33                     | 0.61              |
| 12:M:68:ARG:NH2   | 12:M:279:GLU:OE2  | 2.33                     | 0.61              |
| 19:U:81:LEU:O     | 21:W:59:ARG:NH1   | 2.33                     | 0.61              |
| 15:P:43:THR:HA    | 15:P:47:ILE:HD12  | 1.82                     | 0.61              |
| 17:S:47:LEU:HD22  | 42:u:22:SER:HB2   | 1.81                     | 0.61              |
| 7:H:31:ILE:CD1    | 7:H:88:LEU:HA     | 2.25                     | 0.61              |
| 7:H:96:ARG:HH11   | 7:H:96:ARG:HB3    | 1.64                     | 0.61              |
| 1:A:71:LYS:HD3    | 1:A:75:TRP:CZ3    | 2.36                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:J:65:LEU:HD23   | 9:J:129:LEU:HD22  | 1.83                     | 0.61              |
| 9:J:211:ASP:O     | 9:J:215:ASN:ND2   | 2.33                     | 0.61              |
| 39:p:64:LEU:O     | 39:p:68:GLU:HG2   | 2.00                     | 0.61              |
| 14:O:206:ASP:OD1  | 14:O:207:GLU:N    | 2.33                     | 0.61              |
| 15:P:83:GLU:OE1   | 15:P:142:ARG:NH2  | 2.32                     | 0.61              |
| 16:Q:80:LEU:HD11  | 16:Q:82:LEU:HD21  | 1.82                     | 0.61              |
| 16:Q:82:LEU:HD12  | 16:Q:101:LEU:HD13 | 1.82                     | 0.61              |
| 32:i:163:LEU:HD22 | 32:i:167:TRP:CH2  | 2.36                     | 0.61              |
| 1:A:398:ARG:NH2   | 1:A:408:GLU:OE1   | 2.30                     | 0.61              |
| 4:E:40:TYR:CE2    | 6:G:117:GLU:HG2   | 2.36                     | 0.61              |
| 16:Q:98:VAL:HG23  | 16:Q:110:ASP:HB3  | 1.83                     | 0.61              |
| 41:s:46:LEU:HA    | 41:s:49:ILE:CD1   | 2.29                     | 0.61              |
| 9:J:192:ARG:NH1   | 9:J:198:ALA:O     | 2.33                     | 0.61              |
| 41:s:24:GLU:OE1   | 41:s:271:LEU:HD22 | 2.01                     | 0.60              |
| 1:A:375:LYS:NZ    | 14:O:33:GLY:O     | 2.35                     | 0.60              |
| 32:i:163:LEU:HD22 | 32:i:167:TRP:CZ3  | 2.36                     | 0.60              |
| 3:C:61:SER:OG     | 41:s:54:LYS:HD3   | 2.01                     | 0.60              |
| 10:K:105:ARG:NH1  | 11:L:167:ASN:O    | 2.34                     | 0.60              |
| 27:d:68:PHE:HD1   | 37:n:44:LEU:HD11  | 1.65                     | 0.60              |
| 25:b:110:ILE:HG22 | 25:b:110:ILE:O    | 2.01                     | 0.60              |
| 7:H:94:MET:CE     | 7:H:99:PRO:CG     | 2.75                     | 0.60              |
| 35:l:288:THR:HG21 | 35:l:307:SER:HB2  | 1.83                     | 0.60              |
| 12:M:472:PRO:O    | 12:M:510:TRP:NE1  | 2.30                     | 0.60              |
| 14:O:182:ASN:OD1  | 14:O:222:ARG:NH2  | 2.35                     | 0.60              |
| 24:a:106:VAL:CG1  | 37:n:50:ARG:NH2   | 2.48                     | 0.60              |
| 35:l:90:ILE:HG12  | 35:l:129:MET:CE   | 2.26                     | 0.60              |
| 35:l:419:THR:HA   | 35:l:422:TYR:CE2  | 2.37                     | 0.60              |
| 27:d:69:ARG:NH1   | 37:n:43:LEU:O     | 2.35                     | 0.60              |
| 36:m:1:MET:HE3    | 36:m:4:TYR:H      | 1.67                     | 0.60              |
| 5:F:33:VAL:O      | 5:F:36:PHE:HB3    | 2.01                     | 0.60              |
| 35:l:97:THR:HG21  | 35:l:125:LEU:HD22 | 1.83                     | 0.60              |
| 36:m:57:PHE:CD2   | 41:s:107:ALA:HB1  | 2.37                     | 0.60              |
| 1:A:185:ASN:ND2   | 1:A:187:CYS:O     | 2.34                     | 0.60              |
| 12:M:50:LEU:O     | 12:M:54:GLU:HG3   | 2.02                     | 0.60              |
| 14:O:156:LEU:HB3  | 14:O:158:ILE:HG12 | 1.84                     | 0.60              |
| 32:i:132:THR:CG2  | 32:i:212:THR:HG23 | 2.32                     | 0.60              |
| 9:J:204:SER:OG    | 9:J:238:GLN:O     | 2.20                     | 0.59              |
| 17:S:39:ALA:HA    | 17:S:44:GLN:HG3   | 1.82                     | 0.59              |
| 21:W:120:MET:HE1  | 36:m:126:VAL:HG13 | 1.84                     | 0.59              |
| 15:P:68:ILE:HG21  | 15:P:99:PHE:CE1   | 2.37                     | 0.59              |
| 18:T:39:THR:HG22  | 18:T:62:VAL:HG12  | 1.85                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:347:ASN:HB3  | 49:i:401:PLX:H301 | 1.83                     | 0.59              |
| 35:l:579:ASN:O    | 35:l:579:ASN:OD1  | 2.19                     | 0.59              |
| 1:A:48:ARG:O      | 10:K:74:ARG:NH1   | 2.35                     | 0.59              |
| 11:L:84:ARG:NH1   | 11:L:88:GLN:O     | 2.36                     | 0.59              |
| 30:g:11:VAL:HB    | 30:g:14:GLN:HG3   | 1.83                     | 0.59              |
| 1:A:88:ARG:HG3    | 1:A:246:GLU:OE2   | 2.03                     | 0.59              |
| 41:s:62:ARG:HD3   | 41:s:64:ALA:H     | 1.65                     | 0.59              |
| 44:w:84:ARG:HD3   | 44:w:149:HIS:CD2  | 2.37                     | 0.59              |
| 1:A:282:VAL:HG13  | 1:A:356:VAL:HG21  | 1.84                     | 0.59              |
| 5:F:30:SER:O      | 5:F:31:GLN:C      | 2.46                     | 0.59              |
| 6:G:88:LYS:HD3    | 6:G:98:LEU:HD21   | 1.85                     | 0.59              |
| 25:b:109:THR:HG23 | 27:d:19:ALA:HB3   | 1.84                     | 0.59              |
| 32:i:110:PRO:HG2  | 35:l:594:THR:HG21 | 1.83                     | 0.59              |
| 1:A:181:LEU:O     | 1:A:186:ALA:O     | 2.21                     | 0.59              |
| 4:E:70:ASN:ND2    | 50:G:201:8Q1:O4   | 2.35                     | 0.59              |
| 1:A:157:TYR:CD1   | 1:A:212:LEU:HD11  | 2.36                     | 0.59              |
| 1:A:168:ASN:HA    | 1:A:171:VAL:CG1   | 2.33                     | 0.59              |
| 8:I:9:GLN:O       | 8:I:13:ASN:ND2    | 2.32                     | 0.59              |
| 24:a:155:GLU:OE1  | 24:a:158:ARG:NH2  | 2.33                     | 0.59              |
| 15:P:106:ALA:HB1  | 15:P:108:PHE:CD1  | 2.38                     | 0.59              |
| 6:X:82:ARG:O      | 6:X:86:VAL:HG23   | 2.02                     | 0.59              |
| 29:f:68:GLU:OE2   | 29:f:71:ARG:NH2   | 2.36                     | 0.59              |
| 7:H:38:ILE:O      | 7:H:45:ARG:NH1    | 2.31                     | 0.59              |
| 12:M:58:MET:HE2   | 12:M:60:ILE:HD13  | 1.84                     | 0.59              |
| 12:M:299:ARG:HG2  | 12:M:300:GLN:HG2  | 1.85                     | 0.59              |
| 21:W:144:THR:HB   | 41:s:96:ILE:HG23  | 1.84                     | 0.59              |
| 12:M:495:ASN:O    | 12:M:499:ASN:OD1  | 2.21                     | 0.58              |
| 16:Q:116:LEU:O    | 16:Q:116:LEU:HG   | 2.02                     | 0.58              |
| 27:d:114:GLN:HG3  | 35:l:203:MET:HG2  | 1.84                     | 0.58              |
| 35:l:88:MET:HE1   | 35:l:468:ILE:HD12 | 1.83                     | 0.58              |
| 40:r:243:MET:O    | 40:r:247:THR:HG23 | 2.02                     | 0.58              |
| 1:A:456:GLN:OE1   | 1:A:457:HIS:CE1   | 2.56                     | 0.58              |
| 5:F:30:SER:HB2    | 5:F:63:PRO:HG3    | 1.82                     | 0.58              |
| 9:J:215:ASN:O     | 9:J:219:SER:OG    | 2.20                     | 0.58              |
| 20:V:123:ALA:O    | 20:V:127:MET:HG3  | 2.03                     | 0.58              |
| 1:A:174:ARG:HA    | 10:K:93:LEU:HD21  | 1.86                     | 0.58              |
| 5:F:33:VAL:HG22   | 5:F:87:VAL:HG11   | 1.85                     | 0.58              |
| 8:I:18:ARG:HG3    | 8:I:18:ARG:HH11   | 1.68                     | 0.58              |
| 9:J:234:GLU:OE1   | 9:J:234:GLU:N     | 2.35                     | 0.58              |
| 32:i:132:THR:HG21 | 32:i:212:THR:CG2  | 2.33                     | 0.58              |
| 7:H:93:LYS:HA     | 7:H:96:ARG:HH12   | 1.66                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:150:ARG:NH2  | 16:Q:359:ASP:OD1  | 2.36                     | 0.58              |
| 27:d:26:LEU:HD22  | 43:v:75:PRO:HB2   | 1.84                     | 0.58              |
| 2:B:101:HIS:ND1   | 2:B:149:MET:HE1   | 2.18                     | 0.58              |
| 35:l:8:THR:HB     | 35:l:82:MET:HE3   | 1.86                     | 0.58              |
| 8:I:70:MET:HG2    | 15:P:66:ALA:HB1   | 1.85                     | 0.58              |
| 29:f:39:PRO:HG3   | 44:w:351:TRP:CB   | 2.34                     | 0.58              |
| 12:M:162:ASP:OD1  | 12:M:172:ILE:HA   | 2.03                     | 0.58              |
| 39:p:59:LYS:HA    | 39:p:59:LYS:HE2   | 1.86                     | 0.58              |
| 4:E:15:THR:OG1    | 11:L:55:VAL:O     | 2.22                     | 0.58              |
| 9:J:249:ILE:O     | 9:J:253:ILE:HG13  | 2.04                     | 0.58              |
| 12:M:546:PHE:CE1  | 12:M:567:ILE:HD13 | 2.39                     | 0.58              |
| 15:P:51:ASN:HD22  | 15:P:54:VAL:HG21  | 1.69                     | 0.58              |
| 24:a:152:LYS:HD3  | 30:g:96:VAL:HG21  | 1.86                     | 0.58              |
| 44:w:114:LEU:HD21 | 57:w:401:ADP:H1'  | 1.86                     | 0.58              |
| 12:M:137:CYS:HB3  | 12:M:140:GLN:HB2  | 1.86                     | 0.57              |
| 14:O:67:VAL:HG13  | 14:O:75:LYS:HG3   | 1.86                     | 0.57              |
| 16:Q:152:SER:O    | 16:Q:156:GLU:HG3  | 2.03                     | 0.57              |
| 32:i:149:ILE:HD12 | 32:i:154:MET:CG   | 2.26                     | 0.57              |
| 34:k:27:MET:HE1   | 36:m:68:PHE:HD2   | 1.69                     | 0.57              |
| 44:w:211:VAL:HA   | 44:w:214:ILE:CG2  | 2.34                     | 0.57              |
| 14:O:100:LYS:O    | 14:O:104:ILE:HG13 | 2.03                     | 0.57              |
| 39:p:159:LYS:HB2  | 39:p:162:ASP:OD1  | 2.04                     | 0.57              |
| 3:C:119:LYS:NZ    | 3:C:123:GLN:HE21  | 2.03                     | 0.57              |
| 18:T:37:LYS:HD3   | 18:T:62:VAL:HG21  | 1.87                     | 0.57              |
| 35:l:102:GLU:OE1  | 35:l:456:ARG:NH2  | 2.32                     | 0.57              |
| 12:M:283:GLU:OE2  | 12:M:420:LYS:NZ   | 2.34                     | 0.57              |
| 15:P:113:ASP:OD1  | 15:P:114:LEU:N    | 2.38                     | 0.57              |
| 6:X:108:LEU:HB3   | 6:X:110:LEU:HD23  | 1.85                     | 0.57              |
| 24:a:108:GLU:OE1  | 24:a:110:TRP:NE1  | 2.36                     | 0.57              |
| 24:a:160:MET:HE2  | 30:g:95:TYR:CG    | 2.39                     | 0.57              |
| 35:l:186:MET:CE   | 40:r:379:LEU:HD21 | 2.35                     | 0.57              |
| 15:P:103:HIS:HD2  | 15:P:105:ASN:HB2  | 1.69                     | 0.57              |
| 20:V:4:THR:HG22   | 20:V:8:LYS:HZ3    | 1.62                     | 0.57              |
| 22:Y:44:TYR:HB2   | 23:Z:14:MET:HE1   | 1.87                     | 0.57              |
| 24:a:130:GLU:HB3  | 37:n:45:PHE:CD1   | 2.40                     | 0.57              |
| 41:s:21:THR:HB    | 56:s:401:UQ:HM23  | 1.86                     | 0.57              |
| 13:N:85:GLU:HB2   | 13:N:98:PRO:HB3   | 1.86                     | 0.57              |
| 14:O:182:ASN:HB3  | 14:O:194:GLU:HB3  | 1.87                     | 0.57              |
| 35:l:72:GLN:NE2   | 40:r:459:TYR:O    | 2.38                     | 0.57              |
| 44:w:231:ALA:HA   | 44:w:234:LEU:HD12 | 1.85                     | 0.57              |
| 44:w:118:TYR:OH   | 57:w:401:ADP:O2'  | 2.23                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:L:89:SER:O     | 12:M:59:GLN:NE2   | 2.37                     | 0.57              |
| 16:Q:184:ILE:HD11 | 16:Q:251:PHE:HZ   | 1.69                     | 0.57              |
| 26:c:58:ARG:NH1   | 26:c:61:ASP:OD2   | 2.38                     | 0.57              |
| 44:w:78:ALA:HB2   | 44:w:158:VAL:HG11 | 1.86                     | 0.57              |
| 3:C:79:MET:HE1    | 3:C:177:ILE:HG13  | 1.87                     | 0.56              |
| 37:n:18:PRO:O     | 37:n:22:VAL:HG23  | 2.05                     | 0.56              |
| 3:C:59:ARG:NH1    | 49:C:303:PLX:O3   | 2.30                     | 0.56              |
| 50:X:201:8Q1:N36  | 50:X:201:8Q1:O40  | 2.38                     | 0.56              |
| 24:a:91:VAL:HG13  | 27:d:52:ILE:HD13  | 1.86                     | 0.56              |
| 25:b:74:HIS:O     | 35:l:14:ILE:HD12  | 2.05                     | 0.56              |
| 32:i:221:HIS:HB2  | 32:i:323:MET:HE1  | 1.86                     | 0.56              |
| 4:E:84:ILE:O      | 4:E:88:MET:HG3    | 2.05                     | 0.56              |
| 7:H:58:MET:HG2    | 7:H:71:GLN:OE1    | 2.05                     | 0.56              |
| 10:K:109:ARG:NH2  | 14:O:106:GLN:O    | 2.38                     | 0.56              |
| 18:T:47:ASP:HA    | 18:T:52:ARG:NH1   | 2.20                     | 0.56              |
| 24:a:91:VAL:HG13  | 27:d:52:ILE:CD1   | 2.35                     | 0.56              |
| 28:e:89:VAL:HG21  | 40:r:25:ILE:HG23  | 1.87                     | 0.56              |
| 32:i:42:PRO:HG2   | 36:m:167:VAL:HG22 | 1.88                     | 0.56              |
| 35:l:357:ARG:HG3  | 39:p:32:VAL:HG13  | 1.86                     | 0.56              |
| 35:l:489:THR:O    | 35:l:493:VAL:HG13 | 2.05                     | 0.56              |
| 8:I:14:TRP:O      | 21:W:28:ARG:NH2   | 2.38                     | 0.56              |
| 14:O:41:HIS:NE2   | 14:O:47:ASN:OD1   | 2.32                     | 0.56              |
| 34:k:27:MET:HE1   | 36:m:68:PHE:CD2   | 2.40                     | 0.56              |
| 2:B:130:ILE:HG12  | 2:B:145:TYR:CD1   | 2.41                     | 0.56              |
| 44:w:271:GLU:O    | 44:w:275:TYR:CD1  | 2.58                     | 0.56              |
| 32:i:267:ILE:HG12 | 32:i:279:PRO:HB3  | 1.88                     | 0.56              |
| 7:H:83:GLN:OE1    | 7:H:83:GLN:HA     | 2.06                     | 0.56              |
| 12:M:394:VAL:HG22 | 12:M:473:MET:HE1  | 1.86                     | 0.56              |
| 37:n:42:SER:O     | 37:n:46:LYS:N     | 2.38                     | 0.56              |
| 6:X:91:ASP:OD2    | 23:Z:42:ARG:NH2   | 2.28                     | 0.56              |
| 22:Y:65:MET:HE2   | 35:l:375:ILE:HG12 | 1.88                     | 0.56              |
| 24:a:131:LYS:HE3  | 37:n:32:ASP:OD2   | 2.06                     | 0.56              |
| 41:s:264:LEU:O    | 41:s:268:ILE:HG12 | 2.05                     | 0.56              |
| 2:B:68:ARG:NH2    | 16:Q:260:GLU:OE2  | 2.39                     | 0.56              |
| 21:W:112:HIS:CD2  | 31:h:58:ILE:CD1   | 2.89                     | 0.55              |
| 1:A:87:GLY:N      | 1:A:93:PHE:O      | 2.38                     | 0.55              |
| 40:r:328:CYS:O    | 40:r:332:THR:HG23 | 2.06                     | 0.55              |
| 41:s:89:LEU:HD22  | 41:s:240:ILE:HD12 | 1.88                     | 0.55              |
| 44:w:350:LYS:CB   | 44:w:351:TRP:HE3  | 2.12                     | 0.55              |
| 12:M:407:PRO:HD2  | 12:M:438:LEU:HD21 | 1.89                     | 0.55              |
| 14:O:206:ASP:OD1  | 14:O:206:ASP:C    | 2.49                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:Y:51:THR:HG22  | 22:Y:53:SER:H     | 1.71                     | 0.55              |
| 2:B:146:ASP:OD2   | 11:L:112:MET:CE   | 2.54                     | 0.55              |
| 7:H:83:GLN:NE2    | 15:P:104:THR:HA   | 2.22                     | 0.55              |
| 11:L:132:GLU:CD   | 11:L:132:GLU:H    | 2.14                     | 0.55              |
| 16:Q:293:LEU:HD22 | 16:Q:298:ILE:HD12 | 1.88                     | 0.55              |
| 55:a:201:CDL:H362 | 25:b:80:TRP:HB3   | 1.88                     | 0.55              |
| 12:M:178:GLN:HG2  | 12:M:204:MET:CE   | 2.36                     | 0.55              |
| 14:O:193:TYR:CD2  | 14:O:204:ILE:HD13 | 2.42                     | 0.55              |
| 22:Y:62:SER:HG    | 35:l:371:THR:HG1  | 1.54                     | 0.55              |
| 1:A:181:LEU:O     | 1:A:186:ALA:CB    | 2.54                     | 0.55              |
| 35:l:360:GLY:HA3  | 35:l:435:PRO:HA   | 1.88                     | 0.55              |
| 41:s:86:TRP:CZ2   | 41:s:232:ILE:HG22 | 2.41                     | 0.55              |
| 3:C:125:PRO:HB2   | 41:s:58:LYS:HE3   | 1.88                     | 0.55              |
| 9:J:73:LEU:O      | 9:J:78:SER:OG     | 2.22                     | 0.55              |
| 6:X:69:SER:OG     | 6:X:70:ASP:N      | 2.38                     | 0.55              |
| 24:a:141:GLN:O    | 24:a:145:GLU:HG3  | 2.06                     | 0.55              |
| 25:b:123:PHE:HD2  | 43:v:40:VAL:HG11  | 1.71                     | 0.55              |
| 1:A:290:GLU:HG3   | 1:A:291:GLU:N     | 2.22                     | 0.55              |
| 12:M:117:MET:HE2  | 12:M:143:SER:HA   | 1.89                     | 0.55              |
| 19:U:53:TYR:CD1   | 21:W:72:MET:HE3   | 2.42                     | 0.55              |
| 16:Q:184:ILE:HD11 | 16:Q:251:PHE:CZ   | 2.42                     | 0.55              |
| 6:X:123:GLU:HG2   | 6:X:129:GLU:HA    | 1.89                     | 0.55              |
| 31:h:105:ARG:NH2  | 42:u:17:GLU:OE2   | 2.40                     | 0.55              |
| 33:j:68:GLU:HG2   | 36:m:161:LEU:HD13 | 1.88                     | 0.55              |
| 35:l:108:MET:HE1  | 35:l:240:PRO:HB3  | 1.89                     | 0.55              |
| 39:p:59:LYS:O     | 39:p:59:LYS:HD3   | 2.07                     | 0.55              |
| 41:s:86:TRP:HZ2   | 41:s:232:ILE:HG22 | 1.72                     | 0.55              |
| 2:B:131:GLU:HG3   | 2:B:144:ARG:HD2   | 1.88                     | 0.54              |
| 4:E:98:LYS:HB3    | 4:E:102:HIS:HB2   | 1.89                     | 0.54              |
| 12:M:33:GLU:CB    | 12:M:42:MET:HE1   | 2.32                     | 0.54              |
| 6:X:130:ILE:HG23  | 6:X:147:TYR:CZ    | 2.42                     | 0.54              |
| 27:d:46:THR:O     | 27:d:50:GLU:HG2   | 2.06                     | 0.54              |
| 29:f:44:VAL:O     | 29:f:48:LEU:HD22  | 2.07                     | 0.54              |
| 1:A:157:TYR:CB    | 1:A:212:LEU:HD11  | 2.37                     | 0.54              |
| 6:G:103:HIS:ND1   | 6:G:106:LYS:HG2   | 2.22                     | 0.54              |
| 26:c:158:PRO:HD3  | 43:v:22:MET:HE2   | 1.89                     | 0.54              |
| 35:l:355:ASP:OD1  | 35:l:357:ARG:NE   | 2.34                     | 0.54              |
| 40:r:403:THR:HA   | 40:r:406:TYR:CE2  | 2.42                     | 0.54              |
| 14:O:54:ASP:O     | 14:O:89:GLN:NE2   | 2.41                     | 0.54              |
| 18:T:45:TYR:HE1   | 18:T:51:ARG:HH21  | 1.55                     | 0.54              |
| 27:d:26:LEU:C     | 27:d:26:LEU:HD23  | 2.32                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:s:62:ARG:HH11  | 41:s:64:ALA:HA    | 1.72                     | 0.54              |
| 44:w:108:LEU:HD21 | 44:w:330:LYS:HE3  | 1.89                     | 0.54              |
| 16:Q:182:ASN:ND2  | 16:Q:403:PRO:HB2  | 2.22                     | 0.54              |
| 25:b:103:ARG:NH1  | 43:v:49:ALA:O     | 2.40                     | 0.54              |
| 38:o:121:LEU:HD23 | 38:o:123:GLN:HE21 | 1.72                     | 0.54              |
| 13:N:8:ARG:O      | 13:N:12:GLN:HG2   | 2.08                     | 0.54              |
| 19:U:65:ASP:O     | 19:U:74:GLN:HB3   | 2.08                     | 0.54              |
| 1:A:311:TRP:NE1   | 1:A:333:GLU:OE2   | 2.37                     | 0.54              |
| 9:J:166:HIS:HB3   | 9:J:200:ILE:HD13  | 1.90                     | 0.54              |
| 10:K:100:GLN:HB3  | 14:O:71:PRO:HA    | 1.90                     | 0.54              |
| 11:L:92:ASN:HB3   | 15:P:238:PRO:HA   | 1.89                     | 0.54              |
| 14:O:59:ASN:OD1   | 14:O:62:ARG:NH1   | 2.40                     | 0.54              |
| 43:v:18:ASP:OD1   | 43:v:18:ASP:C     | 2.50                     | 0.54              |
| 6:G:130:ILE:HG22  | 6:G:147:TYR:OH    | 2.07                     | 0.54              |
| 35:l:384:PRO:HA   | 35:l:389:PHE:CG   | 2.43                     | 0.54              |
| 1:A:185:ASN:OD1   | 1:A:190:GLY:N     | 2.20                     | 0.54              |
| 2:B:165:ASP:OD1   | 16:Q:368:ARG:NH2  | 2.41                     | 0.54              |
| 3:C:188:LYS:HB3   | 3:C:191:ARG:HD2   | 1.90                     | 0.54              |
| 9:J:206:ILE:HG12  | 9:J:245:VAL:HG21  | 1.90                     | 0.54              |
| 11:L:111:LEU:HD11 | 13:N:126:PRO:HG2  | 1.89                     | 0.54              |
| 30:g:36:MET:HE2   | 32:i:339:MET:HE2  | 1.88                     | 0.54              |
| 2:B:89:GLU:OE2    | 13:N:34:ARG:NH2   | 2.41                     | 0.54              |
| 6:X:85:TYR:OH     | 23:Z:22:TRP:NE1   | 2.30                     | 0.54              |
| 32:i:289:ASN:HA   | 32:i:292:PHE:CE2  | 2.42                     | 0.54              |
| 33:j:5:LEU:C      | 33:j:5:LEU:HD23   | 2.32                     | 0.54              |
| 35:l:186:MET:HE1  | 40:r:379:LEU:HD21 | 1.90                     | 0.54              |
| 41:s:154:LEU:HD12 | 41:s:159:SER:O    | 2.07                     | 0.54              |
| 25:b:28:LEU:HG    | 25:b:32:GLU:HG2   | 1.90                     | 0.53              |
| 35:l:407:TRP:CZ2  | 35:l:411:MET:HE3  | 2.43                     | 0.53              |
| 7:H:21:HIS:O      | 7:H:25:LYS:HG2    | 2.08                     | 0.53              |
| 25:b:99:GLU:CG    | 35:l:61:MET:HE2   | 2.38                     | 0.53              |
| 40:r:108:MET:HE3  | 40:r:121:LEU:HD11 | 1.91                     | 0.53              |
| 5:F:54:LEU:HD12   | 5:F:54:LEU:H      | 1.74                     | 0.53              |
| 23:Z:43:ASP:OD1   | 23:Z:43:ASP:O     | 2.26                     | 0.53              |
| 26:c:136:PHE:HD1  | 55:l:701:CDL:H851 | 1.74                     | 0.53              |
| 34:k:44:SER:HB2   | 34:k:59:MET:HE1   | 1.90                     | 0.53              |
| 12:M:36:VAL:HB    | 12:M:56:VAL:HG21  | 1.90                     | 0.53              |
| 34:k:8:ILE:HG21   | 34:k:43:MET:HB2   | 1.91                     | 0.53              |
| 35:l:288:THR:HG23 | 35:l:304:PHE:HD1  | 1.73                     | 0.53              |
| 35:l:559:GLU:O    | 35:l:563:PRO:HD2  | 2.09                     | 0.53              |
| 6:G:104:PHE:HA    | 6:G:108:LEU:HD12  | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:142:GLN:C     | 6:G:142:GLN:OE1   | 2.51                     | 0.53              |
| 16:Q:118:2MR:CD   | 16:Q:118:2MR:CQ2  | 2.86                     | 0.53              |
| 19:U:60:ASP:OD1   | 19:U:60:ASP:N     | 2.39                     | 0.53              |
| 1:A:342:LEU:HD22  | 1:A:347:THR:CG2   | 2.37                     | 0.53              |
| 5:F:36:PHE:HZ     | 5:F:91:LEU:HD13   | 1.72                     | 0.53              |
| 6:G:119:ILE:HG22  | 6:G:130:ILE:HD11  | 1.90                     | 0.53              |
| 7:H:96:ARG:NH1    | 7:H:96:ARG:CB     | 2.71                     | 0.53              |
| 9:J:238:GLN:N     | 9:J:326:ASP:OD2   | 2.41                     | 0.53              |
| 35:l:558:LEU:HB3  | 40:r:214:LEU:HD21 | 1.91                     | 0.53              |
| 37:n:50:ARG:HB3   | 37:n:51:PRO:HD2   | 1.91                     | 0.53              |
| 1:A:120:GLY:HA3   | 1:A:204:TYR:HD1   | 1.74                     | 0.53              |
| 4:E:68:MET:HE1    | 50:G:201:8Q1:C30  | 2.39                     | 0.53              |
| 35:l:250:SER:HB2  | 35:l:333:ALA:HA   | 1.89                     | 0.53              |
| 2:B:142:THR:O     | 2:B:187:LYS:NZ    | 2.42                     | 0.53              |
| 21:W:98:MET:CE    | 31:h:79:ILE:HA    | 2.39                     | 0.53              |
| 29:f:44:VAL:O     | 29:f:48:LEU:CD2   | 2.57                     | 0.53              |
| 30:g:122:ARG:O    | 38:o:109:ARG:NH2  | 2.33                     | 0.53              |
| 32:i:208:TYR:HA   | 32:i:211:MET:HE2  | 1.91                     | 0.53              |
| 35:l:111:ASP:OD1  | 39:p:97:TYR:OH    | 2.26                     | 0.53              |
| 44:w:58:LYS:HA    | 44:w:202:HIS:ND1  | 2.24                     | 0.53              |
| 1:A:448:GLU:HA    | 1:A:448:GLU:OE1   | 2.09                     | 0.53              |
| 1:A:456:GLN:CD    | 1:A:457:HIS:HD1   | 2.09                     | 0.53              |
| 5:F:46:LYS:HE2    | 12:M:674:LEU:HD21 | 1.90                     | 0.53              |
| 2:B:130:ILE:HD11  | 2:B:145:TYR:CE1   | 2.31                     | 0.53              |
| 22:Y:94:ASP:OD1   | 22:Y:99:ILE:HB    | 2.08                     | 0.53              |
| 6:G:115:GLN:NE2   | 6:G:138:LEU:O     | 2.41                     | 0.52              |
| 48:Q:501:PEE:H27  | 35:l:563:PRO:HA   | 1.91                     | 0.52              |
| 6:X:83:VAL:HG13   | 6:X:122:MET:HE3   | 1.91                     | 0.52              |
| 31:h:18:MET:HG3   | 31:h:18:MET:O     | 2.08                     | 0.52              |
| 35:l:400:ASN:HD22 | 35:l:409:LEU:HD21 | 1.74                     | 0.52              |
| 41:s:85:MET:CE    | 41:s:233:MET:HE2  | 2.39                     | 0.52              |
| 1:A:149:MET:HE1   | 1:A:241:THR:HB    | 1.92                     | 0.52              |
| 12:M:389:THR:HG21 | 12:M:473:MET:HG3  | 1.90                     | 0.52              |
| 41:s:85:MET:HE2   | 41:s:233:MET:HE2  | 1.91                     | 0.52              |
| 6:X:90:TYR:HE1    | 23:Z:44:PRO:HB2   | 1.74                     | 0.52              |
| 38:o:118:GLU:OE1  | 38:o:120:LYS:NZ   | 2.31                     | 0.52              |
| 15:P:46:THR:HG23  | 16:Q:358:VAL:HG22 | 1.88                     | 0.52              |
| 16:Q:282:ASP:CG   | 16:Q:437:LYS:HE2  | 2.33                     | 0.52              |
| 21:W:120:MET:HE1  | 36:m:126:VAL:CG1  | 2.40                     | 0.52              |
| 34:k:22:TYR:O     | 35:l:585:LYS:NZ   | 2.30                     | 0.52              |
| 35:l:5:ALA:HB2    | 35:l:61:MET:SD    | 2.49                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:159:ARG:NH2   | 14:O:176:CYS:O    | 2.42                     | 0.52              |
| 32:i:43:VAL:HG11  | 32:i:129:LEU:HD23 | 1.90                     | 0.52              |
| 36:m:1:MET:HE1    | 36:m:4:TYR:HA     | 1.90                     | 0.52              |
| 26:c:99:LEU:HD11  | 26:c:109:LEU:HD21 | 1.91                     | 0.52              |
| 3:C:113:MET:HE3   | 3:C:116:ALA:HB3   | 1.91                     | 0.52              |
| 30:g:32:ARG:HB2   | 30:g:78:LEU:HD11  | 1.91                     | 0.52              |
| 35:l:264:TYR:CD2  | 35:l:265:PRO:HD3  | 2.45                     | 0.52              |
| 36:m:165:VAL:O    | 36:m:169:MET:HG2  | 2.10                     | 0.52              |
| 42:u:83:THR:HA    | 42:u:86:TRP:CD1   | 2.45                     | 0.52              |
| 9:J:116:ILE:CG2   | 9:J:155:VAL:HG21  | 2.39                     | 0.52              |
| 12:M:462:PHE:O    | 12:M:466:LEU:HG   | 2.10                     | 0.52              |
| 35:l:272:LEU:O    | 35:l:276:MET:HG3  | 2.10                     | 0.52              |
| 1:A:69:LEU:HD11   | 1:A:143:LEU:HD21  | 1.92                     | 0.52              |
| 4:E:25:MET:O      | 4:E:29:LYS:HG3    | 2.10                     | 0.52              |
| 8:I:18:ARG:HG3    | 8:I:18:ARG:NH1    | 2.23                     | 0.52              |
| 6:X:103:HIS:HE1   | 6:X:105:MET:HG2   | 1.75                     | 0.52              |
| 26:c:148:GLU:OE1  | 35:l:275:THR:HG21 | 2.10                     | 0.52              |
| 26:c:165:ASP:OD2  | 26:c:170:ARG:NH2  | 2.43                     | 0.52              |
| 27:d:81:ASP:O     | 27:d:85:MET:HG3   | 2.10                     | 0.52              |
| 27:d:134:GLN:NE2  | 28:e:135:PRO:O    | 2.42                     | 0.52              |
| 28:e:140:ASN:HD22 | 28:e:144:PRO:HD3  | 1.75                     | 0.52              |
| 35:l:127:THR:HG22 | 35:l:147:VAL:HG13 | 1.92                     | 0.52              |
| 41:s:62:ARG:HH21  | 41:s:68:ILE:HB    | 1.74                     | 0.52              |
| 2:B:211:TYR:CZ    | 8:I:39:PRO:HG3    | 2.45                     | 0.51              |
| 2:B:119:CYS:SG    | 2:B:145:TYR:OH    | 2.62                     | 0.51              |
| 5:F:29:GLY:HA2    | 5:F:81:ASN:OD1    | 2.11                     | 0.51              |
| 35:l:343:SER:O    | 35:l:347:ILE:HG13 | 2.10                     | 0.51              |
| 37:n:46:LYS:NZ    | 37:n:46:LYS:CB    | 2.73                     | 0.51              |
| 9:J:163:LYS:NZ    | 9:J:253:ILE:O     | 2.38                     | 0.51              |
| 12:M:339:ALA:HB3  | 12:M:542:PRO:HG3  | 1.91                     | 0.51              |
| 12:M:400:ILE:HG12 | 12:M:473:MET:HB3  | 1.92                     | 0.51              |
| 13:N:78:ASP:OD1   | 13:N:78:ASP:N     | 2.42                     | 0.51              |
| 1:A:71:LYS:HD3    | 1:A:75:TRP:CE3    | 2.45                     | 0.51              |
| 4:E:114:ARG:HD3   | 4:E:115:PRO:HD2   | 1.93                     | 0.51              |
| 12:M:372:PHE:H    | 12:M:532:PRO:HB2  | 1.75                     | 0.51              |
| 14:O:98:MET:HE2   | 14:O:116:ALA:CB   | 2.41                     | 0.51              |
| 22:Y:47:PHE:HZ    | 35:l:364:LYS:HG3  | 1.74                     | 0.51              |
| 23:Z:57:PHE:O     | 35:l:434:LYS:NZ   | 2.38                     | 0.51              |
| 33:j:6:THR:HG21   | 41:s:87:VAL:HG11  | 1.91                     | 0.51              |
| 3:C:92:VAL:HG12   | 41:s:25:ARG:HH12  | 1.74                     | 0.51              |
| 4:E:22:SER:HB2    | 4:E:27:GLU:HB2    | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:90:LEU:HB2    | 15:P:102:ASP:HB3  | 1.92                     | 0.51              |
| 20:V:107:SER:HB3  | 20:V:110:ILE:HB   | 1.91                     | 0.51              |
| 35:l:51:LEU:O     | 35:l:55:MET:HG3   | 2.11                     | 0.51              |
| 9:J:116:ILE:HG22  | 9:J:155:VAL:HG21  | 1.93                     | 0.51              |
| 12:M:512:VAL:O    | 12:M:514:ASN:ND2  | 2.43                     | 0.51              |
| 13:N:124:TYR:HD1  | 18:T:61:GLU:HG3   | 1.75                     | 0.51              |
| 21:W:85:GLN:O     | 21:W:89:GLU:HG3   | 2.10                     | 0.51              |
| 32:i:279:PRO:HA   | 32:i:282:MET:HG3  | 1.93                     | 0.51              |
| 36:m:173:ARG:HH11 | 36:m:173:ARG:CG   | 2.23                     | 0.51              |
| 7:H:40:LYS:HA     | 7:H:45:ARG:HD3    | 1.93                     | 0.51              |
| 16:Q:259:GLU:HB3  | 21:W:25:LEU:HD11  | 1.92                     | 0.51              |
| 24:a:79:GLY:HA3   | 55:a:201:CDL:H222 | 1.93                     | 0.51              |
| 25:b:117:ILE:HD13 | 25:b:117:ILE:N    | 2.25                     | 0.51              |
| 2:B:130:ILE:CD1   | 2:B:145:TYR:HE1   | 2.18                     | 0.51              |
| 48:Q:502:PEE:H20  | 41:s:183:MET:CE   | 2.41                     | 0.51              |
| 38:o:50:GLN:NE2   | 38:o:60:ILE:HG23  | 2.26                     | 0.51              |
| 1:A:456:GLN:CD    | 1:A:457:HIS:ND1   | 2.65                     | 0.51              |
| 2:B:76:TYR:CE1    | 41:s:33:LEU:HD13  | 2.46                     | 0.51              |
| 43:v:103:GLU:O    | 43:v:107:ARG:HG2  | 2.11                     | 0.51              |
| 2:B:48:MET:O      | 19:U:10:LYS:NZ    | 2.31                     | 0.51              |
| 14:O:130:TYR:HA   | 14:O:189:ASN:HD21 | 1.76                     | 0.51              |
| 21:W:130:ASN:HA   | 21:W:133:ILE:HD12 | 1.91                     | 0.51              |
| 22:Y:96:GLU:CD    | 22:Y:96:GLU:H     | 2.19                     | 0.51              |
| 32:i:245:MET:HE1  | 55:i:402:CDL:H171 | 1.93                     | 0.51              |
| 35:l:245:ALA:O    | 35:l:249:SER:OG   | 2.26                     | 0.51              |
| 1:A:48:ARG:HD2    | 10:K:70:ASN:O     | 2.11                     | 0.50              |
| 5:F:36:PHE:CD2    | 5:F:87:VAL:CG2    | 2.91                     | 0.50              |
| 11:L:90:GLY:HA3   | 15:P:238:PRO:HB2  | 1.91                     | 0.50              |
| 12:M:403:VAL:HG11 | 12:M:452:LEU:HD21 | 1.93                     | 0.50              |
| 15:P:148:ASP:N    | 15:P:148:ASP:OD1  | 2.43                     | 0.50              |
| 20:V:4:THR:CG2    | 20:V:8:LYS:HZ2    | 2.19                     | 0.50              |
| 26:c:149:ILE:HG22 | 26:c:150:TYR:CD1  | 2.46                     | 0.50              |
| 33:j:90:MET:SD    | 36:m:151:THR:HG23 | 2.51                     | 0.50              |
| 35:l:71:LEU:HD23  | 40:r:310:MET:HE1  | 1.93                     | 0.50              |
| 2:B:146:ASP:CG    | 11:L:112:MET:HE1  | 2.36                     | 0.50              |
| 25:b:32:GLU:HG3   | 39:p:115:TYR:HA   | 1.93                     | 0.50              |
| 44:w:65:ASN:OD1   | 44:w:66:ILE:N     | 2.45                     | 0.50              |
| 16:Q:251:PHE:HB3  | 16:Q:341:LEU:HD11 | 1.94                     | 0.50              |
| 32:i:132:THR:HG22 | 32:i:212:THR:CG2  | 2.34                     | 0.50              |
| 34:k:25:HIS:O     | 34:k:28:SER:N     | 2.35                     | 0.50              |
| 35:l:221:ALA:HA   | 35:l:226:GLN:HG2  | 1.92                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:p:11:THR:O     | 39:p:15:LYS:HG3   | 2.11                     | 0.50              |
| 12:M:141:ASP:O    | 12:M:145:MET:HG2  | 2.12                     | 0.50              |
| 14:O:186:VAL:HG12 | 14:O:193:TYR:HB2  | 1.93                     | 0.50              |
| 24:a:131:LYS:HD2  | 37:n:57:TRP:CE3   | 2.46                     | 0.50              |
| 24:a:137:MET:HE1  | 37:n:42:SER:HB3   | 1.93                     | 0.50              |
| 32:i:239:VAL:O    | 32:i:243:LEU:HG   | 2.11                     | 0.50              |
| 55:i:402:CDL:H142 | 40:r:94:LEU:HD13  | 1.93                     | 0.50              |
| 35:l:292:ALA:HB2  | 35:l:304:PHE:HB3  | 1.92                     | 0.50              |
| 1:A:398:ARG:NH1   | 12:M:155:GLU:OE1  | 2.40                     | 0.50              |
| 3:C:83:ARG:NH1    | 16:Q:212:GLU:OE2  | 2.32                     | 0.50              |
| 6:G:103:HIS:CE1   | 6:G:105:MET:HB2   | 2.46                     | 0.50              |
| 11:L:163:ASN:O    | 11:L:171:ARG:HA   | 2.12                     | 0.50              |
| 4:E:40:TYR:HE2    | 6:G:117:GLU:HG2   | 1.76                     | 0.50              |
| 6:G:84:LEU:O      | 6:G:88:LYS:HG2    | 2.12                     | 0.50              |
| 9:J:38:HIS:NE2    | 13:N:132:LYS:HD2  | 2.27                     | 0.50              |
| 12:M:676:ASN:O    | 12:M:678:GLN:NE2  | 2.44                     | 0.50              |
| 14:O:130:TYR:HA   | 14:O:189:ASN:ND2  | 2.27                     | 0.50              |
| 34:k:57:ASN:HB3   | 36:m:143:ILE:HG13 | 1.94                     | 0.50              |
| 39:p:164:PRO:O    | 39:p:167:TRP:HD1  | 1.94                     | 0.50              |
| 40:r:378:GLU:OE2  | 40:r:378:GLU:HA   | 2.12                     | 0.50              |
| 7:H:96:ARG:HH11   | 7:H:96:ARG:CB     | 2.24                     | 0.50              |
| 15:P:106:ALA:HB1  | 15:P:108:PHE:CE1  | 2.47                     | 0.50              |
| 16:Q:39:PRO:HB3   | 16:Q:43:TRP:CD1   | 2.47                     | 0.50              |
| 6:X:110:LEU:HD12  | 6:X:114:ASP:HB3   | 1.92                     | 0.50              |
| 13:N:106:ARG:HB2  | 13:N:109:ILE:HG13 | 1.93                     | 0.50              |
| 16:Q:82:LEU:CD1   | 16:Q:101:LEU:HD13 | 2.41                     | 0.50              |
| 55:i:402:CDL:H662 | 55:i:402:CDL:H612 | 1.93                     | 0.50              |
| 33:j:15:SER:HA    | 41:s:76:ILE:HD12  | 1.94                     | 0.50              |
| 35:l:293:ILE:HG23 | 35:l:294:THR:HG23 | 1.94                     | 0.50              |
| 3:C:71:CYS:HB3    | 16:Q:141:TYR:CG   | 2.47                     | 0.50              |
| 8:I:94:ALA:HB1    | 15:P:105:ASN:HD21 | 1.77                     | 0.50              |
| 9:J:37:HIS:CE1    | 18:T:49:ASP:HA    | 2.47                     | 0.50              |
| 35:l:65:ASN:OD1   | 35:l:66:TRP:N     | 2.42                     | 0.50              |
| 35:l:521:LYS:HB3  | 35:l:525:MET:HE1  | 1.94                     | 0.50              |
| 12:M:29:SER:OG    | 12:M:30:ASN:N     | 2.45                     | 0.49              |
| 15:P:61:PHE:O     | 15:P:65:VAL:HG22  | 2.12                     | 0.49              |
| 24:a:168:TRP:HB3  | 30:g:2:THR:O      | 2.12                     | 0.49              |
| 25:b:19:ARG:HD2   | 39:p:171:VAL:O    | 2.11                     | 0.49              |
| 31:h:69:ARG:O     | 31:h:73:MET:HG3   | 2.12                     | 0.49              |
| 32:i:347:ASN:N    | 32:i:347:ASN:OD1  | 2.45                     | 0.49              |
| 35:l:407:TRP:CE2  | 35:l:411:MET:HE3  | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:r:196:TRP:CD1  | 40:r:250:LEU:HB3  | 2.47                     | 0.49              |
| 40:r:225:ILE:O    | 40:r:229:MET:HG3  | 2.12                     | 0.49              |
| 41:s:25:ARG:HD2   | 56:s:401:UQ:HM21  | 1.94                     | 0.49              |
| 41:s:85:MET:SD    | 41:s:108:MET:HB2  | 2.51                     | 0.49              |
| 41:s:87:VAL:HG22  | 41:s:88:PRO:HD3   | 1.80                     | 0.49              |
| 19:U:14:ALA:O     | 19:U:15:LYS:HG2   | 2.12                     | 0.49              |
| 20:V:4:THR:O      | 20:V:8:LYS:HG3    | 2.12                     | 0.49              |
| 24:a:106:VAL:CG1  | 37:n:50:ARG:HH21  | 2.02                     | 0.49              |
| 35:l:525:MET:CE   | 35:l:528:TYR:HE1  | 2.12                     | 0.49              |
| 42:u:59:GLU:O     | 42:u:63:VAL:HG13  | 2.12                     | 0.49              |
| 43:v:83:GLU:OE1   | 43:v:83:GLU:N     | 2.44                     | 0.49              |
| 1:A:270:ASN:HD21  | 1:A:340:ASP:H     | 1.59                     | 0.49              |
| 4:E:79:VAL:O      | 4:E:83:VAL:HG23   | 2.11                     | 0.49              |
| 4:E:87:LYS:O      | 4:E:91:GLU:HG3    | 2.11                     | 0.49              |
| 7:H:83:GLN:HE21   | 15:P:104:THR:HA   | 1.77                     | 0.49              |
| 24:a:156:VAL:HG13 | 24:a:160:MET:HE3  | 1.94                     | 0.49              |
| 35:l:131:LEU:O    | 35:l:140:LEU:CD1  | 2.61                     | 0.49              |
| 1:A:384:PRO:HB2   | 1:A:423:THR:HG22  | 1.92                     | 0.49              |
| 7:H:7:LYS:HG3     | 7:H:8:THR:HG23    | 1.94                     | 0.49              |
| 7:H:94:MET:HE1    | 7:H:99:PRO:HG2    | 1.93                     | 0.49              |
| 32:i:18:MET:HE3   | 32:i:22:ILE:CG2   | 2.43                     | 0.49              |
| 44:w:84:ARG:HD3   | 44:w:149:HIS:HD2  | 1.77                     | 0.49              |
| 44:w:288:ASP:OD1  | 44:w:289:ARG:N    | 2.45                     | 0.49              |
| 9:J:135:GLU:OE1   | 9:J:179:ARG:NH2   | 2.46                     | 0.49              |
| 16:Q:53:TYR:HE1   | 48:Q:501:PEE:H2   | 1.77                     | 0.49              |
| 38:o:116:ILE:HG12 | 38:o:123:GLN:NE2  | 2.28                     | 0.49              |
| 1:A:115:VAL:HG22  | 1:A:248:VAL:HG21  | 1.94                     | 0.49              |
| 2:B:146:ASP:OD2   | 11:L:112:MET:HE1  | 2.13                     | 0.49              |
| 22:Y:72:ARG:HA    | 22:Y:72:ARG:NE    | 2.28                     | 0.49              |
| 26:c:184:TYR:HA   | 43:v:34:ARG:NH1   | 2.28                     | 0.49              |
| 39:p:100:PRO:HG3  | 40:r:419:TYR:CE1  | 2.48                     | 0.49              |
| 40:r:357:THR:O    | 40:r:361:VAL:HG23 | 2.13                     | 0.49              |
| 44:w:110:GLY:HA2  | 44:w:134:TRP:CD2  | 2.48                     | 0.49              |
| 1:A:131:ILE:HD11  | 1:A:245:VAL:HG21  | 1.95                     | 0.49              |
| 12:M:483:ARG:HB2  | 12:M:483:ARG:NH1  | 2.27                     | 0.49              |
| 32:i:100:MET:HE2  | 32:i:153:LEU:HD21 | 1.94                     | 0.49              |
| 40:r:45:LEU:HD23  | 40:r:45:LEU:H     | 1.77                     | 0.49              |
| 6:G:91:ASP:OD1    | 6:G:91:ASP:N      | 2.42                     | 0.49              |
| 12:M:321:ASP:O    | 12:M:325:ARG:HG3  | 2.13                     | 0.49              |
| 17:S:69:ILE:HD11  | 42:u:68:LEU:HD23  | 1.94                     | 0.49              |
| 24:a:150:ARG:NH1  | 42:u:166:ARG:O    | 2.46                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:l:159:HIS:NE2  | 39:p:96:CYS:HB2   | 2.28                     | 0.49              |
| 35:l:568:PHE:CE1  | 35:l:572:LYS:HE3  | 2.47                     | 0.49              |
| 36:m:1:MET:HE3    | 36:m:4:TYR:N      | 2.28                     | 0.49              |
| 44:w:165:SER:HB3  | 44:w:245:PHE:CZ   | 2.47                     | 0.49              |
| 4:E:44:PRO:HD3    | 4:E:60:ARG:HH12   | 1.77                     | 0.49              |
| 5:F:31:GLN:NE2    | 5:F:35:ASP:OD1    | 2.43                     | 0.49              |
| 8:I:40:LYS:HB3    | 21:W:7:LYS:H      | 1.78                     | 0.49              |
| 9:J:47:GLY:HA3    | 15:P:225:GLU:OE1  | 2.13                     | 0.49              |
| 16:Q:159:LEU:O    | 16:Q:160:ASN:CB   | 2.59                     | 0.49              |
| 16:Q:182:ASN:HD22 | 16:Q:403:PRO:HB2  | 1.78                     | 0.49              |
| 17:S:54:ILE:HD11  | 31:h:106:PRO:HB3  | 1.94                     | 0.49              |
| 20:V:69:ILE:HG21  | 20:V:100:THR:HG21 | 1.94                     | 0.49              |
| 6:X:132:ASP:HB3   | 39:p:18:ARG:NE    | 2.24                     | 0.49              |
| 36:m:17:PHE:HA    | 36:m:20:PHE:CE2   | 2.48                     | 0.49              |
| 20:V:5:LEU:HA     | 20:V:8:LYS:HG3    | 1.94                     | 0.49              |
| 1:A:151:ALA:O     | 1:A:191:TYR:OH    | 2.21                     | 0.48              |
| 15:P:44:ARG:HB3   | 15:P:45:PRO:CD    | 2.43                     | 0.48              |
| 55:a:201:CDL:H541 | 48:l:703:PEE:H16  | 1.95                     | 0.48              |
| 40:r:12:LEU:HB2   | 40:r:13:PRO:HD3   | 1.95                     | 0.48              |
| 33:j:3:ILE:HG12   | 48:m:201:PEE:H50  | 1.95                     | 0.48              |
| 35:l:190:LEU:HD11 | 40:r:307:TRP:CH2  | 2.48                     | 0.48              |
| 5:F:83:SER:O      | 5:F:87:VAL:HG22   | 2.13                     | 0.48              |
| 20:V:106:ARG:NE   | 20:V:106:ARG:CA   | 2.73                     | 0.48              |
| 6:X:117:GLU:OE2   | 39:p:20:TYR:OH    | 2.29                     | 0.48              |
| 26:c:164:ASN:HA   | 26:c:181:VAL:HG12 | 1.95                     | 0.48              |
| 32:i:276:ILE:HG21 | 48:r:501:PEE:H14  | 1.94                     | 0.48              |
| 44:w:350:LYS:HB3  | 44:w:351:TRP:CZ3  | 2.48                     | 0.48              |
| 1:A:195:VAL:O     | 10:K:97:ARG:NH1   | 2.41                     | 0.48              |
| 3:C:55:ASN:ND2    | 3:C:187:GLU:O     | 2.45                     | 0.48              |
| 6:G:103:HIS:HB3   | 6:G:107:ASP:OD1   | 2.13                     | 0.48              |
| 13:N:32:ASP:OD2   | 13:N:58:ARG:NH2   | 2.46                     | 0.48              |
| 48:Q:502:PEE:H51  | 48:Q:502:PEE:H60  | 1.95                     | 0.48              |
| 26:c:152:SER:HA   | 43:v:5:LEU:HD11   | 1.96                     | 0.48              |
| 43:v:17:PRO:HB3   | 43:v:105:GLU:OE1  | 2.13                     | 0.48              |
| 44:w:353:TRP:H    | 44:w:353:TRP:CD1  | 2.31                     | 0.48              |
| 2:B:200:GLU:OE2   | 13:N:88:ARG:HB2   | 2.13                     | 0.48              |
| 12:M:278:HIS:CE1  | 12:M:280:ASP:HB2  | 2.48                     | 0.48              |
| 21:W:120:MET:CE   | 36:m:126:VAL:CG1  | 2.90                     | 0.48              |
| 32:i:106:LEU:HD22 | 32:i:187:MET:HE2  | 1.95                     | 0.48              |
| 38:o:3:PHE:CZ     | 39:p:70:GLU:HG3   | 2.48                     | 0.48              |
| 43:v:18:ASP:OD1   | 43:v:18:ASP:O     | 2.32                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:157:TYR:CD2   | 1:A:212:LEU:CD1   | 2.96                     | 0.48              |
| 3:C:61:SER:HG     | 41:s:54:LYS:HD3   | 1.77                     | 0.48              |
| 48:Q:501:PEE:H37  | 48:Q:501:PEE:H60  | 1.95                     | 0.48              |
| 35:l:62:ILE:HD13  | 35:l:81:LYS:HA    | 1.94                     | 0.48              |
| 41:s:51:ASP:HB3   | 56:s:401:UQ:H8    | 1.96                     | 0.48              |
| 1:A:116:ASN:O     | 1:A:245:VAL:HG23  | 2.14                     | 0.48              |
| 6:G:75:THR:OG1    | 6:G:156:GLU:OE1   | 2.31                     | 0.48              |
| 18:T:29:VAL:HG21  | 18:T:64:GLU:OE1   | 2.13                     | 0.48              |
| 39:p:162:ASP:OD1  | 39:p:162:ASP:N    | 2.47                     | 0.48              |
| 2:B:130:ILE:HG12  | 2:B:145:TYR:HD1   | 1.78                     | 0.48              |
| 9:J:257:ASP:O     | 9:J:261:LYS:NZ    | 2.45                     | 0.48              |
| 15:P:46:THR:HG22  | 15:P:46:THR:O     | 2.13                     | 0.48              |
| 22:Y:47:PHE:HE2   | 22:Y:50:LEU:HD11  | 1.79                     | 0.48              |
| 40:r:433:GLU:O    | 40:r:437:MET:HG2  | 2.14                     | 0.48              |
| 1:A:88:ARG:HB2    | 1:A:247:THR:OG1   | 2.14                     | 0.48              |
| 1:A:296:LEU:HD13  | 1:A:337:MET:SD    | 2.54                     | 0.48              |
| 6:G:74:LEU:H      | 6:G:74:LEU:HD23   | 1.78                     | 0.48              |
| 6:G:74:LEU:HD12   | 6:G:79:ILE:HD11   | 1.96                     | 0.48              |
| 6:G:128:PHE:HE1   | 6:G:148:ILE:CD1   | 2.26                     | 0.48              |
| 13:N:5:GLN:O      | 13:N:9:ARG:HG3    | 2.14                     | 0.48              |
| 14:O:130:TYR:HB2  | 14:O:169:PHE:HD1  | 1.79                     | 0.48              |
| 21:W:51:MET:HA    | 41:s:313:SER:HB2  | 1.95                     | 0.48              |
| 26:c:59:VAL:HG12  | 26:c:60:GLU:OE1   | 2.14                     | 0.48              |
| 35:l:127:THR:HG21 | 35:l:146:GLY:C    | 2.39                     | 0.48              |
| 14:O:56:THR:HG21  | 14:O:58:GLU:OE2   | 2.14                     | 0.47              |
| 15:P:64:TYR:HH    | 15:P:103:HIS:HE2  | 1.61                     | 0.47              |
| 32:i:128:LEU:HD23 | 32:i:128:LEU:O    | 2.13                     | 0.47              |
| 41:s:7:LEU:O      | 41:s:11:ILE:HG12  | 2.14                     | 0.47              |
| 12:M:341:ILE:HD11 | 12:M:537:ILE:HG13 | 1.95                     | 0.47              |
| 15:P:68:ILE:HG22  | 15:P:69:LEU:HG    | 1.96                     | 0.47              |
| 16:Q:133:LEU:HD22 | 16:Q:228:ARG:HD3  | 1.96                     | 0.47              |
| 25:b:120:MET:HE1  | 43:v:61:HIS:HA    | 1.96                     | 0.47              |
| 40:r:150:LEU:O    | 40:r:153:THR:OG1  | 2.25                     | 0.47              |
| 41:s:101:GLY:O    | 41:s:105:MET:HG3  | 2.14                     | 0.47              |
| 1:A:338:ASP:OD1   | 1:A:338:ASP:C     | 2.58                     | 0.47              |
| 2:B:210:LEU:HD12  | 8:I:38:PRO:HB3    | 1.96                     | 0.47              |
| 9:J:369:VAL:HG12  | 9:J:370:LYS:HG2   | 1.96                     | 0.47              |
| 14:O:64:GLU:OE1   | 14:O:64:GLU:O     | 2.32                     | 0.47              |
| 16:Q:192:LEU:HD12 | 16:Q:197:MET:HB2  | 1.95                     | 0.47              |
| 17:S:1:MET:HB2    | 17:S:3:PHE:CE2    | 2.49                     | 0.47              |
| 6:X:88:LYS:HG3    | 6:X:98:LEU:HD21   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:i:146:SER:HA   | 32:i:149:ILE:HG23 | 1.96                     | 0.47              |
| 35:l:1:MET:O      | 35:l:1:MET:SD     | 2.72                     | 0.47              |
| 1:A:256:ARG:CG    | 14:O:245:VAL:HG12 | 2.43                     | 0.47              |
| 17:S:66:LEU:O     | 17:S:69:ILE:HG22  | 2.15                     | 0.47              |
| 24:a:95:GLU:OE2   | 55:a:201:CDL:O1   | 2.23                     | 0.47              |
| 24:a:156:VAL:CG1  | 24:a:160:MET:HE3  | 2.45                     | 0.47              |
| 26:c:36:MET:O     | 26:c:36:MET:HG2   | 2.14                     | 0.47              |
| 32:i:128:LEU:C    | 32:i:128:LEU:CD2  | 2.86                     | 0.47              |
| 33:j:60:ILE:HG21  | 36:m:168:ILE:HG21 | 1.97                     | 0.47              |
| 48:r:501:PEE:H79  | 48:r:501:PEE:H41  | 1.95                     | 0.47              |
| 12:M:178:GLN:HB3  | 12:M:204:MET:HE2  | 1.97                     | 0.47              |
| 15:P:132:LEU:HB2  | 15:P:141:ILE:HG22 | 1.94                     | 0.47              |
| 32:i:236:LYS:NZ   | 32:i:314:LYS:O    | 2.43                     | 0.47              |
| 37:n:50:ARG:HB2   | 37:n:53:GLU:CB    | 2.44                     | 0.47              |
| 39:p:26:HIS:ND1   | 39:p:75:GLN:O     | 2.48                     | 0.47              |
| 39:p:92:GLU:HB3   | 39:p:95:GLU:HG3   | 1.97                     | 0.47              |
| 44:w:57:SER:O     | 44:w:156:GLY:HA3  | 2.14                     | 0.47              |
| 12:M:650:SER:OG   | 12:M:652:ASN:OD1  | 2.31                     | 0.47              |
| 24:a:106:VAL:O    | 37:n:50:ARG:NH2   | 2.48                     | 0.47              |
| 24:a:140:LEU:HD21 | 40:r:177:LEU:HB3  | 1.97                     | 0.47              |
| 35:l:137:LEU:HD13 | 35:l:186:MET:HG2  | 1.95                     | 0.47              |
| 41:s:24:GLU:HA    | 41:s:271:LEU:HD13 | 1.95                     | 0.47              |
| 1:A:213:ILE:HG23  | 1:A:235:VAL:HA    | 1.96                     | 0.47              |
| 2:B:90:LYS:NZ     | 2:B:174:GLU:OE2   | 2.48                     | 0.47              |
| 3:C:166:CYS:SG    | 16:Q:138:ARG:NH2  | 2.76                     | 0.47              |
| 10:K:98:MET:SD    | 10:K:98:MET:N     | 2.88                     | 0.47              |
| 21:W:88:ARG:HG2   | 42:u:10:LEU:HG    | 1.97                     | 0.47              |
| 6:X:115:GLN:NE2   | 6:X:138:LEU:O     | 2.46                     | 0.47              |
| 35:l:233:LEU:HB3  | 35:l:234:PRO:HD3  | 1.97                     | 0.47              |
| 41:s:85:MET:CE    | 41:s:233:MET:CE   | 2.93                     | 0.47              |
| 1:A:244:ASN:O     | 1:A:248:VAL:HG23  | 2.15                     | 0.47              |
| 9:J:243:VAL:HG12  | 9:J:247:LYS:HE2   | 1.96                     | 0.47              |
| 20:V:96:ALA:O     | 20:V:100:THR:HG23 | 2.15                     | 0.47              |
| 23:Z:43:ASP:OD1   | 23:Z:43:ASP:C     | 2.56                     | 0.47              |
| 26:c:58:ARG:NH2   | 26:c:60:GLU:HG3   | 2.30                     | 0.47              |
| 26:c:182:VAL:HG13 | 43:v:34:ARG:NH2   | 2.29                     | 0.47              |
| 27:d:43:ARG:HB3   | 27:d:44:PRO:HD3   | 1.97                     | 0.47              |
| 33:j:24:LEU:HB3   | 33:j:25:PRO:HD3   | 1.97                     | 0.47              |
| 1:A:146:GLY:HA3   | 1:A:193:PHE:CE1   | 2.50                     | 0.47              |
| 2:B:137:ASP:OD1   | 2:B:137:ASP:N     | 2.37                     | 0.47              |
| 12:M:478:SER:O    | 12:M:482:GLN:HG2  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:M:560:LEU:HD23 | 12:M:564:CYS:SG   | 2.55                     | 0.47              |
| 18:T:114:CYS:SG   | 18:T:116:LEU:HG   | 2.55                     | 0.47              |
| 18:T:119:ARG:HH11 | 18:T:119:ARG:HG2  | 1.79                     | 0.47              |
| 21:W:50:MET:HE3   | 21:W:50:MET:HA    | 1.96                     | 0.47              |
| 25:b:10:LEU:HD22  | 25:b:14:GLN:NE2   | 2.30                     | 0.47              |
| 26:c:50:ALA:HA    | 26:c:53:LYS:HD3   | 1.96                     | 0.47              |
| 26:c:149:ILE:O    | 26:c:151:PRO:HD3  | 2.14                     | 0.47              |
| 27:d:68:PHE:CD1   | 37:n:44:LEU:HD11  | 2.48                     | 0.47              |
| 29:f:40:ASP:O     | 29:f:44:VAL:CG2   | 2.62                     | 0.47              |
| 7:H:76:GLN:HB2    | 7:H:79:GLU:OE2    | 2.15                     | 0.47              |
| 16:Q:412:VAL:HB   | 16:Q:421:ARG:HB3  | 1.96                     | 0.47              |
| 19:U:24:ALA:HB2   | 48:U:101:PEE:H72  | 1.97                     | 0.47              |
| 19:U:45:ILE:HD11  | 19:U:81:LEU:HD13  | 1.97                     | 0.47              |
| 39:p:144:THR:HG22 | 39:p:145:PRO:O    | 2.14                     | 0.47              |
| 40:r:48:ASN:N     | 40:r:48:ASN:OD1   | 2.48                     | 0.47              |
| 48:r:501:PEE:H26  | 48:r:501:PEE:H60  | 1.97                     | 0.47              |
| 1:A:410:ASP:OD1   | 1:A:443:ARG:NH2   | 2.32                     | 0.46              |
| 7:H:22:GLU:O      | 7:H:26:ILE:HG13   | 2.14                     | 0.46              |
| 15:P:103:HIS:CD2  | 15:P:105:ASN:HB2  | 2.49                     | 0.46              |
| 32:i:278:MET:O    | 32:i:282:MET:HG3  | 2.15                     | 0.46              |
| 39:p:176:GLU:HG3  | 39:p:177:ARG:HG2  | 1.97                     | 0.46              |
| 41:s:104:PHE:O    | 41:s:108:MET:HG2  | 2.15                     | 0.46              |
| 12:M:133:GLN:HG3  | 12:M:136:GLU:HG3  | 1.96                     | 0.46              |
| 12:M:360:ARG:HH21 | 12:M:632:MET:CA   | 2.26                     | 0.46              |
| 6:X:136:GLU:OE1   | 39:p:18:ARG:NE    | 2.48                     | 0.46              |
| 27:d:78:GLU:CD    | 30:g:108:LYS:HB3  | 2.35                     | 0.46              |
| 29:f:39:PRO:HG2   | 44:w:351:TRP:CG   | 2.51                     | 0.46              |
| 32:i:278:MET:O    | 32:i:282:MET:CG   | 2.63                     | 0.46              |
| 34:k:22:TYR:HB3   | 35:l:585:LYS:HG2  | 1.97                     | 0.46              |
| 40:r:343:ILE:O    | 40:r:346:ARG:NE   | 2.31                     | 0.46              |
| 1:A:157:TYR:CD1   | 1:A:212:LEU:CD1   | 2.98                     | 0.46              |
| 12:M:307:ILE:HG23 | 12:M:317:THR:HG21 | 1.97                     | 0.46              |
| 48:U:101:PEE:H35  | 48:U:101:PEE:H30  | 1.78                     | 0.46              |
| 36:m:23:LYS:N     | 36:m:24:PRO:HD3   | 2.30                     | 0.46              |
| 40:r:447:LEU:HD11 | 49:r:503:PLX:H371 | 1.98                     | 0.46              |
| 2:B:198:GLU:OE1   | 2:B:202:ALA:HB2   | 2.16                     | 0.46              |
| 12:M:381:LEU:HD22 | 12:M:664:TYR:HD2  | 1.80                     | 0.46              |
| 35:l:534:HIS:CD2  | 48:l:702:PEE:H13  | 2.50                     | 0.46              |
| 42:u:40:ASN:O     | 42:u:44:MET:HG2   | 2.15                     | 0.46              |
| 3:C:48:ALA:HB2    | 3:C:191:ARG:HH12  | 1.80                     | 0.46              |
| 3:C:96:SER:HB3    | 3:C:99:GLN:NE2    | 2.31                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 20:V:53:VAL:HA    | 20:V:56:THR:HG22  | 1.98                     | 0.46              |
| 34:k:23:ARG:HD3   | 36:m:23:LYS:HB2   | 1.98                     | 0.46              |
| 35:l:407:TRP:O    | 35:l:411:MET:HG2  | 2.14                     | 0.46              |
| 49:r:503:PLX:H121 | 49:r:503:PLX:H152 | 1.47                     | 0.46              |
| 44:w:59:VAL:HG13  | 44:w:201:PRO:HA   | 1.96                     | 0.46              |
| 2:B:98:ARG:NH2    | 16:Q:224:ALA:O    | 2.42                     | 0.46              |
| 14:O:197:THR:H    | 14:O:200:ASP:HB2  | 1.81                     | 0.46              |
| 16:Q:95:LEU:HB2   | 16:Q:458:PHE:CZ   | 2.50                     | 0.46              |
| 19:U:82:LYS:HB3   | 19:U:82:LYS:HE2   | 1.74                     | 0.46              |
| 21:W:70:ALA:HB2   | 42:u:125:LEU:HD13 | 1.97                     | 0.46              |
| 40:r:445:LEU:O    | 40:r:448:THR:HG22 | 2.16                     | 0.46              |
| 9:J:207:PHE:HB2   | 9:J:214:LEU:HD13  | 1.97                     | 0.46              |
| 12:M:325:ARG:HB3  | 12:M:325:ARG:CZ   | 2.46                     | 0.46              |
| 18:T:104:LYS:HD2  | 18:T:107:LYS:CE   | 2.45                     | 0.46              |
| 21:W:119:PRO:O    | 36:m:130:THR:OG1  | 2.29                     | 0.46              |
| 6:X:91:ASP:OD1    | 6:X:91:ASP:N      | 2.48                     | 0.46              |
| 26:c:56:ASN:ND2   | 38:o:43:LEU:HD21  | 2.31                     | 0.46              |
| 35:l:88:MET:CE    | 35:l:468:ILE:HD12 | 2.45                     | 0.46              |
| 35:l:298:ILE:O    | 35:l:302:VAL:HG23 | 2.16                     | 0.46              |
| 2:B:74:LEU:HB2    | 41:s:272:TRP:CZ2  | 2.49                     | 0.46              |
| 14:O:46:GLU:N     | 14:O:46:GLU:OE2   | 2.49                     | 0.46              |
| 16:Q:443:MET:HE3  | 16:Q:443:MET:HB3  | 1.89                     | 0.46              |
| 43:v:15:LYS:NZ    | 43:v:110:GLN:HE22 | 2.14                     | 0.46              |
| 44:w:182:GLN:HB3  | 44:w:314:LEU:HD21 | 1.98                     | 0.46              |
| 44:w:223:ASN:HB3  | 44:w:226:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:209:GLU:OE1   | 47:A:503:NAI:O3B  | 2.24                     | 0.46              |
| 9:J:243:VAL:O     | 9:J:247:LYS:HG3   | 2.16                     | 0.46              |
| 12:M:178:GLN:HB3  | 12:M:204:MET:CE   | 2.46                     | 0.46              |
| 12:M:354:LEU:HD22 | 12:M:548:LEU:HD22 | 1.97                     | 0.46              |
| 12:M:462:PHE:CE2  | 12:M:466:LEU:HD21 | 2.51                     | 0.46              |
| 32:i:98:MET:HE2   | 32:i:98:MET:HB2   | 1.84                     | 0.46              |
| 37:n:39:ARG:HG3   | 37:n:57:TRP:CE2   | 2.51                     | 0.46              |
| 1:A:162:PHE:HB3   | 1:A:165:GLU:HB2   | 1.97                     | 0.46              |
| 5:F:69:TYR:CE2    | 5:F:75:LYS:HG3    | 2.40                     | 0.46              |
| 19:U:38:TYR:HB2   | 41:s:310:MET:O    | 2.16                     | 0.46              |
| 21:W:10:MET:HE3   | 21:W:11:PRO:HD2   | 1.98                     | 0.46              |
| 24:a:96:ALA:HB2   | 27:d:61:TYR:CE2   | 2.50                     | 0.46              |
| 32:i:334:THR:HG21 | 55:i:402:CDL:H391 | 1.98                     | 0.46              |
| 35:l:241:THR:HG21 | 35:l:344:GLY:HA3  | 1.97                     | 0.46              |
| 43:v:46:MET:HE3   | 43:v:56:ARG:HD3   | 1.97                     | 0.46              |
| 44:w:219:GLN:NE2  | 44:w:227:MET:SD   | 2.84                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:456:GLN:CD    | 1:A:456:GLN:C     | 2.84                     | 0.45              |
| 46:A:502:FMN:H9   | 46:A:502:FMN:H1'1 | 1.75                     | 0.45              |
| 14:O:172:ILE:HD12 | 14:O:173:GLU:H    | 1.80                     | 0.45              |
| 32:i:42:PRO:HG3   | 36:m:167:VAL:HG13 | 1.99                     | 0.45              |
| 35:l:338:MET:HE2  | 35:l:338:MET:HB3  | 1.82                     | 0.45              |
| 41:s:61:LEU:HD12  | 41:s:61:LEU:O     | 2.17                     | 0.45              |
| 1:A:279:SER:OG    | 1:A:280:GLY:N     | 2.49                     | 0.45              |
| 6:G:139:MET:HE2   | 6:G:139:MET:HB2   | 1.85                     | 0.45              |
| 9:J:209:ARG:HB3   | 9:J:210:GLU:OE2   | 2.17                     | 0.45              |
| 20:V:37:SER:O     | 20:V:41:ILE:HG12  | 2.16                     | 0.45              |
| 30:g:49:ALA:HB2   | 55:i:402:CDL:H712 | 1.98                     | 0.45              |
| 30:g:117:GLU:OE1  | 30:g:119:HIS:NE2  | 2.49                     | 0.45              |
| 31:h:2:PRO:HA     | 32:i:140:SER:HB2  | 1.98                     | 0.45              |
| 32:i:95:MET:HE2   | 32:i:149:ILE:HA   | 1.98                     | 0.45              |
| 35:l:389:PHE:O    | 35:l:393:ASP:HB3  | 2.17                     | 0.45              |
| 1:A:85:LEU:HD12   | 1:A:86:ARG:N      | 2.31                     | 0.45              |
| 2:B:198:GLU:HB3   | 13:N:109:ILE:HG12 | 1.98                     | 0.45              |
| 9:J:251:ASN:O     | 9:J:255:ASP:N     | 2.45                     | 0.45              |
| 14:O:154:LYS:HE3  | 14:O:154:LYS:HB2  | 1.71                     | 0.45              |
| 18:T:64:GLU:OE1   | 18:T:64:GLU:HA    | 2.16                     | 0.45              |
| 20:V:107:SER:HB3  | 20:V:110:ILE:CG2  | 2.46                     | 0.45              |
| 21:W:51:MET:HE2   | 41:s:311:THR:HB   | 1.98                     | 0.45              |
| 22:Y:47:PHE:CZ    | 35:l:364:LYS:HG3  | 2.50                     | 0.45              |
| 22:Y:100:LEU:O    | 22:Y:102:ASP:N    | 2.44                     | 0.45              |
| 32:i:265:MET:HE2  | 32:i:343:LEU:HD21 | 1.98                     | 0.45              |
| 35:l:190:LEU:C    | 35:l:190:LEU:HD23 | 2.41                     | 0.45              |
| 38:o:59:VAL:HG22  | 40:r:423:ILE:HG12 | 1.98                     | 0.45              |
| 44:w:254:GLU:OE1  | 44:w:254:GLU:N    | 2.49                     | 0.45              |
| 3:C:193:TRP:HA    | 3:C:196:ARG:HG2   | 1.98                     | 0.45              |
| 19:U:66:VAL:HG13  | 42:u:130:LYS:HD3  | 1.97                     | 0.45              |
| 29:f:61:GLN:O     | 29:f:65:ASP:OD2   | 2.34                     | 0.45              |
| 55:l:701:CDL:H742 | 55:l:701:CDL:H711 | 1.78                     | 0.45              |
| 1:A:339:PHE:CE1   | 1:A:349:LEU:HD23  | 2.51                     | 0.45              |
| 1:A:413:TRP:O     | 1:A:416:SER:OG    | 2.23                     | 0.45              |
| 12:M:133:GLN:O    | 12:M:137:CYS:HB2  | 2.17                     | 0.45              |
| 16:Q:232:VAL:HG23 | 16:Q:356:ILE:HB   | 1.98                     | 0.45              |
| 27:d:26:LEU:HD22  | 43:v:75:PRO:CB    | 2.45                     | 0.45              |
| 28:e:149:LEU:HD12 | 28:e:149:LEU:H    | 1.81                     | 0.45              |
| 35:l:152:PHE:CD1  | 35:l:168:ALA:HB1  | 2.52                     | 0.45              |
| 35:l:533:MET:HE3  | 48:l:702:PEE:H24  | 1.97                     | 0.45              |
| 36:m:55:MET:HA    | 36:m:55:MET:HE2   | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:r:310:MET:HB3  | 40:r:455:LEU:HD22 | 1.97                     | 0.45              |
| 44:w:295:ARG:HA   | 44:w:298:VAL:HG22 | 1.98                     | 0.45              |
| 1:A:272:GLY:O     | 1:A:292:MET:HB2   | 2.17                     | 0.45              |
| 6:G:128:PHE:CE1   | 6:G:148:ILE:CD1   | 3.00                     | 0.45              |
| 14:O:172:ILE:HD12 | 14:O:173:GLU:N    | 2.32                     | 0.45              |
| 16:Q:139:LEU:HD13 | 16:Q:424:ILE:HG21 | 1.98                     | 0.45              |
| 20:V:40:SER:OG    | 20:V:55:ARG:NH1   | 2.50                     | 0.45              |
| 32:i:129:LEU:HD12 | 32:i:133:TRP:HB3  | 1.98                     | 0.45              |
| 43:v:28:ASP:OD1   | 43:v:28:ASP:N     | 2.43                     | 0.45              |
| 12:M:203:ASP:OD1  | 12:M:203:ASP:N    | 2.45                     | 0.45              |
| 28:e:53:ILE:O     | 44:w:315:PRO:HB3  | 2.17                     | 0.45              |
| 30:g:4:MET:HG2    | 30:g:7:ARG:HD2    | 1.98                     | 0.45              |
| 1:A:89:GLY:O      | 47:A:503:NAI:H2N  | 2.17                     | 0.45              |
| 2:B:76:TYR:HE1    | 41:s:33:LEU:HD13  | 1.81                     | 0.45              |
| 16:Q:232:VAL:CG2  | 16:Q:356:ILE:HB   | 2.47                     | 0.45              |
| 48:U:101:PEE:H59  | 48:U:101:PEE:H64  | 1.74                     | 0.45              |
| 20:V:2:ALA:HA     | 35:l:601:LEU:HD12 | 1.99                     | 0.45              |
| 20:V:47:ALA:HB3   | 20:V:51:GLU:CD    | 2.42                     | 0.45              |
| 25:b:22:TRP:CE2   | 39:p:172:THR:HG22 | 2.50                     | 0.45              |
| 28:e:121:GLU:O    | 28:e:124:ARG:HG2  | 2.17                     | 0.45              |
| 29:f:39:PRO:CG    | 44:w:351:TRP:CB   | 2.95                     | 0.45              |
| 35:l:66:TRP:HZ3   | 48:l:703:PEE:H38  | 1.82                     | 0.45              |
| 9:J:329:LEU:HD23  | 9:J:331:HIS:HE1   | 1.82                     | 0.45              |
| 15:P:69:LEU:HD11  | 15:P:99:PHE:CD2   | 2.52                     | 0.45              |
| 16:Q:152:SER:HB3  | 16:Q:229:PRO:HA   | 1.98                     | 0.45              |
| 16:Q:156:GLU:OE1  | 16:Q:229:PRO:O    | 2.35                     | 0.45              |
| 17:S:22:ALA:O     | 17:S:26:ILE:HG13  | 2.17                     | 0.45              |
| 26:c:108:ASP:HB3  | 26:c:111:MET:HB3  | 1.99                     | 0.45              |
| 26:c:111:MET:HE1  | 35:l:543:SER:OG   | 2.17                     | 0.45              |
| 30:g:12:PRO:HG2   | 31:h:8:LYS:HB3    | 1.98                     | 0.45              |
| 30:g:92:MET:O     | 30:g:96:VAL:HG23  | 2.16                     | 0.45              |
| 56:s:401:UQ:H101  | 56:s:401:UQ:H121  | 1.60                     | 0.45              |
| 1:A:181:LEU:HA    | 1:A:186:ALA:O     | 2.17                     | 0.45              |
| 17:S:21:MET:SD    | 41:s:253:GLU:HG3  | 2.56                     | 0.45              |
| 17:S:69:ILE:HD11  | 42:u:68:LEU:CD2   | 2.46                     | 0.45              |
| 26:c:169:GLU:N    | 26:c:169:GLU:OE2  | 2.50                     | 0.45              |
| 27:d:30:VAL:O     | 27:d:34:THR:HG22  | 2.17                     | 0.45              |
| 35:l:286:LEU:HD22 | 35:l:411:MET:SD   | 2.57                     | 0.45              |
| 38:o:8:PRO:HG3    | 38:o:14:LEU:HD13  | 1.99                     | 0.45              |
| 38:o:81:ARG:HB3   | 38:o:81:ARG:NH1   | 2.32                     | 0.45              |
| 44:w:54:THR:O     | 44:w:54:THR:OG1   | 2.34                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:U:42:ALA:HB2   | 41:s:312:ALA:HA   | 1.99                     | 0.44              |
| 32:i:222:SER:CB   | 32:i:237:MET:HE3  | 2.47                     | 0.44              |
| 1:A:408:GLU:O     | 1:A:411:SER:HB3   | 2.17                     | 0.44              |
| 21:W:57:ARG:HB3   | 41:s:316:PRO:HG3  | 1.98                     | 0.44              |
| 25:b:88:TYR:CE1   | 27:d:49:ARG:HG2   | 2.52                     | 0.44              |
| 26:c:81:ARG:HD3   | 26:c:85:GLU:OE2   | 2.17                     | 0.44              |
| 28:e:128:TYR:CD1  | 28:e:128:TYR:C    | 2.95                     | 0.44              |
| 30:g:12:PRO:HB3   | 31:h:5:ASP:HB3    | 1.99                     | 0.44              |
| 42:u:121:ASP:N    | 42:u:124:GLU:OE1  | 2.43                     | 0.44              |
| 1:A:127:ASP:HA    | 1:A:130:ILE:HG12  | 1.99                     | 0.44              |
| 9:J:235:THR:HG23  | 9:J:325:SER:HA    | 1.98                     | 0.44              |
| 17:S:69:ILE:HG13  | 17:S:69:ILE:O     | 2.18                     | 0.44              |
| 18:T:79:VAL:O     | 18:T:121:PRO:HD3  | 2.17                     | 0.44              |
| 24:a:136:THR:HG21 | 40:r:48:ASN:HD22  | 1.81                     | 0.44              |
| 55:a:201:CDL:H372 | 55:a:201:CDL:H341 | 1.60                     | 0.44              |
| 40:r:248:THR:HG23 | 40:r:249:ILE:HG23 | 2.00                     | 0.44              |
| 12:M:370:GLU:OE2  | 12:M:518:ARG:NH2  | 2.40                     | 0.44              |
| 32:i:326:LEU:HB3  | 32:i:327:PRO:HD3  | 1.99                     | 0.44              |
| 33:j:51:PHE:CE2   | 36:m:74:MET:HB3   | 2.52                     | 0.44              |
| 35:l:174:TYR:CD2  | 35:l:232:TRP:HB3  | 2.52                     | 0.44              |
| 35:l:327:LEU:O    | 35:l:331:MET:HG2  | 2.17                     | 0.44              |
| 35:l:536:LEU:HB3  | 35:l:537:PRO:HD3  | 1.99                     | 0.44              |
| 6:G:112:SER:CB    | 50:G:201:8Q1:O2   | 2.65                     | 0.44              |
| 12:M:495:ASN:O    | 12:M:499:ASN:CG   | 2.61                     | 0.44              |
| 14:O:133:GLN:HG3  | 14:O:172:ILE:HG23 | 1.99                     | 0.44              |
| 20:V:50:LEU:O     | 20:V:53:VAL:HG12  | 2.18                     | 0.44              |
| 21:W:93:GLU:HG3   | 31:h:98:HIS:NE2   | 2.32                     | 0.44              |
| 34:k:26:LEU:HD23  | 34:k:78:LEU:HD12  | 1.98                     | 0.44              |
| 55:l:701:CDL:H351 | 55:l:701:CDL:H382 | 1.67                     | 0.44              |
| 44:w:125:ASP:OD1  | 44:w:125:ASP:N    | 2.37                     | 0.44              |
| 1:A:185:ASN:C     | 1:A:187:CYS:H     | 2.26                     | 0.44              |
| 1:A:214:GLU:OE2   | 1:A:224:ARG:NE    | 2.39                     | 0.44              |
| 12:M:222:ILE:HA   | 12:M:225:ILE:HG12 | 2.00                     | 0.44              |
| 16:Q:116:LEU:HD23 | 16:Q:459:GLY:HA2  | 1.99                     | 0.44              |
| 20:V:106:ARG:HE   | 20:V:106:ARG:CA   | 2.30                     | 0.44              |
| 25:b:32:GLU:HG3   | 39:p:115:TYR:HD1  | 1.83                     | 0.44              |
| 35:l:37:LYS:HD3   | 35:l:98:TRP:HE1   | 1.83                     | 0.44              |
| 36:m:25:SER:O     | 36:m:27:ILE:N     | 2.49                     | 0.44              |
| 36:m:51:PHE:CD2   | 36:m:143:ILE:HD13 | 2.52                     | 0.44              |
| 40:r:216:LEU:HD23 | 40:r:287:ALA:HB1  | 1.99                     | 0.44              |
| 3:C:79:MET:CE     | 3:C:86:MET:HE2    | 2.44                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:55:LYS:HA     | 7:H:58:MET:HE3    | 1.99                     | 0.44              |
| 12:M:304:GLN:HG2  | 12:M:615:LEU:HD12 | 1.99                     | 0.44              |
| 28:e:63:ASP:OD1   | 28:e:63:ASP:C     | 2.61                     | 0.44              |
| 36:m:1:MET:CE     | 36:m:4:TYR:HA     | 2.47                     | 0.44              |
| 37:n:46:LYS:HZ3   | 37:n:46:LYS:HB3   | 1.83                     | 0.44              |
| 40:r:207:MET:HE1  | 40:r:297:VAL:HG12 | 1.99                     | 0.44              |
| 44:w:350:LYS:HA   | 44:w:350:LYS:HD3  | 1.82                     | 0.44              |
| 1:A:296:LEU:HD12  | 1:A:296:LEU:HA    | 1.86                     | 0.44              |
| 16:Q:150:ALA:HB2  | 16:Q:400:ILE:HG12 | 2.00                     | 0.44              |
| 29:f:39:PRO:CG    | 44:w:351:TRP:HB3  | 2.47                     | 0.44              |
| 31:h:21:GLN:HA    | 34:k:53:PHE:CE1   | 2.53                     | 0.44              |
| 49:i:401:PLX:H311 | 49:i:401:PLX:H341 | 1.73                     | 0.44              |
| 35:l:49:VAL:HB    | 35:l:50:PRO:HD3   | 2.00                     | 0.44              |
| 35:l:292:ALA:HB2  | 35:l:304:PHE:CB   | 2.48                     | 0.44              |
| 39:p:63:LEU:C     | 39:p:65:ARG:H     | 2.25                     | 0.44              |
| 42:u:84:GLU:HB2   | 42:u:106:LYS:NZ   | 2.33                     | 0.44              |
| 44:w:123:SER:OG   | 44:w:125:ASP:OD1  | 2.32                     | 0.44              |
| 2:B:117:LYS:HE3   | 2:B:130:ILE:HG22  | 2.00                     | 0.44              |
| 12:M:47:THR:HG23  | 12:M:51:GLN:HB2   | 1.99                     | 0.44              |
| 16:Q:463:ARG:HE   | 16:Q:463:ARG:HB2  | 1.72                     | 0.44              |
| 17:S:43:TYR:CZ    | 21:W:68:ARG:HG3   | 2.53                     | 0.44              |
| 23:Z:13:LYS:HA    | 23:Z:13:LYS:HD2   | 1.81                     | 0.44              |
| 23:Z:57:PHE:CG    | 35:l:435:PRO:HG3  | 2.53                     | 0.44              |
| 32:i:38:LEU:HD12  | 34:k:73:LEU:HD22  | 2.00                     | 0.44              |
| 32:i:97:MET:HG2   | 35:l:599:MET:HE1  | 2.00                     | 0.44              |
| 35:l:384:PRO:HA   | 35:l:389:PHE:CD1  | 2.53                     | 0.44              |
| 40:r:191:SER:HB3  | 48:r:501:PEE:H3   | 1.99                     | 0.44              |
| 41:s:267:THR:O    | 41:s:271:LEU:HG   | 2.18                     | 0.44              |
| 1:A:88:ARG:CG     | 1:A:246:GLU:OE2   | 2.65                     | 0.43              |
| 2:B:65:GLU:HG3    | 16:Q:264:ASN:O    | 2.18                     | 0.43              |
| 6:G:118:ILE:O     | 6:G:122:MET:HG2   | 2.19                     | 0.43              |
| 9:J:151:ALA:O     | 9:J:155:VAL:HG22  | 2.18                     | 0.43              |
| 6:X:131:PRO:HB3   | 26:c:89:TRP:CD2   | 2.52                     | 0.43              |
| 25:b:121:LYS:C    | 25:b:122:GLU:HG3  | 2.42                     | 0.43              |
| 40:r:218:LYS:O    | 40:r:222:GLU:HG2  | 2.17                     | 0.43              |
| 1:A:168:ASN:HA    | 1:A:171:VAL:HG12  | 1.99                     | 0.43              |
| 2:B:198:GLU:HG2   | 13:N:108:TYR:HE1  | 1.83                     | 0.43              |
| 4:E:120:SER:O     | 4:E:124:VAL:HG13  | 2.17                     | 0.43              |
| 10:K:87:LEU:HD11  | 14:O:66:ILE:HD11  | 2.00                     | 0.43              |
| 2:B:122:VAL:HG21  | 16:Q:385:TYR:HD1  | 1.83                     | 0.43              |
| 3:C:92:VAL:HG12   | 41:s:25:ARG:NH1   | 2.33                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:H:7:LYS:HA      | 7:H:16:VAL:HG21   | 2.00                     | 0.43              |
| 14:O:146:ASP:OD1  | 14:O:146:ASP:N    | 2.48                     | 0.43              |
| 14:O:166:ASP:OD1  | 14:O:166:ASP:N    | 2.34                     | 0.43              |
| 6:X:80:LYS:HE3    | 6:X:80:LYS:HB3    | 1.73                     | 0.43              |
| 22:Y:103:ASP:C    | 22:Y:103:ASP:OD1  | 2.61                     | 0.43              |
| 25:b:109:THR:HG23 | 27:d:19:ALA:CB    | 2.47                     | 0.43              |
| 32:i:129:LEU:HD12 | 32:i:129:LEU:O    | 2.17                     | 0.43              |
| 34:k:37:MET:HG3   | 34:k:67:ALA:CB    | 2.48                     | 0.43              |
| 35:l:492:ILE:O    | 35:l:496:MET:HG2  | 2.18                     | 0.43              |
| 1:A:312:ASP:HA    | 1:A:329:LYS:NZ    | 2.33                     | 0.43              |
| 4:E:41:ARG:HG3    | 4:E:41:ARG:HH11   | 1.83                     | 0.43              |
| 5:F:41:TYR:O      | 5:F:44:LEU:HB2    | 2.18                     | 0.43              |
| 12:M:217:GLU:C    | 12:M:288:ASP:OD1  | 2.61                     | 0.43              |
| 14:O:193:TYR:HE1  | 14:O:216:PRO:HA   | 1.82                     | 0.43              |
| 35:l:290:LEU:HD23 | 35:l:290:LEU:O    | 2.18                     | 0.43              |
| 5:F:35:ASP:OD1    | 5:F:35:ASP:N      | 2.50                     | 0.43              |
| 12:M:48:THR:HA    | 12:M:95:PRO:HA    | 1.99                     | 0.43              |
| 20:V:76:ILE:O     | 20:V:80:VAL:HG23  | 2.18                     | 0.43              |
| 25:b:99:GLU:HG3   | 35:l:61:MET:HE2   | 1.99                     | 0.43              |
| 27:d:114:GLN:OE1  | 35:l:199:GLN:HG3  | 2.19                     | 0.43              |
| 32:i:284:MET:HE1  | 40:r:159:PRO:HD3  | 2.00                     | 0.43              |
| 40:r:121:LEU:O    | 40:r:125:THR:HG23 | 2.18                     | 0.43              |
| 1:A:177:TYR:OH    | 1:A:194:ASP:OD1   | 2.34                     | 0.43              |
| 3:C:98:ARG:HA     | 3:C:98:ARG:HD3    | 1.81                     | 0.43              |
| 7:H:69:GLU:HG3    | 7:H:77:ILE:HG12   | 2.00                     | 0.43              |
| 7:H:96:ARG:NH1    | 7:H:96:ARG:HB2    | 2.33                     | 0.43              |
| 9:J:204:SER:OG    | 9:J:204:SER:O     | 2.33                     | 0.43              |
| 15:P:61:PHE:HZ    | 15:P:106:ALA:HB2  | 1.83                     | 0.43              |
| 16:Q:65:PRO:HB2   | 16:Q:67:ASN:O     | 2.19                     | 0.43              |
| 6:X:113:LEU:O     | 6:X:117:GLU:HG3   | 2.19                     | 0.43              |
| 25:b:87:LYS:HD3   | 25:b:88:TYR:CZ    | 2.54                     | 0.43              |
| 26:c:96:ASP:OD1   | 26:c:96:ASP:N     | 2.51                     | 0.43              |
| 37:n:46:LYS:CB    | 37:n:46:LYS:HZ3   | 2.31                     | 0.43              |
| 39:p:63:LEU:O     | 39:p:64:LEU:HB3   | 2.18                     | 0.43              |
| 1:A:126:LYS:NZ    | 1:A:127:ASP:OD1   | 2.48                     | 0.43              |
| 21:W:30:LEU:HD23  | 21:W:35:MET:HG2   | 1.99                     | 0.43              |
| 26:c:157:GLY:HA2  | 43:v:22:MET:CE    | 2.49                     | 0.43              |
| 31:h:32:ARG:NH2   | 31:h:66:CYS:O     | 2.51                     | 0.43              |
| 33:j:71:LEU:HD23  | 33:j:71:LEU:HA    | 1.86                     | 0.43              |
| 35:l:468:ILE:O    | 35:l:472:ILE:HG12 | 2.19                     | 0.43              |
| 40:r:373:ILE:HD11 | 40:r:444:LEU:HD23 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:r:501:PEE:H68  | 48:r:501:PEE:H62  | 1.82                     | 0.43              |
| 18:T:105:GLU:OE1  | 18:T:105:GLU:O    | 2.37                     | 0.43              |
| 20:V:91:PHE:HE1   | 20:V:120:LEU:HD22 | 1.82                     | 0.43              |
| 21:W:66:GLU:OE2   | 42:u:123:GLY:N    | 2.41                     | 0.43              |
| 22:Y:100:LEU:H    | 43:v:111:ARG:NH1  | 2.17                     | 0.43              |
| 24:a:134:GLU:OE2  | 37:n:40:ASN:N     | 2.50                     | 0.43              |
| 25:b:104:ILE:HD13 | 27:d:18:PRO:HG3   | 2.00                     | 0.43              |
| 26:c:149:ILE:HG22 | 26:c:150:TYR:HD1  | 1.83                     | 0.43              |
| 27:d:97:LYS:NZ    | 28:e:114:MET:HE3  | 2.34                     | 0.43              |
| 41:s:26:LYS:HD2   | 41:s:36:GLY:HA3   | 2.01                     | 0.43              |
| 44:w:181:LYS:O    | 44:w:184:VAL:HG22 | 2.18                     | 0.43              |
| 1:A:329:LYS:HA    | 1:A:332:CYS:SG    | 2.58                     | 0.43              |
| 5:F:19:ILE:HG23   | 5:F:53:ILE:HA     | 2.00                     | 0.43              |
| 5:F:20:ARG:O      | 5:F:65:LEU:HD12   | 2.19                     | 0.43              |
| 12:M:394:VAL:HG11 | 12:M:418:ILE:HG12 | 2.01                     | 0.43              |
| 16:Q:159:LEU:O    | 16:Q:160:ASN:HB3  | 2.19                     | 0.43              |
| 16:Q:351:MET:HE2  | 16:Q:351:MET:HB2  | 1.85                     | 0.43              |
| 26:c:156:VAL:HG11 | 43:v:95:TYR:CZ    | 2.53                     | 0.43              |
| 32:i:81:SER:O     | 32:i:83:GLN:N     | 2.49                     | 0.43              |
| 49:j:201:PLX:H312 | 49:j:201:PLX:H282 | 1.74                     | 0.43              |
| 35:l:222:GLY:HA2  | 35:l:229:LEU:HD12 | 2.00                     | 0.43              |
| 48:m:201:PEE:H52  | 41:s:104:PHE:HE1  | 1.83                     | 0.43              |
| 40:r:420:THR:HB   | 40:r:423:ILE:HD12 | 2.01                     | 0.43              |
| 41:s:26:LYS:HA    | 41:s:36:GLY:HA3   | 2.01                     | 0.43              |
| 56:s:401:UQ:HM53  | 56:s:401:UQ:H72   | 1.73                     | 0.43              |
| 1:A:118:ASP:HB3   | 46:A:502:FMN:O4   | 2.18                     | 0.43              |
| 12:M:64:CYS:O     | 12:M:184:ARG:NH2  | 2.34                     | 0.43              |
| 14:O:75:LYS:HB2   | 14:O:75:LYS:HE3   | 1.80                     | 0.43              |
| 16:Q:220:ALA:HB3  | 16:Q:224:ALA:HA   | 2.00                     | 0.43              |
| 50:X:201:8Q1:O3   | 39:p:13:GLN:NE2   | 2.52                     | 0.43              |
| 32:i:170:LEU:HD11 | 32:i:288:LEU:HD22 | 1.99                     | 0.43              |
| 32:i:268:GLN:HE21 | 32:i:268:GLN:HB3  | 1.65                     | 0.43              |
| 32:i:292:PHE:CE1  | 32:i:293:TYR:CE1  | 3.07                     | 0.43              |
| 39:p:173:ARG:O    | 39:p:174:PRO:C    | 2.62                     | 0.43              |
| 41:s:2:PHE:O      | 41:s:6:ILE:HG12   | 2.19                     | 0.43              |
| 8:I:33:LYS:N      | 8:I:33:LYS:HD3    | 2.34                     | 0.42              |
| 12:M:382:ARG:HA   | 12:M:385:TYR:CE1  | 2.54                     | 0.42              |
| 14:O:164:THR:CG2  | 14:O:169:PHE:H    | 2.32                     | 0.42              |
| 15:P:44:ARG:NE    | 15:P:45:PRO:HD3   | 2.30                     | 0.42              |
| 25:b:80:TRP:HE1   | 27:d:41:VAL:HA    | 1.84                     | 0.42              |
| 35:l:309:GLN:O    | 35:l:313:MET:HG3  | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:l:356:ILE:HA   | 35:l:359:MET:HE2  | 2.00                     | 0.42              |
| 42:u:39:PRO:HG2   | 42:u:66:CYS:SG    | 2.59                     | 0.42              |
| 2:B:150:THR:HG21  | 2:B:180:HIS:CD2   | 2.54                     | 0.42              |
| 8:I:27:ARG:HH21   | 13:N:56:PHE:HD2   | 1.65                     | 0.42              |
| 9:J:275:ASP:OD1   | 9:J:275:ASP:N     | 2.41                     | 0.42              |
| 15:P:106:ALA:HB1  | 15:P:108:PHE:HD1  | 1.83                     | 0.42              |
| 16:Q:450:ILE:O    | 16:Q:453:THR:HG22 | 2.19                     | 0.42              |
| 23:Z:49:GLU:OE1   | 39:p:34:ARG:NE    | 2.46                     | 0.42              |
| 55:i:402:CDL:H362 | 55:i:402:CDL:H392 | 1.84                     | 0.42              |
| 55:l:701:CDL:H511 | 55:l:701:CDL:H542 | 1.81                     | 0.42              |
| 36:m:25:SER:O     | 36:m:28:TYR:N     | 2.50                     | 0.42              |
| 1:A:244:ASN:N     | 46:A:502:FMN:O1P  | 2.36                     | 0.42              |
| 1:A:347:THR:HG23  | 1:A:348:GLY:N     | 2.33                     | 0.42              |
| 11:L:96:LYS:HA    | 11:L:96:LYS:HD3   | 1.94                     | 0.42              |
| 14:O:100:LYS:HA   | 14:O:103:GLU:HG2  | 2.00                     | 0.42              |
| 16:Q:278:VAL:HG12 | 16:Q:329:ARG:HH21 | 1.85                     | 0.42              |
| 25:b:16:ARG:O     | 25:b:20:ARG:HG3   | 2.20                     | 0.42              |
| 33:j:53:MET:HG3   | 33:j:57:LEU:HD23  | 2.01                     | 0.42              |
| 34:k:37:MET:CE    | 36:m:64:MET:HE1   | 2.48                     | 0.42              |
| 35:l:327:LEU:HD12 | 35:l:327:LEU:HA   | 1.85                     | 0.42              |
| 4:E:88:MET:HE2    | 15:P:184:LEU:O    | 2.19                     | 0.42              |
| 5:F:23:LEU:O      | 5:F:57:GLU:HA     | 2.19                     | 0.42              |
| 9:J:116:ILE:O     | 9:J:120:VAL:HG22  | 2.20                     | 0.42              |
| 12:M:166:GLY:HA2  | 12:M:213:MET:SD   | 2.60                     | 0.42              |
| 6:X:119:ILE:HG21  | 6:X:135:ALA:HB1   | 2.00                     | 0.42              |
| 33:j:94:LEU:HD23  | 33:j:94:LEU:HA    | 1.93                     | 0.42              |
| 37:n:42:SER:O     | 37:n:46:LYS:HB2   | 2.20                     | 0.42              |
| 40:r:126:LEU:HD12 | 40:r:126:LEU:HA   | 1.89                     | 0.42              |
| 1:A:119:GLU:OE2   | 1:A:128:ARG:HB2   | 2.20                     | 0.42              |
| 3:C:49:LYS:HD2    | 3:C:49:LYS:HA     | 1.62                     | 0.42              |
| 3:C:167:PRO:HG3   | 16:Q:222:MET:SD   | 2.59                     | 0.42              |
| 16:Q:263:THR:HG23 | 16:Q:264:ASN:OD1  | 2.18                     | 0.42              |
| 16:Q:315:GLU:OE1  | 16:Q:316:PHE:N    | 2.51                     | 0.42              |
| 27:d:12:GLU:HB3   | 27:d:15:ARG:HH21  | 1.84                     | 0.42              |
| 35:l:7:LEU:O      | 35:l:11:THR:HG23  | 2.19                     | 0.42              |
| 1:A:380:GLY:O     | 1:A:386:ARG:NH1   | 2.52                     | 0.42              |
| 46:A:502:FMN:N1   | 46:A:502:FMN:O3'  | 2.48                     | 0.42              |
| 3:C:124:MET:HA    | 3:C:125:PRO:HD3   | 1.64                     | 0.42              |
| 5:F:35:ASP:O      | 5:F:36:PHE:C      | 2.62                     | 0.42              |
| 12:M:250:SER:OG   | 12:M:251:ILE:N    | 2.52                     | 0.42              |
| 13:N:8:ARG:HE     | 13:N:8:ARG:HB2    | 1.67                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:N:72:ASP:C     | 13:N:72:ASP:OD1   | 2.62                     | 0.42              |
| 14:O:177:LEU:HD12 | 14:O:185:MET:SD   | 2.60                     | 0.42              |
| 44:w:41:LEU:O     | 44:w:45:LEU:HD13  | 2.18                     | 0.42              |
| 44:w:54:THR:C     | 44:w:56:THR:H     | 2.28                     | 0.42              |
| 3:C:119:LYS:HZ2   | 3:C:123:GLN:HE21  | 1.68                     | 0.42              |
| 5:F:30:SER:HB2    | 5:F:63:PRO:CG     | 2.50                     | 0.42              |
| 20:V:97:GLY:O     | 20:V:100:THR:OG1  | 2.27                     | 0.42              |
| 22:Y:45:ARG:HA    | 23:Z:51:TRP:CE3   | 2.55                     | 0.42              |
| 24:a:168:TRP:CD2  | 30:g:2:THR:HG23   | 2.54                     | 0.42              |
| 39:p:25:ARG:HD3   | 39:p:25:ARG:HA    | 1.93                     | 0.42              |
| 40:r:184:HIS:ND1  | 40:r:184:HIS:N    | 2.67                     | 0.42              |
| 1:A:394:LYS:HD3   | 12:M:155:GLU:HB3  | 2.00                     | 0.42              |
| 8:I:74:LYS:HD2    | 8:I:74:LYS:HA     | 1.76                     | 0.42              |
| 6:X:112:SER:O     | 6:X:116:VAL:HG13  | 2.19                     | 0.42              |
| 22:Y:103:ASP:OD1  | 22:Y:104:GLU:N    | 2.52                     | 0.42              |
| 32:i:41:ILE:HG13  | 34:k:73:LEU:HD21  | 2.02                     | 0.42              |
| 33:j:53:MET:HE2   | 33:j:53:MET:HB2   | 1.81                     | 0.42              |
| 35:l:142:ILE:HG12 | 40:r:370:PRO:HB2  | 2.02                     | 0.42              |
| 41:s:41:GLY:HA2   | 41:s:46:LEU:HD12  | 2.02                     | 0.42              |
| 41:s:85:MET:HE3   | 41:s:233:MET:CE   | 2.50                     | 0.42              |
| 41:s:183:MET:O    | 41:s:187:ILE:HG12 | 2.20                     | 0.42              |
| 41:s:199:ASP:OD1  | 41:s:199:ASP:N    | 2.48                     | 0.42              |
| 6:G:115:GLN:O     | 6:G:118:ILE:HG12  | 2.20                     | 0.42              |
| 9:J:143:ASP:O     | 9:J:148:ILE:HG12  | 2.20                     | 0.42              |
| 13:N:11:LEU:HD12  | 13:N:11:LEU:HA    | 1.76                     | 0.42              |
| 14:O:181:VAL:HG12 | 14:O:222:ARG:HH22 | 1.85                     | 0.42              |
| 32:i:18:MET:HE3   | 32:i:22:ILE:HG21  | 2.01                     | 0.42              |
| 36:m:7:PHE:O      | 36:m:11:THR:HG23  | 2.20                     | 0.42              |
| 37:n:46:LYS:NZ    | 37:n:46:LYS:HB2   | 2.33                     | 0.42              |
| 38:o:121:LEU:HD12 | 38:o:121:LEU:O    | 2.19                     | 0.42              |
| 40:r:329:LEU:HG   | 40:r:437:MET:HE2  | 2.01                     | 0.42              |
| 1:A:338:ASP:OD1   | 1:A:341:ALA:N     | 2.45                     | 0.42              |
| 16:Q:114:GLY:N    | 16:Q:462:ASP:OD1  | 2.48                     | 0.42              |
| 17:S:42:SER:O     | 17:S:42:SER:OG    | 2.35                     | 0.42              |
| 19:U:32:LEU:N     | 19:U:33:PRO:HD2   | 2.35                     | 0.42              |
| 28:e:92:PHE:O     | 28:e:96:SER:HB3   | 2.20                     | 0.42              |
| 28:e:137:MET:HB2  | 28:e:137:MET:HE3  | 1.75                     | 0.42              |
| 39:p:150:ARG:HE   | 39:p:150:ARG:HB3  | 1.70                     | 0.42              |
| 40:r:126:LEU:HD12 | 40:r:149:PHE:CZ   | 2.54                     | 0.42              |
| 41:s:71:PHE:CD1   | 41:s:71:PHE:C     | 2.98                     | 0.42              |
| 42:u:83:THR:HA    | 42:u:86:TRP:NE1   | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:w:55:GLU:OE2   | 44:w:277:LYS:NZ   | 2.31                     | 0.42              |
| 8:I:107:SER:C     | 8:I:109:ASP:H     | 2.28                     | 0.41              |
| 27:d:83:LEU:O     | 27:d:87:GLU:OE1   | 2.37                     | 0.41              |
| 32:i:291:TYR:HA   | 40:r:151:PHE:HZ   | 1.85                     | 0.41              |
| 55:i:402:CDL:H772 | 55:i:402:CDL:H741 | 1.74                     | 0.41              |
| 34:k:45:THR:HG23  | 36:m:52:LEU:HD13  | 2.01                     | 0.41              |
| 37:n:54:GLU:HG3   | 37:n:55:VAL:HG22  | 2.02                     | 0.41              |
| 12:M:249:GLU:HG3  | 12:M:262:VAL:HG22 | 2.03                     | 0.41              |
| 15:P:125:ARG:HD3  | 15:P:126:PHE:CZ   | 2.55                     | 0.41              |
| 16:Q:204:PHE:HA   | 16:Q:207:ARG:HB2  | 2.02                     | 0.41              |
| 16:Q:253:PHE:O    | 16:Q:257:GLU:HG3  | 2.20                     | 0.41              |
| 6:X:146:ASP:HB3   | 25:b:16:ARG:CZ    | 2.51                     | 0.41              |
| 24:a:184:LYS:HB3  | 31:h:30:PRO:HB3   | 2.02                     | 0.41              |
| 28:e:87:MET:HE3   | 28:e:87:MET:HB3   | 1.96                     | 0.41              |
| 35:l:76:LEU:HD21  | 35:l:196:TRP:HE3  | 1.84                     | 0.41              |
| 35:l:99:SER:HB3   | 35:l:341:MET:HE1  | 2.02                     | 0.41              |
| 35:l:108:MET:HE2  | 35:l:240:PRO:HB3  | 2.02                     | 0.41              |
| 38:o:57:LEU:HD23  | 38:o:57:LEU:O     | 2.20                     | 0.41              |
| 43:v:106:ARG:O    | 43:v:110:GLN:HG2  | 2.20                     | 0.41              |
| 3:C:79:MET:HG2    | 3:C:86:MET:HE3    | 2.02                     | 0.41              |
| 4:E:123:TYR:CZ    | 12:M:320:GLU:HG3  | 2.56                     | 0.41              |
| 14:O:193:TYR:CE1  | 14:O:216:PRO:HA   | 2.56                     | 0.41              |
| 16:Q:144:MET:HE2  | 16:Q:144:MET:HB2  | 1.95                     | 0.41              |
| 48:Q:502:PEE:H20  | 41:s:183:MET:HE2  | 2.03                     | 0.41              |
| 48:Q:502:PEE:H36  | 48:Q:502:PEE:H41  | 1.82                     | 0.41              |
| 17:S:49:GLU:OE1   | 17:S:52:ARG:NH2   | 2.40                     | 0.41              |
| 19:U:31:ILE:HD13  | 19:U:31:ILE:HA    | 1.89                     | 0.41              |
| 27:d:9:VAL:HG11   | 28:e:123:GLU:HG2  | 2.02                     | 0.41              |
| 35:l:88:MET:HE1   | 35:l:468:ILE:CD1  | 2.50                     | 0.41              |
| 35:l:198:LEU:HD23 | 35:l:198:LEU:HA   | 1.87                     | 0.41              |
| 36:m:129:ASP:OD1  | 36:m:129:ASP:N    | 2.38                     | 0.41              |
| 37:n:30:ARG:O     | 37:n:33:GLU:HG2   | 2.20                     | 0.41              |
| 38:o:62:ASP:O     | 38:o:66:ILE:HG12  | 2.20                     | 0.41              |
| 39:p:108:HIS:CD2  | 39:p:109:PRO:HD2  | 2.55                     | 0.41              |
| 40:r:437:MET:HA   | 40:r:437:MET:HE3  | 2.01                     | 0.41              |
| 1:A:168:ASN:CA    | 1:A:171:VAL:HG12  | 2.51                     | 0.41              |
| 1:A:290:GLU:HG2   | 1:A:294:VAL:HG11  | 2.02                     | 0.41              |
| 6:G:119:ILE:O     | 6:G:123:GLU:HG2   | 2.20                     | 0.41              |
| 12:M:29:SER:HG    | 12:M:30:ASN:H     | 1.68                     | 0.41              |
| 12:M:329:MET:HE2  | 12:M:329:MET:HB3  | 1.95                     | 0.41              |
| 20:V:73:THR:HB    | 20:V:93:GLY:HA2   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 39:p:68:GLU:OE2   | 39:p:68:GLU:HA    | 2.20                     | 0.41              |
| 1:A:118:ASP:O     | 1:A:159:ARG:HD2   | 2.20                     | 0.41              |
| 3:C:70:ALA:HB1    | 16:Q:118:2MR:CQ1  | 2.51                     | 0.41              |
| 12:M:144:MET:HG3  | 16:Q:383:LYS:HG3  | 2.02                     | 0.41              |
| 14:O:137:THR:HG22 | 14:O:138:THR:H    | 1.85                     | 0.41              |
| 16:Q:199:PRO:HB3  | 16:Q:258:LEU:HD13 | 2.02                     | 0.41              |
| 16:Q:295:GLY:O    | 16:Q:324:GLY:HA2  | 2.21                     | 0.41              |
| 21:W:43:LEU:HG    | 41:s:179:TRP:HE1  | 1.86                     | 0.41              |
| 6:X:147:TYR:CD1   | 6:X:147:TYR:C     | 2.99                     | 0.41              |
| 32:i:20:VAL:HG11  | 32:i:137:ALA:HB1  | 2.03                     | 0.41              |
| 49:j:201:PLX:H342 | 49:j:201:PLX:H372 | 1.53                     | 0.41              |
| 35:l:20:MET:HA    | 49:r:503:PLX:H211 | 2.03                     | 0.41              |
| 36:m:173:ARG:HG2  | 36:m:173:ARG:NH1  | 2.28                     | 0.41              |
| 39:p:127:ARG:HG3  | 39:p:128:LEU:N    | 2.33                     | 0.41              |
| 40:r:272:THR:HA   | 40:r:275:ILE:HD12 | 2.02                     | 0.41              |
| 42:u:58:GLU:O     | 42:u:62:LEU:HD23  | 2.20                     | 0.41              |
| 44:w:275:TYR:CD1  | 44:w:275:TYR:N    | 2.86                     | 0.41              |
| 44:w:302:LEU:HD23 | 44:w:302:LEU:HA   | 1.93                     | 0.41              |
| 17:S:3:PHE:HA     | 17:S:6:LEU:HD23   | 2.02                     | 0.41              |
| 22:Y:43:ARG:HD2   | 22:Y:46:GLN:HB2   | 2.02                     | 0.41              |
| 22:Y:65:MET:HE3   | 22:Y:65:MET:HB3   | 1.95                     | 0.41              |
| 39:p:24:LEU:HD23  | 39:p:24:LEU:HA    | 1.84                     | 0.41              |
| 42:u:38:LYS:HB3   | 42:u:39:PRO:HD3   | 2.02                     | 0.41              |
| 43:v:57:ASP:OD1   | 43:v:57:ASP:N     | 2.52                     | 0.41              |
| 44:w:235:GLN:NE2  | 44:w:239:ASN:OD1  | 2.54                     | 0.41              |
| 1:A:35:LEU:HD23   | 1:A:40:ARG:NH1    | 2.36                     | 0.41              |
| 1:A:337:MET:HE3   | 1:A:337:MET:HB3   | 1.84                     | 0.41              |
| 5:F:79:LEU:HG     | 5:F:87:VAL:HG12   | 2.03                     | 0.41              |
| 15:P:119:VAL:HG12 | 15:P:121:THR:HG22 | 2.01                     | 0.41              |
| 6:X:88:LYS:HB2    | 6:X:88:LYS:HE3    | 1.91                     | 0.41              |
| 26:c:49:ALA:HA    | 26:c:59:VAL:HG23  | 2.02                     | 0.41              |
| 32:i:91:ASN:OD1   | 32:i:92:PRO:HD2   | 2.21                     | 0.41              |
| 35:l:71:LEU:HD23  | 40:r:310:MET:CE   | 2.50                     | 0.41              |
| 35:l:383:MET:HG2  | 35:l:384:PRO:HD2  | 2.01                     | 0.41              |
| 49:r:502:PLX:H22  | 49:r:502:PLX:H1C3 | 1.74                     | 0.41              |
| 41:s:285:LEU:C    | 41:s:285:LEU:CD1  | 2.91                     | 0.41              |
| 42:u:60:GLY:O     | 42:u:63:VAL:HG22  | 2.21                     | 0.41              |
| 1:A:456:GLN:C     | 1:A:456:GLN:NE2   | 2.78                     | 0.41              |
| 3:C:98:ARG:HD2    | 41:s:61:LEU:HD21  | 2.02                     | 0.41              |
| 4:E:98:LYS:HD3    | 4:E:102:HIS:HB3   | 2.03                     | 0.41              |
| 26:c:70:MET:H     | 26:c:70:MET:HG2   | 1.66                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:e:73:SER:C     | 28:e:75:GLY:H     | 2.28                     | 0.41              |
| 35:l:16:THR:HG22  | 35:l:126:ILE:HD13 | 2.02                     | 0.41              |
| 35:l:61:MET:HE3   | 35:l:61:MET:HB2   | 1.88                     | 0.41              |
| 35:l:245:ALA:HB2  | 35:l:340:PHE:HB3  | 2.03                     | 0.41              |
| 38:o:35:GLU:O     | 38:o:39:ILE:HG23  | 2.21                     | 0.41              |
| 40:r:122:PHE:HD1  | 40:r:238:LEU:HD13 | 1.86                     | 0.41              |
| 4:e:16:SER:HA     | 11:L:54:ALA:HA    | 2.03                     | 0.41              |
| 8:I:42:PRO:HD3    | 21:W:6:VAL:HG13   | 2.03                     | 0.41              |
| 9:J:344:PRO:HG2   | 9:J:347:LEU:HG    | 2.03                     | 0.41              |
| 10:K:70:ASN:OD1   | 10:K:70:ASN:N     | 2.54                     | 0.41              |
| 12:M:58:MET:HE1   | 12:M:104:THR:HB   | 2.03                     | 0.41              |
| 12:M:483:ARG:HB2  | 12:M:483:ARG:HH11 | 1.85                     | 0.41              |
| 14:O:68:LYS:HE3   | 14:O:68:LYS:HB2   | 1.86                     | 0.41              |
| 14:O:193:TYR:HB3  | 14:O:196:LEU:HD11 | 2.03                     | 0.41              |
| 14:O:236:GLU:HG2  | 14:O:237:PRO:HD2  | 2.03                     | 0.41              |
| 16:Q:133:LEU:CD2  | 16:Q:228:ARG:HD3  | 2.50                     | 0.41              |
| 16:Q:188:THR:HG21 | 16:Q:203:MET:HB2  | 2.03                     | 0.41              |
| 18:T:119:ARG:HD2  | 18:T:122:HIS:HD2  | 1.86                     | 0.41              |
| 19:U:78:LEU:O     | 19:U:82:LYS:HG3   | 2.21                     | 0.41              |
| 23:Z:60:ASN:OD1   | 23:Z:60:ASN:N     | 2.54                     | 0.41              |
| 24:a:117:ILE:HD13 | 49:a:202:PLX:H211 | 2.03                     | 0.41              |
| 28:e:97:ILE:O     | 28:e:101:LEU:HB2  | 2.20                     | 0.41              |
| 29:f:73:ASN:HB3   | 29:f:75:LEU:HD23  | 2.02                     | 0.41              |
| 31:h:65:GLU:OE1   | 31:h:71:LYS:HB2   | 2.21                     | 0.41              |
| 33:j:107:THR:O    | 33:j:107:THR:HG22 | 2.21                     | 0.41              |
| 35:l:128:MET:HG2  | 35:l:251:THR:HG22 | 2.01                     | 0.41              |
| 35:l:149:ILE:HD13 | 35:l:149:ILE:HA   | 1.91                     | 0.41              |
| 35:l:288:THR:HG21 | 35:l:307:SER:CB   | 2.48                     | 0.41              |
| 35:l:554:ASP:OD1  | 40:r:213:HIS:NE2  | 2.53                     | 0.41              |
| 40:r:133:ILE:HD11 | 40:r:231:LEU:HD11 | 2.02                     | 0.41              |
| 40:r:216:LEU:HB3  | 40:r:217:PRO:HD3  | 2.02                     | 0.41              |
| 41:s:38:ASN:OD1   | 41:s:38:ASN:N     | 2.54                     | 0.41              |
| 41:s:162:LEU:HD23 | 41:s:165:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:179:ALA:HB1   | 1:A:181:LEU:HD23  | 2.03                     | 0.41              |
| 1:A:392:MET:HE1   | 1:A:432:ALA:HA    | 2.01                     | 0.41              |
| 46:A:502:FMN:N5   | 47:A:503:NAI:H4N  | 2.36                     | 0.41              |
| 2:B:68:ARG:NH1    | 21:W:28:ARG:HG2   | 2.36                     | 0.41              |
| 4:E:127:ASP:OD2   | 9:J:45:LYS:NZ     | 2.53                     | 0.41              |
| 7:H:31:ILE:HA     | 7:H:31:ILE:HD12   | 1.81                     | 0.41              |
| 10:K:79:HIS:ND1   | 14:O:216:PRO:HD2  | 2.35                     | 0.41              |
| 12:M:646:LEU:HD12 | 12:M:646:LEU:HA   | 1.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:Q:102:SER:OG   | 16:Q:107:ARG:NH1  | 2.54                     | 0.41              |
| 19:U:78:LEU:HD23  | 19:U:78:LEU:HA    | 1.83                     | 0.41              |
| 20:V:69:ILE:HG21  | 20:V:100:THR:CG2  | 2.51                     | 0.41              |
| 27:d:146:LEU:HD23 | 27:d:146:LEU:HA   | 1.92                     | 0.41              |
| 32:i:245:MET:HE3  | 32:i:245:MET:HB3  | 1.89                     | 0.41              |
| 33:j:1:MET:N      | 33:j:4:MET:HE3    | 2.36                     | 0.41              |
| 40:r:150:LEU:HG   | 40:r:154:LEU:HD12 | 2.03                     | 0.41              |
| 40:r:457:PRO:HG2  | 40:r:458:LEU:HD12 | 2.02                     | 0.41              |
| 1:A:185:ASN:O     | 1:A:187:CYS:N     | 2.54                     | 0.40              |
| 2:B:210:LEU:HD23  | 2:B:210:LEU:HA    | 1.88                     | 0.40              |
| 5:F:82:PHE:HB3    | 5:F:87:VAL:HG13   | 2.03                     | 0.40              |
| 9:J:71:ASN:OD1    | 9:J:75:ARG:NH2    | 2.50                     | 0.40              |
| 9:J:114:ASP:O     | 9:J:118:LYS:HG2   | 2.21                     | 0.40              |
| 9:J:269:ASN:HB2   | 9:J:271:TYR:CZ    | 2.56                     | 0.40              |
| 6:X:110:LEU:HD12  | 6:X:114:ASP:CB    | 2.51                     | 0.40              |
| 6:X:113:LEU:O     | 6:X:116:VAL:HG22  | 2.21                     | 0.40              |
| 26:c:184:TYR:OH   | 43:v:104:ARG:NH1  | 2.54                     | 0.40              |
| 31:h:32:ARG:NH1   | 34:k:50:ASN:OD1   | 2.53                     | 0.40              |
| 31:h:74:LYS:HE3   | 31:h:74:LYS:HB2   | 1.94                     | 0.40              |
| 2:B:105:ARG:HD2   | 13:N:108:TYR:CG   | 2.56                     | 0.40              |
| 9:J:148:ILE:HB    | 9:J:149:PRO:HD3   | 2.03                     | 0.40              |
| 12:M:360:ARG:HE   | 12:M:632:MET:HB3  | 1.87                     | 0.40              |
| 16:Q:237:PRO:HD2  | 16:Q:240:LEU:HD22 | 2.03                     | 0.40              |
| 22:Y:99:ILE:HD11  | 43:v:108:LEU:HD12 | 2.03                     | 0.40              |
| 24:a:127:ASP:OD1  | 49:a:202:PLX:H12  | 2.22                     | 0.40              |
| 33:j:81:THR:C     | 33:j:83:ASN:H     | 2.29                     | 0.40              |
| 49:j:201:PLX:H182 | 49:j:201:PLX:H131 | 2.02                     | 0.40              |
| 34:k:43:MET:HE2   | 34:k:47:ILE:HD11  | 2.04                     | 0.40              |
| 35:l:140:LEU:HD12 | 35:l:140:LEU:HA   | 1.84                     | 0.40              |
| 39:p:30:TRP:NE1   | 39:p:76:HIS:HB2   | 2.36                     | 0.40              |
| 39:p:155:PRO:O    | 39:p:165:PRO:HD2  | 2.21                     | 0.40              |
| 41:s:81:LEU:HA    | 41:s:84:THR:HG22  | 2.03                     | 0.40              |
| 43:v:25:PHE:CD2   | 43:v:108:LEU:HD23 | 2.50                     | 0.40              |
| 1:A:35:LEU:HD23   | 1:A:40:ARG:HH11   | 1.86                     | 0.40              |
| 2:B:100:GLU:O     | 2:B:170:GLY:N     | 2.46                     | 0.40              |
| 6:G:119:ILE:HG23  | 6:G:130:ILE:HD11  | 2.01                     | 0.40              |
| 9:J:175:LYS:HB2   | 9:J:175:LYS:HE3   | 1.85                     | 0.40              |
| 12:M:217:GLU:O    | 12:M:288:ASP:OD1  | 2.39                     | 0.40              |
| 12:M:624:ARG:NH2  | 12:M:637:ASP:OD1  | 2.40                     | 0.40              |
| 13:N:10:GLY:O     | 13:N:14:VAL:HG23  | 2.21                     | 0.40              |
| 25:b:76:LEU:HD12  | 25:b:76:LEU:HA    | 1.80                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:e:114:MET:HB3  | 28:e:117:TRP:HB3  | 2.04                     | 0.40              |
| 31:h:54:LYS:HD3   | 31:h:54:LYS:HA    | 1.71                     | 0.40              |
| 31:h:76:LEU:HD23  | 31:h:76:LEU:HA    | 1.73                     | 0.40              |
| 35:l:51:LEU:HG    | 35:l:55:MET:HE2   | 2.04                     | 0.40              |
| 40:r:196:TRP:CE3  | 40:r:257:MET:HE3  | 2.56                     | 0.40              |
| 41:s:47:GLN:HB3   | 41:s:48:PRO:HD3   | 2.03                     | 0.40              |
| 42:u:80:GLU:O     | 42:u:84:GLU:HG3   | 2.20                     | 0.40              |
| 44:w:211:VAL:CA   | 44:w:214:ILE:HG22 | 2.45                     | 0.40              |
| 1:A:140:GLU:CD    | 1:A:252:PRO:HB3   | 2.46                     | 0.40              |
| 49:C:303:PLX:H31  | 13:N:75:TRP:CD2   | 2.56                     | 0.40              |
| 7:H:28:TYR:O      | 7:H:31:ILE:HG22   | 2.22                     | 0.40              |
| 12:M:89:VAL:HG11  | 12:M:94:MET:HE3   | 2.03                     | 0.40              |
| 12:M:556:THR:HG22 | 12:M:557:ARG:H    | 1.86                     | 0.40              |
| 18:T:119:ARG:HD2  | 18:T:122:HIS:CD2  | 2.56                     | 0.40              |
| 6:X:93:ILE:O      | 6:X:93:ILE:HG13   | 2.20                     | 0.40              |
| 26:c:110:ASP:OD1  | 26:c:110:ASP:N    | 2.53                     | 0.40              |
| 32:i:347:ASN:HB3  | 49:i:401:PLX:H282 | 2.04                     | 0.40              |
| 1:A:201:ALA:O     | 14:O:119:TYR:HB3  | 2.21                     | 0.40              |
| 3:C:119:LYS:NZ    | 3:C:123:GLN:NE2   | 2.68                     | 0.40              |
| 5:F:56:ARG:NH1    | 12:M:382:ARG:HG3  | 2.36                     | 0.40              |
| 6:G:149:ALA:O     | 6:G:153:ASP:N     | 2.52                     | 0.40              |
| 14:O:185:MET:SD   | 14:O:185:MET:C    | 3.05                     | 0.40              |
| 48:Q:502:PEE:H21  | 48:Q:502:PEE:H16  | 1.75                     | 0.40              |
| 21:W:58:ARG:HA    | 21:W:58:ARG:HD2   | 1.87                     | 0.40              |
| 23:Z:20:LYS:HE3   | 23:Z:20:LYS:HB3   | 1.72                     | 0.40              |
| 31:h:17:TRP:CZ3   | 31:h:18:MET:HB2   | 2.57                     | 0.40              |
| 41:s:66:SER:HB2   | 41:s:122:ALA:O    | 2.22                     | 0.40              |
| 42:u:108:ASP:O    | 42:u:111:VAL:HG12 | 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     | 429/433 (99%)  | 415 (97%) | 14 (3%)  | 0        | 100         | 100 |
| 2   | B     | 174/176 (99%)  | 169 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 3   | C     | 154/156 (99%)  | 149 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 4   | E     | 113/115 (98%)  | 110 (97%) | 3 (3%)   | 0        | 100         | 100 |
| 5   | F     | 84/86 (98%)    | 81 (96%)  | 2 (2%)   | 1 (1%)   | 10          | 42  |
| 6   | G     | 86/88 (98%)    | 85 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 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     | 289/342 (84%)  | 276 (96%) | 13 (4%)  | 0        | 100         | 100 |
| 10  | K     | 40/43 (93%)    | 40 (100%) | 0        | 0        | 100         | 100 |
| 11  | L     | 123/125 (98%)  | 121 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 12  | M     | 688/690 (100%) | 669 (97%) | 18 (3%)  | 1 (0%)   | 48          | 79  |
| 13  | N     | 142/144 (99%)  | 137 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 14  | O     | 215/217 (99%)  | 206 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 15  | P     | 206/208 (99%)  | 197 (96%) | 9 (4%)   | 0        | 100         | 100 |
| 16  | Q     | 412/430 (96%)  | 398 (97%) | 13 (3%)  | 1 (0%)   | 43          | 73  |
| 17  | S     | 68/70 (97%)    | 64 (94%)  | 4 (6%)   | 0        | 100         | 100 |
| 18  | T     | 94/96 (98%)    | 92 (98%)  | 2 (2%)   | 0        | 100         | 100 |
| 19  | U     | 81/83 (98%)    | 78 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 20  | V     | 138/140 (99%)  | 131 (95%) | 6 (4%)   | 1 (1%)   | 18          | 52  |
| 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%)    | 82 (100%) | 0        | 0        | 100         | 100 |
| 24  | a     | 138/140 (99%)  | 134 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 25  | b     | 99/126 (79%)   | 93 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 45  |
| 26  | c     | 154/156 (99%)  | 146 (95%) | 8 (5%)   | 0        | 100         | 100 |
| 27  | d     | 173/175 (99%)  | 169 (98%) | 4 (2%)   | 0        | 100         | 100 |
| 28  | e     | 105/107 (98%)  | 100 (95%) | 5 (5%)   | 0        | 100         | 100 |
| 29  | f     | 40/49 (82%)    | 40 (100%) | 0        | 0        | 100         | 100 |
| 30  | g     | 119/122 (98%)  | 114 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 31  | h     | 103/105 (98%)  | 99 (96%)  | 4 (4%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 32  | i     | 345/347 (99%)   | 334 (97%)  | 11 (3%)  | 0        | 100         | 100 |
| 33  | j     | 95/115 (83%)    | 89 (94%)   | 6 (6%)   | 0        | 100         | 100 |
| 34  | k     | 96/98 (98%)     | 91 (95%)   | 5 (5%)   | 0        | 100         | 100 |
| 35  | l     | 601/603 (100%)  | 570 (95%)  | 31 (5%)  | 0        | 100         | 100 |
| 36  | m     | 125/175 (71%)   | 115 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 37  | n     | 54/56 (96%)     | 53 (98%)   | 1 (2%)   | 0        | 100         | 100 |
| 38  | o     | 126/128 (98%)   | 120 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 39  | p     | 176/178 (99%)   | 167 (95%)  | 8 (4%)   | 1 (1%)   | 21          | 56  |
| 40  | r     | 457/459 (100%)  | 440 (96%)  | 17 (4%)  | 0        | 100         | 100 |
| 41  | s     | 299/318 (94%)   | 282 (94%)  | 17 (6%)  | 0        | 100         | 100 |
| 42  | u     | 169/171 (99%)   | 161 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 43  | v     | 122/124 (98%)   | 115 (94%)  | 7 (6%)   | 0        | 100         | 100 |
| 44  | w     | 318/320 (99%)   | 303 (95%)  | 15 (5%)  | 0        | 100         | 100 |
| All | All   | 8029/8322 (96%) | 7702 (96%) | 321 (4%) | 6 (0%)   | 49          | 79  |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 31  | GLN  |
| 39  | p     | 175 | ARG  |
| 12  | M     | 283 | GLU  |
| 16  | Q     | 160 | ASN  |
| 25  | b     | 110 | ILE  |
| 20  | V     | 46  | 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     | 343/346 (99%)  | 337 (98%)  | 6 (2%)   | 53          | 75  |
| 2   | B     | 151/151 (100%) | 151 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | C     | 132/132 (100%) | 132 (100%) | 0        | 100         | 100 |
| 4   | E     | 107/107 (100%) | 107 (100%) | 0        | 100         | 100 |
| 5   | F     | 72/76 (95%)    | 72 (100%)  | 0        | 100         | 100 |
| 6   | G     | 75/81 (93%)    | 75 (100%)  | 0        | 100         | 100 |
| 6   | X     | 77/81 (95%)    | 77 (100%)  | 0        | 100         | 100 |
| 7   | H     | 98/99 (99%)    | 98 (100%)  | 0        | 100         | 100 |
| 8   | I     | 87/97 (90%)    | 87 (100%)  | 0        | 100         | 100 |
| 9   | J     | 254/296 (86%)  | 254 (100%) | 0        | 100         | 100 |
| 10  | K     | 41/42 (98%)    | 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%) | 182 (100%) | 1 (0%)   | 81          | 85  |
| 15  | P     | 190/190 (100%) | 190 (100%) | 0        | 100         | 100 |
| 16  | Q     | 361/370 (98%)  | 357 (99%)  | 4 (1%)   | 65          | 79  |
| 17  | S     | 58/58 (100%)   | 57 (98%)   | 1 (2%)   | 53          | 75  |
| 18  | T     | 79/79 (100%)   | 78 (99%)   | 1 (1%)   | 61          | 78  |
| 19  | U     | 68/69 (99%)    | 68 (100%)  | 0        | 100         | 100 |
| 20  | V     | 100/101 (99%)  | 95 (95%)   | 5 (5%)   | 22          | 55  |
| 21  | W     | 123/123 (100%) | 123 (100%) | 0        | 100         | 100 |
| 22  | Y     | 62/63 (98%)    | 61 (98%)   | 1 (2%)   | 55          | 75  |
| 23  | Z     | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 24  | a     | 122/122 (100%) | 122 (100%) | 0        | 100         | 100 |
| 25  | b     | 95/119 (80%)   | 95 (100%)  | 0        | 100         | 100 |
| 26  | c     | 140/141 (99%)  | 140 (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     | 35/45 (78%)    | 35 (100%)  | 0        | 100         | 100 |
| 30  | g     | 108/109 (99%)  | 108 (100%) | 0        | 100         | 100 |
| 31  | h     | 93/93 (100%)   | 93 (100%)  | 0        | 100         | 100 |
| 32  | i     | 310/311 (100%) | 308 (99%)  | 2 (1%)   | 78          | 84  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 33  | j     | 88/100 (88%)    | 88 (100%)   | 0        | 100         | 100 |
| 34  | k     | 85/85 (100%)    | 85 (100%)   | 0        | 100         | 100 |
| 35  | l     | 536/537 (100%)  | 536 (100%)  | 0        | 100         | 100 |
| 36  | m     | 98/141 (70%)    | 96 (98%)    | 2 (2%)   | 48          | 72  |
| 37  | n     | 50/53 (94%)     | 49 (98%)    | 1 (2%)   | 48          | 72  |
| 38  | o     | 113/113 (100%)  | 113 (100%)  | 0        | 100         | 100 |
| 39  | p     | 158/159 (99%)   | 158 (100%)  | 0        | 100         | 100 |
| 40  | r     | 410/410 (100%)  | 408 (100%)  | 2 (0%)   | 81          | 85  |
| 41  | s     | 263/275 (96%)   | 261 (99%)   | 2 (1%)   | 73          | 82  |
| 42  | u     | 153/153 (100%)  | 153 (100%)  | 0        | 100         | 100 |
| 43  | v     | 104/111 (94%)   | 104 (100%)  | 0        | 100         | 100 |
| 44  | w     | 280/283 (99%)   | 279 (100%)  | 1 (0%)   | 84          | 86  |
| All | All   | 7044/7246 (97%) | 7015 (100%) | 29 (0%)  | 81          | 86  |

All (29) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | VAL  |
| 1   | A     | 208 | GLU  |
| 1   | A     | 210 | THR  |
| 1   | A     | 351 | THR  |
| 1   | A     | 410 | ASP  |
| 1   | A     | 455 | LEU  |
| 14  | O     | 166 | ASP  |
| 16  | Q     | 156 | GLU  |
| 16  | Q     | 234 | GLN  |
| 16  | Q     | 253 | PHE  |
| 16  | Q     | 263 | THR  |
| 17  | S     | 68  | ASN  |
| 18  | T     | 49  | ASP  |
| 20  | V     | 95  | CYS  |
| 20  | V     | 101 | LEU  |
| 20  | V     | 106 | ARG  |
| 20  | V     | 108 | TYR  |
| 20  | V     | 110 | ILE  |
| 22  | Y     | 81  | LEU  |
| 32  | i     | 128 | LEU  |
| 32  | i     | 268 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | m     | 1   | MET  |
| 36  | m     | 56  | VAL  |
| 37  | n     | 46  | LYS  |
| 40  | r     | 180 | HIS  |
| 40  | r     | 204 | MET  |
| 41  | s     | 84  | THR  |
| 41  | s     | 285 | LEU  |
| 44  | w     | 54  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 49  | HIS  |
| 1   | A     | 136 | HIS  |
| 1   | A     | 168 | ASN  |
| 1   | A     | 422 | HIS  |
| 1   | A     | 436 | GLN  |
| 3   | C     | 123 | GLN  |
| 9   | J     | 376 | ASN  |
| 11  | L     | 86  | ASN  |
| 12  | M     | 278 | HIS  |
| 12  | M     | 304 | GLN  |
| 12  | M     | 667 | GLN  |
| 13  | N     | 116 | ASN  |
| 13  | N     | 123 | GLN  |
| 14  | O     | 69  | ASN  |
| 14  | O     | 133 | GLN  |
| 15  | P     | 51  | ASN  |
| 15  | P     | 77  | GLN  |
| 15  | P     | 105 | ASN  |
| 15  | P     | 107 | GLN  |
| 15  | P     | 196 | HIS  |
| 16  | Q     | 60  | HIS  |
| 16  | Q     | 131 | GLN  |
| 16  | Q     | 160 | ASN  |
| 16  | Q     | 234 | GLN  |
| 16  | Q     | 250 | ASN  |
| 16  | Q     | 306 | GLN  |
| 18  | T     | 63  | ASN  |
| 20  | V     | 134 | GLN  |
| 24  | a     | 50  | HIS  |
| 25  | b     | 89  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | c     | 83  | GLN  |
| 29  | f     | 62  | HIS  |
| 30  | g     | 18  | ASN  |
| 30  | g     | 48  | ASN  |
| 30  | g     | 63  | GLN  |
| 32  | i     | 77  | ASN  |
| 32  | i     | 134 | GLN  |
| 32  | i     | 172 | GLN  |
| 32  | i     | 310 | ASN  |
| 34  | k     | 57  | ASN  |
| 35  | l     | 34  | ASN  |
| 35  | l     | 56  | HIS  |
| 35  | l     | 192 | HIS  |
| 35  | l     | 210 | ASN  |
| 35  | l     | 270 | ASN  |
| 35  | l     | 309 | GLN  |
| 35  | l     | 400 | ASN  |
| 35  | l     | 447 | ASN  |
| 35  | l     | 470 | ASN  |
| 37  | n     | 3   | ASN  |
| 38  | o     | 50  | GLN  |
| 38  | o     | 123 | GLN  |
| 39  | p     | 12  | HIS  |
| 40  | r     | 144 | ASN  |
| 40  | r     | 415 | GLN  |
| 41  | s     | 47  | GLN  |
| 41  | s     | 124 | ASN  |
| 41  | s     | 235 | ASN  |
| 41  | s     | 247 | HIS  |
| 41  | s     | 317 | GLN  |
| 42  | u     | 35  | GLN  |
| 42  | u     | 151 | ASN  |
| 43  | v     | 84  | GLN  |
| 43  | v     | 110 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 16  | 2MR  | Q     | 118 | 16   | 10,12,13     | 1.24 | 1 (10%)     | 5,13,15     | 1.22 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 16  | 2MR  | Q     | 118 | 16   | -       | 5/10/13/15 | -     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 16  | Q     | 118 | 2MR  | CZ-NH2 | -3.40 | 1.26        | 1.33     |

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 16  | Q     | 118 | 2MR  | NH1-CZ-NE-CD |
| 16  | Q     | 118 | 2MR  | NH2-CZ-NE-CD |
| 16  | Q     | 118 | 2MR  | CA-CB-CG-CD  |
| 16  | Q     | 118 | 2MR  | NE-CD-CG-CB  |
| 16  | Q     | 118 | 2MR  | N-CA-CB-CG   |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 16  | Q     | 118 | 2MR  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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 |
| 49  | PLX  | j     | 201 | -    | 51,51,51     | 1.21 | 5 (9%)   | 53,59,59    | 0.61 | 1 (1%)   |
| 49  | PLX  | a     | 202 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.62 | 1 (1%)   |
| 55  | CDL  | i     | 402 | -    | 99,99,99     | 1.11 | 8 (8%)   | 105,111,111 | 0.88 | 4 (3%)   |
| 45  | SF4  | M     | 802 | 12   | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PEE  | r     | 501 | -    | 50,50,50     | 1.18 | 6 (12%)  | 53,55,55    | 0.99 | 2 (3%)   |
| 47  | NAI  | A     | 503 | -    | 47,48,48     | 4.02 | 22 (46%) | 64,73,73    | 1.69 | 12 (18%) |
| 45  | SF4  | C     | 301 | 3,16 | 0,12,12      | -    | -        | -           | -    | -        |
| 45  | SF4  | B     | 301 | 2    | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PEE  | U     | 101 | -    | 50,50,50     | 1.17 | 6 (12%)  | 53,55,55    | 0.97 | 2 (3%)   |
| 52  | FES  | M     | 803 | 12   | 0,4,4        | -    | -        | -           | -    | -        |
| 55  | CDL  | a     | 201 | -    | 90,90,99     | 1.16 | 9 (10%)  | 96,102,111  | 0.94 | 4 (4%)   |
| 50  | 8Q1  | X     | 201 | -    | 32,34,34     | 1.61 | 6 (18%)  | 39,43,43    | 1.53 | 6 (15%)  |
| 48  | PEE  | l     | 702 | -    | 45,45,50     | 1.24 | 6 (13%)  | 48,50,55    | 0.98 | 2 (4%)   |
| 56  | UQ   | s     | 401 | -    | 28,28,63     | 3.32 | 7 (25%)  | 36,37,79    | 2.66 | 11 (30%) |
| 48  | PEE  | Q     | 501 | -    | 46,46,50     | 1.23 | 6 (13%)  | 49,51,55    | 1.00 | 2 (4%)   |
| 55  | CDL  | l     | 701 | -    | 99,99,99     | 1.11 | 9 (9%)   | 105,111,111 | 0.86 | 4 (3%)   |
| 48  | PEE  | l     | 703 | -    | 45,45,50     | 1.24 | 6 (13%)  | 48,50,55    | 0.97 | 2 (4%)   |
| 49  | PLX  | C     | 303 | -    | 51,51,51     | 1.21 | 4 (7%)   | 53,59,59    | 0.63 | 1 (1%)   |
| 50  | 8Q1  | G     | 201 | -    | 32,34,34     | 1.62 | 6 (18%)  | 39,43,43    | 1.57 | 6 (15%)  |
| 48  | PEE  | C     | 302 | -    | 46,46,50     | 1.24 | 6 (13%)  | 49,51,55    | 0.99 | 2 (4%)   |
| 52  | FES  | O     | 301 | 14   | 0,4,4        | -    | -        | -           | -    | -        |
| 45  | SF4  | A     | 501 | 1    | 0,12,12      | -    | -        | -           | -    | -        |
| 48  | PEE  | m     | 201 | -    | 40,40,50     | 1.17 | 5 (12%)  | 43,45,55    | 1.02 | 2 (4%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 49  | PLX  | r     | 503 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.60 | 1 (1%)   |
| 51  | NDP  | J     | 401 | -    | 51,52,52     | 4.29 | 25 (49%) | 71,80,80    | 2.18 | 18 (25%) |
| 48  | PEE  | Q     | 502 | -    | 50,50,50     | 1.18 | 6 (12%)  | 53,55,55    | 0.97 | 2 (3%)   |
| 45  | SF4  | B     | 302 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 45  | SF4  | M     | 801 | 12   | 0,12,12      | -    | -        | -           |      |          |
| 49  | PLX  | r     | 502 | -    | 51,51,51     | 1.20 | 4 (7%)   | 53,59,59    | 0.62 | 1 (1%)   |
| 57  | ADP  | w     | 401 | -    | 28,29,29     | 3.15 | 9 (32%)  | 43,45,45    | 1.91 | 10 (23%) |
| 46  | FMN  | A     | 502 | -    | 33,33,33     | 1.07 | 2 (6%)   | 48,50,50    | 1.23 | 7 (14%)  |
| 49  | PLX  | i     | 401 | -    | 51,51,51     | 1.20 | 3 (5%)   | 53,59,59    | 0.62 | 1 (1%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 49  | PLX  | j     | 201 | -    | -       | 28/55/55/55    | -       |
| 49  | PLX  | a     | 202 | -    | -       | 19/55/55/55    | -       |
| 55  | CDL  | i     | 402 | -    | -       | 63/110/110/110 | -       |
| 48  | PEE  | r     | 501 | -    | -       | 24/54/54/54    | -       |
| 45  | SF4  | M     | 802 | 12   | -       | -              | 0/6/5/5 |
| 47  | NAI  | A     | 503 | -    | -       | 5/29/72/72     | 0/5/5/5 |
| 45  | SF4  | C     | 301 | 3,16 | -       | -              | 0/6/5/5 |
| 45  | SF4  | B     | 301 | 2    | -       | -              | 0/6/5/5 |
| 48  | PEE  | U     | 101 | -    | -       | 26/54/54/54    | -       |
| 52  | FES  | M     | 803 | 12   | -       | -              | 0/1/1/1 |
| 55  | CDL  | a     | 201 | -    | -       | 40/101/101/110 | -       |
| 50  | 8Q1  | X     | 201 | -    | -       | 22/41/41/41    | -       |
| 48  | PEE  | l     | 702 | -    | -       | 28/49/49/54    | -       |
| 56  | UQ   | s     | 401 | -    | -       | 9/21/45/87     | 0/1/1/1 |
| 48  | PEE  | Q     | 501 | -    | -       | 23/50/50/54    | -       |
| 55  | CDL  | l     | 701 | -    | -       | 53/110/110/110 | -       |
| 48  | PEE  | l     | 703 | -    | -       | 23/49/49/54    | -       |
| 49  | PLX  | C     | 303 | -    | -       | 25/55/55/55    | -       |
| 50  | 8Q1  | G     | 201 | -    | -       | 20/41/41/41    | -       |
| 48  | PEE  | C     | 302 | -    | -       | 20/50/50/54    | -       |
| 52  | FES  | O     | 301 | 14   | -       | -              | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|-----|------|---------|-------------|---------|
| 45  | SF4  | A     | 501 | 1    | -       | -           | 0/6/5/5 |
| 48  | PEE  | m     | 201 | -    | -       | 18/44/44/54 | -       |
| 49  | PLX  | r     | 503 | -    | -       | 32/55/55/55 | -       |
| 51  | NDP  | J     | 401 | -    | -       | 9/34/77/77  | 0/5/5/5 |
| 48  | PEE  | Q     | 502 | -    | -       | 19/54/54/54 | -       |
| 45  | SF4  | B     | 302 | 2    | -       | -           | 0/6/5/5 |
| 49  | PLX  | r     | 502 | -    | -       | 33/55/55/55 | -       |
| 45  | SF4  | M     | 801 | 12   | -       | -           | 0/6/5/5 |
| 57  | ADP  | w     | 401 | -    | -       | 4/16/32/32  | 0/3/3/3 |
| 46  | FMN  | A     | 502 | -    | -       | 4/18/18/18  | 0/3/3/3 |
| 49  | PLX  | i     | 401 | -    | -       | 26/55/55/55 | -       |

All (174) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 51  | J     | 401 | NDP  | C3B-C2B | -12.97 | 1.24        | 1.53     |
| 51  | J     | 401 | NDP  | O4D-C4D | 10.72  | 1.68        | 1.45     |
| 47  | A     | 503 | NAI  | C3D-C4D | -10.38 | 1.26        | 1.53     |
| 51  | J     | 401 | NDP  | C3D-C4D | -9.92  | 1.27        | 1.53     |
| 56  | s     | 401 | UQ   | C13-C14 | 9.70   | 1.55        | 1.33     |
| 47  | A     | 503 | NAI  | O4B-C1B | 9.40   | 1.63        | 1.42     |
| 56  | s     | 401 | UQ   | C8-C9   | 9.20   | 1.54        | 1.33     |
| 57  | w     | 401 | ADP  | C3'-C4' | -8.93  | 1.30        | 1.53     |
| 47  | A     | 503 | NAI  | O4B-C4B | -8.39  | 1.26        | 1.45     |
| 51  | J     | 401 | NDP  | O4B-C4B | -8.05  | 1.27        | 1.45     |
| 56  | s     | 401 | UQ   | C18-C19 | 7.94   | 1.56        | 1.32     |
| 47  | A     | 503 | NAI  | C2D-C1D | -7.69  | 1.29        | 1.53     |
| 57  | w     | 401 | ADP  | O4'-C4' | 7.68   | 1.62        | 1.45     |
| 51  | J     | 401 | NDP  | C2N-C3N | 7.65   | 1.56        | 1.35     |
| 47  | A     | 503 | NAI  | C2B-C1B | -7.41  | 1.30        | 1.53     |
| 51  | J     | 401 | NDP  | C6N-C5N | 7.31   | 1.55        | 1.33     |
| 47  | A     | 503 | NAI  | O4D-C4D | 6.93   | 1.60        | 1.45     |
| 51  | J     | 401 | NDP  | PN-O3   | 6.59   | 1.66        | 1.59     |
| 47  | A     | 503 | NAI  | PA-O3   | 6.30   | 1.66        | 1.59     |
| 57  | w     | 401 | ADP  | PA-O3A  | 6.27   | 1.66        | 1.59     |
| 51  | J     | 401 | NDP  | P2B-O2B | 6.05   | 1.70        | 1.59     |
| 47  | A     | 503 | NAI  | C2D-C3D | 6.04   | 1.69        | 1.53     |
| 51  | J     | 401 | NDP  | C6A-N6A | 5.78   | 1.49        | 1.34     |
| 47  | A     | 503 | NAI  | O4D-C1D | 5.60   | 1.54        | 1.42     |
| 51  | J     | 401 | NDP  | PA-O3   | 5.56   | 1.65        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 47  | A     | 503 | NAI  | PN-O3   | 5.55  | 1.65        | 1.59     |
| 51  | J     | 401 | NDP  | C3B-C4B | 5.50  | 1.66        | 1.53     |
| 57  | w     | 401 | ADP  | C6-N6   | 5.39  | 1.48        | 1.34     |
| 47  | A     | 503 | NAI  | C7N-N7N | 5.31  | 1.48        | 1.33     |
| 47  | A     | 503 | NAI  | C4N-C3N | -5.30 | 1.40        | 1.50     |
| 50  | X     | 201 | 8Q1  | C39-N41 | 5.13  | 1.45        | 1.33     |
| 47  | A     | 503 | NAI  | C6A-N6A | 5.12  | 1.47        | 1.34     |
| 51  | J     | 401 | NDP  | C6N-N1N | 5.12  | 1.49        | 1.37     |
| 50  | G     | 201 | 8Q1  | C34-N36 | 5.07  | 1.45        | 1.33     |
| 50  | G     | 201 | 8Q1  | C39-N41 | 5.06  | 1.45        | 1.33     |
| 51  | J     | 401 | NDP  | O4D-C1D | -5.06 | 1.30        | 1.42     |
| 50  | X     | 201 | 8Q1  | C34-N36 | 5.01  | 1.45        | 1.33     |
| 51  | J     | 401 | NDP  | C1B-N9A | -4.58 | 1.33        | 1.46     |
| 51  | J     | 401 | NDP  | O4B-C1B | 4.57  | 1.52        | 1.42     |
| 57  | w     | 401 | ADP  | O4'-C1' | -4.55 | 1.31        | 1.42     |
| 47  | A     | 503 | NAI  | O2B-C2B | 4.31  | 1.53        | 1.43     |
| 51  | J     | 401 | NDP  | O2D-C2D | -3.92 | 1.33        | 1.43     |
| 51  | J     | 401 | NDP  | C7N-N7N | 3.87  | 1.44        | 1.33     |
| 48  | C     | 302 | PEE  | C18-C19 | 3.85  | 1.53        | 1.31     |
| 48  | m     | 201 | PEE  | C18-C19 | 3.84  | 1.53        | 1.31     |
| 48  | l     | 703 | PEE  | C18-C19 | 3.83  | 1.53        | 1.31     |
| 48  | r     | 501 | PEE  | C18-C19 | 3.81  | 1.53        | 1.31     |
| 48  | l     | 702 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | Q     | 501 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | Q     | 502 | PEE  | C18-C19 | 3.80  | 1.53        | 1.31     |
| 48  | U     | 101 | PEE  | C18-C19 | 3.78  | 1.53        | 1.31     |
| 48  | C     | 302 | PEE  | C39-C38 | 3.77  | 1.53        | 1.31     |
| 48  | Q     | 501 | PEE  | C39-C38 | 3.75  | 1.53        | 1.31     |
| 48  | r     | 501 | PEE  | C39-C38 | 3.73  | 1.52        | 1.31     |
| 48  | l     | 702 | PEE  | C39-C38 | 3.73  | 1.52        | 1.31     |
| 48  | U     | 101 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | l     | 703 | PEE  | C39-C38 | 3.72  | 1.52        | 1.31     |
| 48  | Q     | 502 | PEE  | C39-C38 | 3.71  | 1.52        | 1.31     |
| 47  | A     | 503 | NAI  | C7N-C3N | 3.58  | 1.56        | 1.48     |
| 46  | A     | 502 | FMN  | C4A-N5  | 3.50  | 1.38        | 1.30     |
| 47  | A     | 503 | NAI  | C4N-C5N | -3.44 | 1.40        | 1.49     |
| 55  | l     | 701 | CDL  | OA8-CA7 | 3.42  | 1.43        | 1.33     |
| 55  | i     | 402 | CDL  | OA8-CA7 | 3.41  | 1.43        | 1.33     |
| 55  | a     | 201 | CDL  | OA8-CA7 | 3.36  | 1.43        | 1.33     |
| 57  | w     | 401 | ADP  | C8-N9   | -3.33 | 1.31        | 1.37     |
| 51  | J     | 401 | NDP  | C7N-C3N | 3.21  | 1.55        | 1.48     |
| 51  | J     | 401 | NDP  | C8A-N9A | -3.20 | 1.32        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 57  | w     | 401 | ADP  | O2'-C2' | -3.20 | 1.35        | 1.43     |
| 51  | J     | 401 | NDP  | C5A-N7A | -3.09 | 1.33        | 1.39     |
| 55  | i     | 402 | CDL  | OB6-CB5 | 3.08  | 1.43        | 1.34     |
| 55  | l     | 701 | CDL  | OB6-CB5 | 3.06  | 1.42        | 1.34     |
| 55  | a     | 201 | CDL  | OB6-CB5 | 3.04  | 1.42        | 1.34     |
| 55  | l     | 701 | CDL  | OA6-CA5 | 3.04  | 1.42        | 1.34     |
| 55  | a     | 201 | CDL  | OB8-CB7 | 3.03  | 1.42        | 1.33     |
| 55  | i     | 402 | CDL  | OB8-CB7 | 2.98  | 1.42        | 1.33     |
| 57  | w     | 401 | ADP  | O3'-C3' | 2.98  | 1.50        | 1.43     |
| 55  | l     | 701 | CDL  | OB8-CB7 | 2.96  | 1.42        | 1.33     |
| 55  | a     | 201 | CDL  | OA6-CA5 | 2.96  | 1.42        | 1.34     |
| 51  | J     | 401 | NDP  | O3D-C3D | 2.95  | 1.50        | 1.43     |
| 55  | i     | 402 | CDL  | OA6-CA5 | 2.94  | 1.42        | 1.34     |
| 49  | a     | 202 | PLX  | O6-C4   | -2.92 | 1.40        | 1.44     |
| 49  | i     | 401 | PLX  | O6-C4   | -2.90 | 1.40        | 1.44     |
| 49  | C     | 303 | PLX  | O6-C4   | -2.88 | 1.40        | 1.44     |
| 49  | r     | 503 | PLX  | O6-C4   | -2.83 | 1.41        | 1.44     |
| 48  | Q     | 502 | PEE  | O2-C2   | -2.68 | 1.40        | 1.46     |
| 56  | s     | 401 | UQ   | C6-C1   | 2.67  | 1.54        | 1.46     |
| 47  | A     | 503 | NAI  | C8A-N9A | -2.67 | 1.33        | 1.37     |
| 49  | j     | 201 | PLX  | O6-C4   | -2.66 | 1.41        | 1.44     |
| 48  | C     | 302 | PEE  | O2-C2   | -2.63 | 1.40        | 1.46     |
| 48  | r     | 501 | PEE  | O2-C2   | -2.62 | 1.40        | 1.46     |
| 55  | i     | 402 | CDL  | OA6-CA4 | -2.60 | 1.40        | 1.46     |
| 51  | J     | 401 | NDP  | O2B-C2B | 2.60  | 1.52        | 1.44     |
| 48  | Q     | 501 | PEE  | O2-C2   | -2.58 | 1.40        | 1.46     |
| 55  | a     | 201 | CDL  | OA6-CA4 | -2.55 | 1.40        | 1.46     |
| 48  | l     | 703 | PEE  | O3-C30  | 2.55  | 1.40        | 1.33     |
| 48  | l     | 703 | PEE  | O2-C2   | -2.55 | 1.40        | 1.46     |
| 48  | U     | 101 | PEE  | O2-C2   | -2.53 | 1.40        | 1.46     |
| 48  | Q     | 501 | PEE  | O3-C30  | 2.51  | 1.40        | 1.33     |
| 47  | A     | 503 | NAI  | PN-O5D  | 2.51  | 1.69        | 1.59     |
| 48  | l     | 702 | PEE  | O2-C2   | -2.49 | 1.40        | 1.46     |
| 48  | Q     | 502 | PEE  | O3-C30  | 2.46  | 1.40        | 1.33     |
| 48  | r     | 501 | PEE  | O3-C30  | 2.46  | 1.40        | 1.33     |
| 48  | C     | 302 | PEE  | O3-C30  | 2.45  | 1.40        | 1.33     |
| 49  | r     | 502 | PLX  | C7-C6   | 2.45  | 1.55        | 1.50     |
| 55  | l     | 701 | CDL  | OA6-CA4 | -2.44 | 1.40        | 1.46     |
| 49  | r     | 502 | PLX  | O6-C4   | -2.43 | 1.41        | 1.44     |
| 48  | U     | 101 | PEE  | O3-C30  | 2.43  | 1.40        | 1.33     |
| 46  | A     | 502 | FMN  | C10-N1  | 2.42  | 1.38        | 1.33     |
| 48  | m     | 201 | PEE  | O2-C10  | 2.41  | 1.41        | 1.34     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 48  | l     | 702 | PEE  | O3-C30  | 2.41  | 1.40        | 1.33     |
| 50  | X     | 201 | 8Q1  | C1-S44  | 2.40  | 1.81        | 1.76     |
| 48  | m     | 201 | PEE  | O3-C30  | 2.40  | 1.40        | 1.33     |
| 50  | G     | 201 | 8Q1  | C1-S44  | 2.39  | 1.81        | 1.76     |
| 48  | m     | 201 | PEE  | O2-C2   | -2.39 | 1.41        | 1.46     |
| 51  | J     | 401 | NDP  | C2D-C3D | 2.39  | 1.59        | 1.53     |
| 47  | A     | 503 | NAI  | C6N-C5N | 2.39  | 1.40        | 1.33     |
| 49  | j     | 201 | PLX  | C7-C6   | 2.38  | 1.55        | 1.50     |
| 49  | C     | 303 | PLX  | C7-C6   | 2.36  | 1.55        | 1.50     |
| 55  | l     | 701 | CDL  | OB6-CB4 | -2.35 | 1.41        | 1.46     |
| 57  | w     | 401 | ADP  | C5-N7   | -2.35 | 1.34        | 1.39     |
| 50  | G     | 201 | 8Q1  | O40-C39 | -2.35 | 1.18        | 1.23     |
| 49  | a     | 202 | PLX  | C7-C6   | 2.33  | 1.55        | 1.50     |
| 49  | r     | 503 | PLX  | C7-C6   | 2.33  | 1.55        | 1.50     |
| 48  | l     | 702 | PEE  | O2-C10  | 2.33  | 1.40        | 1.34     |
| 49  | i     | 401 | PLX  | C7-C6   | 2.32  | 1.55        | 1.50     |
| 47  | A     | 503 | NAI  | O3B-C3B | -2.28 | 1.37        | 1.43     |
| 50  | G     | 201 | 8Q1  | O35-C34 | -2.28 | 1.19        | 1.23     |
| 48  | U     | 101 | PEE  | O2-C10  | 2.28  | 1.40        | 1.34     |
| 50  | X     | 201 | 8Q1  | O40-C39 | -2.28 | 1.18        | 1.23     |
| 48  | Q     | 501 | PEE  | O2-C10  | 2.27  | 1.40        | 1.34     |
| 48  | C     | 302 | PEE  | O2-C10  | 2.26  | 1.40        | 1.34     |
| 48  | l     | 703 | PEE  | O2-C10  | 2.26  | 1.40        | 1.34     |
| 47  | A     | 503 | NAI  | C5B-C4B | 2.25  | 1.58        | 1.51     |
| 50  | X     | 201 | 8Q1  | O35-C34 | -2.25 | 1.19        | 1.23     |
| 48  | Q     | 502 | PEE  | O2-C10  | 2.25  | 1.40        | 1.34     |
| 55  | a     | 201 | CDL  | PB2-OB2 | 2.25  | 1.68        | 1.59     |
| 55  | i     | 402 | CDL  | PB2-OB2 | 2.24  | 1.68        | 1.59     |
| 55  | l     | 701 | CDL  | PB2-OB2 | 2.24  | 1.68        | 1.59     |
| 50  | X     | 201 | 8Q1  | C6-C1   | 2.23  | 1.53        | 1.50     |
| 55  | i     | 402 | CDL  | PB2-OB5 | 2.23  | 1.68        | 1.59     |
| 49  | j     | 201 | PLX  | P1-O4   | 2.21  | 1.68        | 1.59     |
| 55  | i     | 402 | CDL  | OB6-CB4 | -2.21 | 1.41        | 1.46     |
| 55  | a     | 201 | CDL  | PB2-OB5 | 2.19  | 1.68        | 1.59     |
| 55  | a     | 201 | CDL  | OB6-CB4 | -2.19 | 1.41        | 1.46     |
| 48  | r     | 501 | PEE  | O2-C10  | 2.17  | 1.40        | 1.34     |
| 50  | G     | 201 | 8Q1  | C6-C1   | 2.17  | 1.53        | 1.50     |
| 48  | U     | 101 | PEE  | O3-C3   | -2.17 | 1.40        | 1.45     |
| 51  | J     | 401 | NDP  | PA-O5B  | 2.17  | 1.67        | 1.59     |
| 48  | l     | 702 | PEE  | O3-C3   | -2.16 | 1.40        | 1.45     |
| 48  | Q     | 502 | PEE  | O3-C3   | -2.16 | 1.40        | 1.45     |
| 49  | r     | 502 | PLX  | P1-O4   | 2.15  | 1.67        | 1.59     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | a     | 202 | PLX  | P1-O4   | 2.15  | 1.67        | 1.59     |
| 49  | r     | 503 | PLX  | P1-O4   | 2.14  | 1.67        | 1.59     |
| 48  | m     | 201 | PEE  | O3-C3   | -2.14 | 1.40        | 1.45     |
| 56  | s     | 401 | UQ   | O4-C4   | -2.13 | 1.18        | 1.23     |
| 49  | C     | 303 | PLX  | P1-O4   | 2.13  | 1.67        | 1.59     |
| 48  | C     | 302 | PEE  | O3-C3   | -2.13 | 1.40        | 1.45     |
| 49  | i     | 401 | PLX  | P1-O4   | 2.13  | 1.67        | 1.59     |
| 55  | l     | 701 | CDL  | PB2-OB5 | 2.12  | 1.67        | 1.59     |
| 48  | r     | 501 | PEE  | O3-C3   | -2.12 | 1.40        | 1.45     |
| 51  | J     | 401 | NDP  | O7N-C7N | -2.12 | 1.19        | 1.24     |
| 49  | r     | 502 | PLX  | P1-O1   | 2.11  | 1.67        | 1.59     |
| 49  | r     | 503 | PLX  | P1-O1   | 2.10  | 1.67        | 1.59     |
| 48  | l     | 703 | PEE  | O3-C3   | -2.10 | 1.40        | 1.45     |
| 49  | j     | 201 | PLX  | P1-O1   | 2.10  | 1.67        | 1.59     |
| 47  | A     | 503 | NAI  | C5A-N7A | -2.08 | 1.35        | 1.39     |
| 48  | Q     | 501 | PEE  | O3-C3   | -2.07 | 1.40        | 1.45     |
| 56  | s     | 401 | UQ   | O3-CM3  | -2.07 | 1.40        | 1.45     |
| 49  | a     | 202 | PLX  | P1-O1   | 2.06  | 1.67        | 1.59     |
| 49  | C     | 303 | PLX  | P1-O1   | 2.04  | 1.67        | 1.59     |
| 56  | s     | 401 | UQ   | C7-C8   | 2.04  | 1.53        | 1.50     |
| 55  | l     | 701 | CDL  | C11-CA5 | 2.02  | 1.56        | 1.50     |
| 55  | a     | 201 | CDL  | C11-CA5 | 2.02  | 1.56        | 1.50     |
| 49  | j     | 201 | PLX  | C1-C2   | 2.01  | 1.57        | 1.51     |

All (104) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | s     | 401 | UQ   | C7-C8-C9    | -9.05 | 111.24      | 126.83   |
| 51  | J     | 401 | NDP  | C3N-C2N-N1N | -7.46 | 112.25      | 123.20   |
| 51  | J     | 401 | NDP  | C1D-N1N-C2N | -6.56 | 110.34      | 121.14   |
| 56  | s     | 401 | UQ   | C12-C13-C14 | -6.17 | 113.50      | 127.62   |
| 50  | G     | 201 | 8Q1  | C6-C1-S44   | 5.81  | 120.33      | 113.40   |
| 50  | X     | 201 | 8Q1  | C6-C1-S44   | 5.74  | 120.24      | 113.40   |
| 47  | A     | 503 | NAI  | C5A-C4A-N3A | -5.57 | 119.05      | 126.72   |
| 51  | J     | 401 | NDP  | C1D-N1N-C6N | -5.56 | 109.02      | 120.77   |
| 51  | J     | 401 | NDP  | C5A-C4A-N3A | -5.52 | 119.12      | 126.72   |
| 57  | w     | 401 | ADP  | C5-C4-N3    | -5.45 | 119.21      | 126.72   |
| 51  | J     | 401 | NDP  | C6N-N1N-C2N | -5.36 | 113.58      | 119.32   |
| 56  | s     | 401 | UQ   | C10-C9-C8   | -4.60 | 111.82      | 123.63   |
| 57  | w     | 401 | ADP  | N3-C2-N1    | -4.55 | 121.69      | 128.58   |
| 47  | A     | 503 | NAI  | N3A-C2A-N1A | -4.37 | 121.97      | 128.58   |
| 57  | w     | 401 | ADP  | N3-C4-N9    | 4.27  | 134.43      | 127.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 55  | a     | 201 | CDL  | OA6-CA5-C11 | 4.21  | 120.60      | 111.48   |
| 56  | s     | 401 | UQ   | C11-C9-C8   | -4.21 | 111.72      | 121.17   |
| 55  | a     | 201 | CDL  | OB6-CB5-C51 | 4.19  | 120.53      | 111.48   |
| 48  | m     | 201 | PEE  | O2-C10-C11  | 4.17  | 120.49      | 111.48   |
| 51  | J     | 401 | NDP  | N3A-C2A-N1A | -4.12 | 122.35      | 128.58   |
| 55  | i     | 402 | CDL  | OB6-CB5-C51 | 4.11  | 120.37      | 111.48   |
| 56  | s     | 401 | UQ   | C17-C18-C19 | -4.05 | 114.14      | 127.64   |
| 55  | l     | 701 | CDL  | OA6-CA5-C11 | 4.04  | 120.22      | 111.48   |
| 48  | r     | 501 | PEE  | O2-C10-C11  | 4.02  | 120.18      | 111.48   |
| 56  | s     | 401 | UQ   | C15-C14-C13 | -4.00 | 113.36      | 123.63   |
| 48  | Q     | 501 | PEE  | O2-C10-C11  | 3.98  | 120.09      | 111.48   |
| 48  | C     | 302 | PEE  | O2-C10-C11  | 3.96  | 120.04      | 111.48   |
| 55  | i     | 402 | CDL  | OA6-CA5-C11 | 3.93  | 119.99      | 111.48   |
| 51  | J     | 401 | NDP  | N3A-C4A-N9A | 3.93  | 133.86      | 127.17   |
| 47  | A     | 503 | NAI  | N3A-C4A-N9A | 3.90  | 133.79      | 127.17   |
| 48  | U     | 101 | PEE  | O2-C10-C11  | 3.85  | 119.82      | 111.48   |
| 48  | Q     | 502 | PEE  | O2-C10-C11  | 3.83  | 119.76      | 111.48   |
| 48  | l     | 703 | PEE  | O2-C10-C11  | 3.78  | 119.67      | 111.48   |
| 47  | A     | 503 | NAI  | C2A-N3A-C4A | 3.71  | 120.89      | 111.83   |
| 48  | l     | 702 | PEE  | O2-C10-C11  | 3.70  | 119.49      | 111.48   |
| 55  | l     | 701 | CDL  | OB6-CB5-C51 | 3.65  | 119.38      | 111.48   |
| 57  | w     | 401 | ADP  | C2-N3-C4    | 3.59  | 120.59      | 111.83   |
| 56  | s     | 401 | UQ   | C16-C14-C13 | -3.58 | 113.13      | 121.17   |
| 51  | J     | 401 | NDP  | C2A-N3A-C4A | 3.57  | 120.56      | 111.83   |
| 47  | A     | 503 | NAI  | C4A-C5A-N7A | -3.54 | 106.54      | 110.58   |
| 50  | X     | 201 | 8Q1  | O4-C1-C6    | -3.52 | 119.92      | 123.98   |
| 57  | w     | 401 | ADP  | N9-C8-N7    | -3.49 | 108.99      | 113.94   |
| 50  | G     | 201 | 8Q1  | C37-C38-C39 | 3.45  | 118.14      | 112.39   |
| 47  | A     | 503 | NAI  | C5A-N7A-C8A | 3.43  | 108.85      | 103.45   |
| 50  | G     | 201 | 8Q1  | O4-C1-C6    | -3.42 | 120.04      | 123.98   |
| 47  | A     | 503 | NAI  | C3D-C2D-C1D | 3.41  | 107.92      | 101.46   |
| 56  | s     | 401 | UQ   | C21-C19-C18 | -3.27 | 112.84      | 122.66   |
| 47  | A     | 503 | NAI  | N9A-C8A-N7A | -3.23 | 109.35      | 113.94   |
| 46  | A     | 502 | FMN  | C4-N3-C2    | -3.20 | 119.96      | 125.64   |
| 57  | w     | 401 | ADP  | C4-N9-C8    | 3.16  | 109.05      | 105.74   |
| 57  | w     | 401 | ADP  | C5-N7-C8    | 3.15  | 108.41      | 103.45   |
| 51  | J     | 401 | NDP  | C4A-C5A-N7A | -3.15 | 106.98      | 110.58   |
| 51  | J     | 401 | NDP  | N9A-C8A-N7A | -3.13 | 109.49      | 113.94   |
| 51  | J     | 401 | NDP  | C5A-N7A-C8A | 3.00  | 108.17      | 103.45   |
| 57  | w     | 401 | ADP  | C4-C5-N7    | -2.97 | 107.19      | 110.58   |
| 56  | s     | 401 | UQ   | C7-C6-C5    | -2.90 | 119.91      | 124.89   |
| 56  | s     | 401 | UQ   | C20-C19-C18 | -2.86 | 114.07      | 122.66   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 48  | r     | 501 | PEE  | O3-C30-C31  | 2.84  | 120.48      | 111.83   |
| 56  | s     | 401 | UQ   | CM5-C5-C6   | -2.79 | 119.86      | 124.45   |
| 48  | l     | 702 | PEE  | O3-C30-C31  | 2.78  | 120.30      | 111.83   |
| 55  | a     | 201 | CDL  | OB8-CB7-C71 | 2.75  | 120.22      | 111.83   |
| 47  | A     | 503 | NAI  | C2D-C3D-C4D | 2.75  | 107.92      | 102.61   |
| 48  | m     | 201 | PEE  | O3-C30-C31  | 2.72  | 120.13      | 111.83   |
| 48  | C     | 302 | PEE  | O3-C30-C31  | 2.71  | 120.11      | 111.83   |
| 48  | l     | 703 | PEE  | O3-C30-C31  | 2.70  | 120.07      | 111.83   |
| 48  | Q     | 501 | PEE  | O3-C30-C31  | 2.68  | 120.01      | 111.83   |
| 55  | l     | 701 | CDL  | OB8-CB7-C71 | 2.67  | 119.98      | 111.83   |
| 51  | J     | 401 | NDP  | C2B-C3B-C4B | 2.67  | 107.73      | 101.99   |
| 48  | Q     | 502 | PEE  | O3-C30-C31  | 2.66  | 119.95      | 111.83   |
| 55  | i     | 402 | CDL  | OA8-CA7-C31 | 2.65  | 119.91      | 111.83   |
| 46  | A     | 502 | FMN  | C4A-C4-N3   | 2.64  | 119.98      | 113.25   |
| 55  | i     | 402 | CDL  | OB8-CB7-C71 | 2.59  | 119.73      | 111.83   |
| 48  | U     | 101 | PEE  | O3-C30-C31  | 2.57  | 119.68      | 111.83   |
| 46  | A     | 502 | FMN  | O4-C4-C4A   | -2.57 | 119.76      | 126.53   |
| 55  | a     | 201 | CDL  | OA8-CA7-C31 | 2.55  | 119.61      | 111.83   |
| 55  | l     | 701 | CDL  | OA8-CA7-C31 | 2.55  | 119.60      | 111.83   |
| 51  | J     | 401 | NDP  | C4B-O4B-C1B | -2.49 | 103.97      | 109.47   |
| 49  | r     | 502 | PLX  | C1A-N1-C1   | 2.48  | 119.78      | 109.91   |
| 49  | i     | 401 | PLX  | C1A-N1-C1   | 2.48  | 119.78      | 109.91   |
| 47  | A     | 503 | NAI  | C4D-O4D-C1D | -2.48 | 103.99      | 109.47   |
| 51  | J     | 401 | NDP  | C4A-N9A-C8A | 2.47  | 108.33      | 105.74   |
| 46  | A     | 502 | FMN  | C5A-C9A-N10 | 2.47  | 120.20      | 117.97   |
| 49  | j     | 201 | PLX  | C1A-N1-C1   | 2.45  | 119.64      | 109.91   |
| 49  | a     | 202 | PLX  | C1A-N1-C1   | 2.44  | 119.61      | 109.91   |
| 50  | G     | 201 | 8Q1  | O4-C1-S44   | -2.40 | 119.63      | 122.68   |
| 51  | J     | 401 | NDP  | C2B-C1B-N9A | -2.38 | 109.83      | 113.75   |
| 49  | r     | 503 | PLX  | C1A-N1-C1   | 2.38  | 119.37      | 109.91   |
| 46  | A     | 502 | FMN  | C4A-C10-N10 | 2.38  | 119.88      | 116.48   |
| 46  | A     | 502 | FMN  | C9A-C5A-N5  | -2.32 | 119.99      | 122.45   |
| 50  | X     | 201 | 8Q1  | C43-S44-C1  | 2.30  | 108.65      | 101.84   |
| 50  | X     | 201 | 8Q1  | C37-C38-C39 | 2.28  | 116.19      | 112.39   |
| 49  | C     | 303 | PLX  | C1A-N1-C1   | 2.26  | 118.89      | 109.91   |
| 47  | A     | 503 | NAI  | C4A-N9A-C8A | 2.25  | 108.10      | 105.74   |
| 50  | X     | 201 | 8Q1  | O4-C1-S44   | -2.24 | 119.84      | 122.68   |
| 46  | A     | 502 | FMN  | C10-C4A-N5  | -2.20 | 120.31      | 124.81   |
| 50  | G     | 201 | 8Q1  | C43-S44-C1  | 2.17  | 108.26      | 101.84   |
| 50  | X     | 201 | 8Q1  | C38-C39-N41 | 2.16  | 120.28      | 116.34   |
| 57  | w     | 401 | ADP  | C4'-O4'-C1' | -2.15 | 104.72      | 109.47   |
| 50  | G     | 201 | 8Q1  | C38-C39-N41 | 2.11  | 120.18      | 116.34   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 51  | J     | 401 | NDP  | O4B-C1B-C2B | -2.06 | 103.04      | 106.59   |
| 57  | w     | 401 | ADP  | C2'-C3'-C4' | 2.05  | 106.58      | 102.61   |
| 51  | J     | 401 | NDP  | P2B-O2B-C2B | -2.03 | 118.02      | 123.43   |
| 47  | A     | 503 | NAI  | C6N-N1N-C2N | 2.02  | 121.48      | 119.32   |
| 51  | J     | 401 | NDP  | C2D-C3D-C4D | 2.01  | 106.49      | 102.61   |

There are no chirality outliers.

All (573) 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' |
| 47  | A     | 503 | NAI  | C5B-O5B-PA-O1A  |
| 48  | C     | 302 | PEE  | C1-O3P-P-O2P    |
| 48  | C     | 302 | PEE  | C1-O3P-P-O1P    |
| 48  | C     | 302 | PEE  | C1-O3P-P-O4P    |
| 48  | Q     | 501 | PEE  | C11-C10-O2-C2   |
| 48  | Q     | 501 | PEE  | C4-O4P-P-O1P    |
| 48  | Q     | 502 | PEE  | C1-O3P-P-O1P    |
| 48  | U     | 101 | PEE  | C1-O3P-P-O2P    |
| 48  | U     | 101 | PEE  | C1-O3P-P-O1P    |
| 48  | U     | 101 | PEE  | C1-O3P-P-O4P    |
| 48  | l     | 702 | PEE  | C11-C10-O2-C2   |
| 48  | l     | 702 | PEE  | O4-C10-O2-C2    |
| 48  | l     | 702 | PEE  | C4-O4P-P-O3P    |
| 48  | l     | 702 | PEE  | C4-O4P-P-O2P    |
| 48  | l     | 702 | PEE  | C4-O4P-P-O1P    |
| 48  | m     | 201 | PEE  | C11-C10-O2-C2   |
| 48  | m     | 201 | PEE  | O4-C10-O2-C2    |
| 48  | m     | 201 | PEE  | C4-O4P-P-O3P    |
| 48  | m     | 201 | PEE  | C4-O4P-P-O2P    |
| 48  | m     | 201 | PEE  | C4-O4P-P-O1P    |
| 48  | m     | 201 | PEE  | O4P-C4-C5-N     |
| 48  | r     | 501 | PEE  | C1-O3P-P-O2P    |
| 48  | r     | 501 | PEE  | C1-O3P-P-O1P    |
| 48  | r     | 501 | PEE  | C1-O3P-P-O4P    |
| 49  | C     | 303 | PLX  | C3-O4-P1-O1     |
| 49  | C     | 303 | PLX  | C3-O4-P1-O3     |
| 49  | C     | 303 | PLX  | N1-C1-C2-O1     |
| 49  | a     | 202 | PLX  | O7-C6-C7-C8     |
| 49  | i     | 401 | PLX  | O7-C6-O6-C4     |
| 49  | j     | 201 | PLX  | O7-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | r     | 502 | PLX  | O7-C6-O6-C4     |
| 49  | r     | 502 | PLX  | C5-C4-O6-C6     |
| 49  | r     | 502 | PLX  | O9-C24-O8-C5    |
| 49  | r     | 502 | PLX  | O9-C24-C25-C26  |
| 49  | r     | 503 | PLX  | C3-O4-P1-O1     |
| 49  | r     | 503 | PLX  | O9-C24-O8-C5    |
| 49  | r     | 503 | PLX  | O9-C24-C25-C26  |
| 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  | C28-C29-C32-C34 |
| 50  | G     | 201 | 8Q1  | C28-C29-C32-O33 |
| 50  | G     | 201 | 8Q1  | N41-C42-C43-S44 |
| 50  | G     | 201 | 8Q1  | C42-C43-S44-C1  |
| 50  | X     | 201 | 8Q1  | C1-C6-C7-C8     |
| 50  | X     | 201 | 8Q1  | O4-C1-S44-C43   |
| 50  | X     | 201 | 8Q1  | C6-C1-S44-C43   |
| 50  | X     | 201 | 8Q1  | O27-C28-C29-C30 |
| 50  | X     | 201 | 8Q1  | O27-C28-C29-C31 |
| 50  | X     | 201 | 8Q1  | O27-C28-C29-C32 |
| 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  | C31-C29-C32-O33 |
| 50  | X     | 201 | 8Q1  | N36-C37-C38-C39 |
| 50  | X     | 201 | 8Q1  | C42-C43-S44-C1  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O2  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O1  |
| 51  | J     | 401 | NDP  | C5B-O5B-PA-O1A  |
| 51  | J     | 401 | NDP  | C5B-O5B-PA-O3   |
| 51  | J     | 401 | NDP  | O4B-C4B-C5B-O5B |
| 51  | J     | 401 | NDP  | C2N-C3N-C7N-N7N |
| 55  | a     | 201 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | a     | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | a     | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | a     | 201 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | a     | 201 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | a     | 201 | CDL  | CB3-OB5-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | i     | 402 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | i     | 402 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | i     | 402 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | i     | 402 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | i     | 402 | CDL  | CA3-OA5-PA1-OA3 |
| 55  | i     | 402 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | i     | 402 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | i     | 402 | CDL  | CB3-OB5-PB2-OB4 |
| 55  | l     | 701 | CDL  | CA2-OA2-PA1-OA3 |
| 55  | l     | 701 | CDL  | CA2-OA2-PA1-OA4 |
| 55  | l     | 701 | CDL  | CA2-OA2-PA1-OA5 |
| 55  | l     | 701 | CDL  | CA3-OA5-PA1-OA2 |
| 55  | l     | 701 | CDL  | CA3-OA5-PA1-OA4 |
| 55  | l     | 701 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | l     | 701 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | l     | 701 | CDL  | CB2-OB2-PB2-OB5 |
| 56  | s     | 401 | UQ   | C7-C8-C9-C11    |
| 56  | s     | 401 | UQ   | C12-C13-C14-C16 |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O2A  |
| 56  | s     | 401 | UQ   | C17-C18-C19-C21 |
| 56  | s     | 401 | UQ   | C12-C11-C9-C10  |
| 56  | s     | 401 | UQ   | C13-C14-C16-C17 |
| 48  | l     | 703 | PEE  | C31-C30-O3-C3   |
| 56  | s     | 401 | UQ   | C7-C8-C9-C10    |
| 48  | Q     | 502 | PEE  | C37-C38-C39-C40 |
| 48  | U     | 101 | PEE  | C17-C18-C19-C20 |
| 48  | Q     | 501 | PEE  | O4-C10-O2-C2    |
| 48  | l     | 702 | PEE  | C31-C30-O3-C3   |
| 48  | m     | 201 | PEE  | C31-C30-O3-C3   |
| 55  | i     | 402 | CDL  | C71-CB7-OB8-CB6 |
| 48  | l     | 703 | PEE  | O5-C30-O3-C3    |
| 51  | J     | 401 | NDP  | C2D-C1D-N1N-C6N |
| 48  | l     | 702 | PEE  | O5-C30-O3-C3    |
| 48  | m     | 201 | PEE  | O5-C30-O3-C3    |
| 55  | i     | 402 | CDL  | OB9-CB7-OB8-CB6 |
| 56  | s     | 401 | UQ   | C9-C11-C12-C13  |
| 56  | s     | 401 | UQ   | C14-C16-C17-C18 |
| 55  | l     | 701 | CDL  | C59-C60-C61-C62 |
| 49  | i     | 401 | PLX  | C7-C8-C9-C10    |
| 48  | l     | 703 | PEE  | C37-C38-C39-C40 |
| 48  | r     | 501 | PEE  | C17-C18-C19-C20 |
| 49  | a     | 202 | PLX  | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | r     | 502 | PLX  | C9-C10-C11-C12  |
| 49  | r     | 503 | PLX  | C12-C13-C14-C15 |
| 55  | i     | 402 | CDL  | CB2-C1-CA2-OA2  |
| 48  | U     | 101 | PEE  | C31-C30-O3-C3   |
| 55  | a     | 201 | CDL  | C71-CB7-OB8-CB6 |
| 55  | l     | 701 | CDL  | C71-CB7-OB8-CB6 |
| 49  | j     | 201 | PLX  | C28-C29-C30-C31 |
| 48  | Q     | 502 | PEE  | C12-C13-C14-C15 |
| 55  | i     | 402 | CDL  | OA6-CA4-CA6-OA8 |
| 55  | a     | 201 | CDL  | C34-C35-C36-C37 |
| 49  | r     | 502 | PLX  | C30-C31-C32-C33 |
| 48  | U     | 101 | PEE  | O5-C30-O3-C3    |
| 49  | i     | 401 | PLX  | C31-C32-C33-C34 |
| 51  | J     | 401 | NDP  | C3B-C4B-C5B-O5B |
| 55  | i     | 402 | CDL  | C78-C79-C80-C81 |
| 55  | l     | 701 | CDL  | C35-C36-C37-C38 |
| 48  | r     | 501 | PEE  | C10-C11-C12-C13 |
| 55  | a     | 201 | CDL  | CA7-C31-C32-C33 |
| 55  | a     | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 55  | i     | 402 | CDL  | CB7-C71-C72-C73 |
| 55  | l     | 701 | CDL  | OB9-CB7-OB8-CB6 |
| 49  | j     | 201 | PLX  | C15-C16-C17-C18 |
| 49  | j     | 201 | PLX  | C34-C35-C36-C37 |
| 49  | r     | 502 | PLX  | C11-C12-C13-C14 |
| 55  | i     | 402 | CDL  | C74-C75-C76-C77 |
| 55  | i     | 402 | CDL  | O1-C1-CA2-OA2   |
| 49  | C     | 303 | PLX  | C28-C29-C30-C31 |
| 48  | U     | 101 | PEE  | C34-C35-C36-C37 |
| 55  | l     | 701 | CDL  | C11-C12-C13-C14 |
| 49  | C     | 303 | PLX  | O6-C6-C7-C8     |
| 55  | i     | 402 | CDL  | C51-CB5-OB6-CB4 |
| 55  | l     | 701 | CDL  | C39-C40-C41-C42 |
| 55  | i     | 402 | CDL  | OB7-CB5-OB6-CB4 |
| 48  | Q     | 501 | PEE  | C17-C18-C19-C20 |
| 55  | i     | 402 | CDL  | CB5-C51-C52-C53 |
| 48  | r     | 501 | PEE  | C11-C10-O2-C2   |
| 49  | a     | 202 | PLX  | C28-C29-C30-C31 |
| 49  | i     | 401 | PLX  | C27-C28-C29-C30 |
| 49  | r     | 503 | PLX  | C33-C34-C35-C36 |
| 55  | a     | 201 | CDL  | C73-C74-C75-C76 |
| 48  | C     | 302 | PEE  | C37-C38-C39-C40 |
| 49  | a     | 202 | PLX  | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | l     | 701 | CDL  | C51-C52-C53-C54 |
| 49  | C     | 303 | PLX  | O7-C6-C7-C8     |
| 49  | C     | 303 | PLX  | C17-C18-C19-C20 |
| 48  | Q     | 502 | PEE  | C14-C15-C16-C17 |
| 49  | r     | 503 | PLX  | C13-C14-C15-C16 |
| 48  | U     | 101 | PEE  | C40-C41-C42-C43 |
| 49  | i     | 401 | PLX  | C10-C11-C12-C13 |
| 49  | r     | 502 | PLX  | C27-C28-C29-C30 |
| 48  | Q     | 502 | PEE  | C34-C35-C36-C37 |
| 49  | i     | 401 | PLX  | C11-C10-C9-C8   |
| 55  | l     | 701 | CDL  | C52-C53-C54-C55 |
| 55  | l     | 701 | CDL  | C75-C76-C77-C78 |
| 48  | C     | 302 | PEE  | C11-C10-O2-C2   |
| 48  | U     | 101 | PEE  | C11-C10-O2-C2   |
| 49  | r     | 503 | PLX  | C14-C15-C16-C17 |
| 49  | a     | 202 | PLX  | C10-C11-C12-C13 |
| 55  | a     | 201 | CDL  | C35-C36-C37-C38 |
| 55  | a     | 201 | CDL  | CB5-C51-C52-C53 |
| 48  | l     | 703 | PEE  | C33-C34-C35-C36 |
| 49  | j     | 201 | PLX  | C7-C8-C9-C10    |
| 55  | i     | 402 | CDL  | C17-C18-C19-C20 |
| 55  | i     | 402 | CDL  | CA7-C31-C32-C33 |
| 55  | l     | 701 | CDL  | C37-C38-C39-C40 |
| 49  | i     | 401 | PLX  | C25-C26-C27-C28 |
| 49  | r     | 503 | PLX  | C25-C26-C27-C28 |
| 55  | i     | 402 | CDL  | C55-C56-C57-C58 |
| 48  | r     | 501 | PEE  | O4-C10-O2-C2    |
| 55  | l     | 701 | CDL  | CB3-CB4-CB6-OB8 |
| 48  | r     | 501 | PEE  | C31-C32-C33-C34 |
| 49  | a     | 202 | PLX  | C7-C8-C9-C10    |
| 55  | i     | 402 | CDL  | C73-C74-C75-C76 |
| 48  | l     | 703 | PEE  | C12-C13-C14-C15 |
| 49  | j     | 201 | PLX  | C27-C28-C29-C30 |
| 50  | G     | 201 | 8Q1  | C7-C8-C9-C10    |
| 48  | C     | 302 | PEE  | C42-C43-C44-C45 |
| 49  | i     | 401 | PLX  | C9-C10-C11-C12  |
| 49  | a     | 202 | PLX  | C14-C15-C16-C17 |
| 49  | r     | 502 | PLX  | C7-C8-C9-C10    |
| 48  | Q     | 502 | PEE  | C33-C34-C35-C36 |
| 55  | l     | 701 | CDL  | CB7-C71-C72-C73 |
| 48  | Q     | 501 | PEE  | C22-C23-C24-C25 |
| 49  | a     | 202 | PLX  | C29-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 49  | i     | 401 | PLX  | C32-C33-C34-C35 |
| 55  | i     | 402 | CDL  | C75-C76-C77-C78 |
| 48  | Q     | 502 | PEE  | C30-C31-C32-C33 |
| 55  | a     | 201 | CDL  | C17-C18-C19-C20 |
| 48  | m     | 201 | PEE  | C11-C12-C13-C14 |
| 49  | C     | 303 | PLX  | C14-C15-C16-C17 |
| 55  | a     | 201 | CDL  | C75-C76-C77-C78 |
| 48  | C     | 302 | PEE  | O4-C10-O2-C2    |
| 48  | U     | 101 | PEE  | O4-C10-O2-C2    |
| 49  | i     | 401 | PLX  | C30-C31-C32-C33 |
| 55  | i     | 402 | CDL  | C43-C44-C45-C46 |
| 55  | l     | 701 | CDL  | C73-C74-C75-C76 |
| 49  | C     | 303 | PLX  | C13-C14-C15-C16 |
| 49  | i     | 401 | PLX  | C33-C34-C35-C36 |
| 49  | j     | 201 | PLX  | C10-C11-C12-C13 |
| 49  | r     | 503 | PLX  | C28-C29-C30-C31 |
| 55  | a     | 201 | CDL  | C21-C22-C23-C24 |
| 55  | i     | 402 | CDL  | C71-C72-C73-C74 |
| 48  | r     | 501 | PEE  | C12-C13-C14-C15 |
| 55  | a     | 201 | CDL  | C37-C38-C39-C40 |
| 55  | l     | 701 | CDL  | C40-C41-C42-C43 |
| 55  | a     | 201 | CDL  | C31-C32-C33-C34 |
| 49  | i     | 401 | PLX  | C28-C29-C30-C31 |
| 49  | j     | 201 | PLX  | C25-C26-C27-C28 |
| 50  | X     | 201 | 8Q1  | C6-C7-C8-C9     |
| 55  | a     | 201 | CDL  | C11-C12-C13-C14 |
| 48  | Q     | 501 | PEE  | C21-C22-C23-C24 |
| 49  | C     | 303 | PLX  | C16-C17-C18-C19 |
| 49  | r     | 503 | PLX  | C29-C30-C31-C32 |
| 55  | l     | 701 | CDL  | C51-CB5-OB6-CB4 |
| 48  | l     | 702 | PEE  | C31-C32-C33-C34 |
| 49  | r     | 502 | PLX  | C28-C29-C30-C31 |
| 48  | Q     | 501 | PEE  | C35-C36-C37-C38 |
| 48  | l     | 703 | PEE  | C31-C32-C33-C34 |
| 48  | Q     | 501 | PEE  | C10-C11-C12-C13 |
| 49  | r     | 503 | PLX  | C2-C1-N1-C1C    |
| 49  | r     | 503 | PLX  | C2-C1-N1-C1A    |
| 48  | U     | 101 | PEE  | C21-C22-C23-C24 |
| 49  | j     | 201 | PLX  | C12-C13-C14-C15 |
| 49  | r     | 502 | PLX  | C16-C17-C18-C19 |
| 49  | r     | 503 | PLX  | C10-C11-C12-C13 |
| 48  | l     | 702 | PEE  | O3P-C1-C2-O2    |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | l     | 701 | CDL  | C58-C59-C60-C61 |
| 49  | j     | 201 | PLX  | C35-C36-C37-C38 |
| 48  | l     | 702 | PEE  | C30-C31-C32-C33 |
| 55  | i     | 402 | CDL  | C56-C57-C58-C59 |
| 48  | U     | 101 | PEE  | O2-C2-C3-O3     |
| 55  | l     | 701 | CDL  | OA6-CA4-CA6-OA8 |
| 55  | l     | 701 | CDL  | OB6-CB4-CB6-OB8 |
| 48  | Q     | 502 | PEE  | C31-C30-O3-C3   |
| 48  | r     | 501 | PEE  | C20-C21-C22-C23 |
| 49  | C     | 303 | PLX  | C9-C10-C11-C12  |
| 49  | i     | 401 | PLX  | C14-C15-C16-C17 |
| 49  | r     | 503 | PLX  | C11-C12-C13-C14 |
| 49  | C     | 303 | PLX  | C25-C26-C27-C28 |
| 49  | r     | 503 | PLX  | C27-C28-C29-C30 |
| 55  | i     | 402 | CDL  | C41-C42-C43-C44 |
| 48  | U     | 101 | PEE  | C36-C37-C38-C39 |
| 55  | l     | 701 | CDL  | OB7-CB5-OB6-CB4 |
| 55  | a     | 201 | CDL  | C52-C53-C54-C55 |
| 55  | l     | 701 | CDL  | C60-C61-C62-C63 |
| 49  | a     | 202 | PLX  | C25-C26-C27-C28 |
| 49  | r     | 503 | PLX  | C30-C31-C32-C33 |
| 49  | j     | 201 | PLX  | C13-C14-C15-C16 |
| 48  | Q     | 502 | PEE  | C20-C21-C22-C23 |
| 48  | Q     | 502 | PEE  | C19-C20-C21-C22 |
| 55  | i     | 402 | CDL  | C59-C60-C61-C62 |
| 49  | C     | 303 | PLX  | C7-C8-C9-C10    |
| 49  | C     | 303 | PLX  | C33-C34-C35-C36 |
| 49  | r     | 503 | PLX  | C31-C32-C33-C34 |
| 55  | i     | 402 | CDL  | C62-C63-C64-C65 |
| 48  | l     | 702 | PEE  | C14-C15-C16-C17 |
| 49  | a     | 202 | PLX  | C9-C10-C11-C12  |
| 48  | r     | 501 | PEE  | C36-C37-C38-C39 |
| 55  | a     | 201 | CDL  | C32-C33-C34-C35 |
| 55  | l     | 701 | CDL  | C32-C33-C34-C35 |
| 49  | j     | 201 | PLX  | C3-C4-C5-O8     |
| 49  | r     | 502 | PLX  | C3-C4-C5-O8     |
| 55  | i     | 402 | CDL  | CA3-CA4-CA6-OA8 |
| 55  | i     | 402 | CDL  | CB3-CB4-CB6-OB8 |
| 55  | l     | 701 | CDL  | C55-C56-C57-C58 |
| 49  | r     | 503 | PLX  | C18-C19-C20-C21 |
| 48  | C     | 302 | PEE  | C11-C12-C13-C14 |
| 48  | Q     | 502 | PEE  | C42-C43-C44-C45 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 702 | PEE  | C23-C24-C25-C26 |
| 49  | a     | 202 | PLX  | C11-C10-C9-C8   |
| 49  | r     | 503 | PLX  | C2-C1-N1-C1B    |
| 48  | C     | 302 | PEE  | C13-C14-C15-C16 |
| 49  | C     | 303 | PLX  | C27-C28-C29-C30 |
| 55  | a     | 201 | CDL  | C33-C34-C35-C36 |
| 48  | r     | 501 | PEE  | C40-C41-C42-C43 |
| 50  | G     | 201 | 8Q1  | C11-C12-C13-C14 |
| 48  | Q     | 502 | PEE  | O5-C30-O3-C3    |
| 50  | G     | 201 | 8Q1  | C28-O27-P24-O3  |
| 50  | X     | 201 | 8Q1  | C28-O27-P24-O3  |
| 48  | C     | 302 | PEE  | C15-C16-C17-C18 |
| 48  | Q     | 501 | PEE  | C19-C20-C21-C22 |
| 48  | Q     | 501 | PEE  | C15-C16-C17-C18 |
| 55  | l     | 701 | CDL  | C56-C57-C58-C59 |
| 48  | Q     | 502 | PEE  | C17-C18-C19-C20 |
| 48  | l     | 703 | PEE  | C17-C18-C19-C20 |
| 49  | r     | 502 | PLX  | C33-C34-C35-C36 |
| 55  | i     | 402 | CDL  | C14-C15-C16-C17 |
| 55  | a     | 201 | CDL  | OA5-CA3-CA4-OA6 |
| 55  | i     | 402 | CDL  | C60-C61-C62-C63 |
| 55  | l     | 701 | CDL  | C64-C65-C66-C67 |
| 49  | a     | 202 | PLX  | C30-C31-C32-C33 |
| 49  | r     | 502 | PLX  | C18-C19-C20-C21 |
| 49  | a     | 202 | PLX  | C11-C12-C13-C14 |
| 49  | j     | 201 | PLX  | C33-C34-C35-C36 |
| 48  | C     | 302 | PEE  | O2-C2-C3-O3     |
| 55  | i     | 402 | CDL  | OB6-CB4-CB6-OB8 |
| 55  | i     | 402 | CDL  | C52-C53-C54-C55 |
| 49  | r     | 502 | PLX  | C12-C13-C14-C15 |
| 55  | i     | 402 | CDL  | C84-C85-C86-C87 |
| 50  | G     | 201 | 8Q1  | C12-C13-C14-C15 |
| 55  | i     | 402 | CDL  | C31-CA7-OA8-CA6 |
| 50  | G     | 201 | 8Q1  | C6-C7-C8-C9     |
| 49  | i     | 401 | PLX  | C13-C14-C15-C16 |
| 55  | i     | 402 | CDL  | C13-C14-C15-C16 |
| 55  | a     | 201 | CDL  | C71-C72-C73-C74 |
| 55  | i     | 402 | CDL  | C23-C24-C25-C26 |
| 48  | l     | 702 | PEE  | O3P-C1-C2-C3    |
| 55  | l     | 701 | CDL  | OA5-CA3-CA4-CA6 |
| 48  | Q     | 501 | PEE  | C31-C32-C33-C34 |
| 48  | Q     | 502 | PEE  | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | i     | 402 | CDL  | C35-C36-C37-C38 |
| 49  | r     | 502 | PLX  | C14-C15-C16-C17 |
| 49  | j     | 201 | PLX  | C14-C15-C16-C17 |
| 55  | l     | 701 | CDL  | C77-C78-C79-C80 |
| 48  | C     | 302 | PEE  | C1-C2-C3-O3     |
| 48  | Q     | 501 | PEE  | C1-C2-C3-O3     |
| 48  | U     | 101 | PEE  | C1-C2-C3-O3     |
| 49  | i     | 401 | PLX  | C3-C4-C5-O8     |
| 55  | l     | 701 | CDL  | CA3-CA4-CA6-OA8 |
| 49  | j     | 201 | PLX  | C9-C10-C11-C12  |
| 49  | j     | 201 | PLX  | C31-C32-C33-C34 |
| 49  | r     | 502 | PLX  | C31-C32-C33-C34 |
| 55  | i     | 402 | CDL  | C82-C83-C84-C85 |
| 48  | m     | 201 | PEE  | C24-C25-C26-C27 |
| 49  | r     | 502 | PLX  | C13-C14-C15-C16 |
| 48  | C     | 302 | PEE  | C39-C40-C41-C42 |
| 55  | i     | 402 | CDL  | C64-C65-C66-C67 |
| 48  | l     | 702 | PEE  | C11-C12-C13-C14 |
| 48  | l     | 702 | PEE  | C32-C33-C34-C35 |
| 49  | r     | 502 | PLX  | C15-C16-C17-C18 |
| 50  | X     | 201 | 8Q1  | C10-C11-C12-C13 |
| 49  | C     | 303 | PLX  | C11-C12-C13-C14 |
| 48  | r     | 501 | PEE  | C38-C39-C40-C41 |
| 48  | Q     | 501 | PEE  | C32-C33-C34-C35 |
| 49  | C     | 303 | PLX  | C30-C31-C32-C33 |
| 55  | i     | 402 | CDL  | C42-C43-C44-C45 |
| 50  | G     | 201 | 8Q1  | C1-C6-C7-C8     |
| 49  | r     | 503 | PLX  | C7-C8-C9-C10    |
| 49  | r     | 502 | PLX  | C32-C33-C34-C35 |
| 49  | i     | 401 | PLX  | C19-C20-C21-C22 |
| 49  | j     | 201 | PLX  | C30-C31-C32-C33 |
| 49  | r     | 503 | PLX  | C15-C16-C17-C18 |
| 48  | Q     | 502 | PEE  | O3P-C1-C2-C3    |
| 49  | j     | 201 | PLX  | O4-C3-C4-C5     |
| 55  | a     | 201 | CDL  | OA5-CA3-CA4-CA6 |
| 55  | i     | 402 | CDL  | CB4-CB3-OB5-PB2 |
| 55  | i     | 402 | CDL  | OA9-CA7-OA8-CA6 |
| 49  | j     | 201 | PLX  | C18-C19-C20-C21 |
| 48  | m     | 201 | PEE  | C3-C2-O2-C10    |
| 48  | m     | 201 | PEE  | O3-C30-C31-C32  |
| 48  | Q     | 502 | PEE  | O3P-C1-C2-O2    |
| 49  | j     | 201 | PLX  | O4-C3-C4-O6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | l     | 701 | CDL  | OA5-CA3-CA4-OA6 |
| 49  | i     | 401 | PLX  | C12-C13-C14-C15 |
| 49  | r     | 502 | PLX  | C29-C30-C31-C32 |
| 48  | r     | 501 | PEE  | C1-C2-C3-O3     |
| 49  | r     | 503 | PLX  | C3-C4-C5-O8     |
| 50  | G     | 201 | 8Q1  | C31-C29-C32-C34 |
| 48  | Q     | 501 | PEE  | O2-C2-C3-O3     |
| 49  | j     | 201 | PLX  | O6-C4-C5-O8     |
| 49  | r     | 503 | PLX  | O6-C4-C5-O8     |
| 49  | C     | 303 | PLX  | C31-C32-C33-C34 |
| 55  | l     | 701 | CDL  | C62-C63-C64-C65 |
| 49  | r     | 503 | PLX  | C26-C27-C28-C29 |
| 55  | i     | 402 | CDL  | C20-C21-C22-C23 |
| 50  | X     | 201 | 8Q1  | C7-C8-C9-C10    |
| 46  | A     | 502 | FMN  | C3'-C4'-C5'-O5' |
| 49  | i     | 401 | PLX  | C17-C18-C19-C20 |
| 48  | U     | 101 | PEE  | C23-C24-C25-C26 |
| 55  | a     | 201 | CDL  | C54-C55-C56-C57 |
| 49  | i     | 401 | PLX  | C35-C36-C37-C38 |
| 49  | C     | 303 | PLX  | O9-C24-C25-C26  |
| 48  | r     | 501 | PEE  | C41-C42-C43-C44 |
| 49  | j     | 201 | PLX  | C25-C24-O8-C5   |
| 48  | Q     | 501 | PEE  | C23-C24-C25-C26 |
| 48  | Q     | 501 | PEE  | C30-C31-C32-C33 |
| 49  | C     | 303 | PLX  | C11-C10-C9-C8   |
| 48  | U     | 101 | PEE  | C41-C42-C43-C44 |
| 49  | i     | 401 | PLX  | O4-C3-C4-C5     |
| 48  | U     | 101 | PEE  | C37-C38-C39-C40 |
| 55  | i     | 402 | CDL  | CA5-C11-C12-C13 |
| 48  | l     | 703 | PEE  | C21-C22-C23-C24 |
| 55  | a     | 201 | CDL  | C55-C56-C57-C58 |
| 49  | C     | 303 | PLX  | O8-C24-C25-C26  |
| 49  | a     | 202 | PLX  | O6-C6-C7-C8     |
| 49  | r     | 503 | PLX  | O8-C24-C25-C26  |
| 49  | i     | 401 | PLX  | O4-C3-C4-O6     |
| 48  | l     | 702 | PEE  | C24-C25-C26-C27 |
| 55  | i     | 402 | CDL  | C81-C82-C83-C84 |
| 50  | G     | 201 | 8Q1  | C11-C10-C9-C8   |
| 51  | J     | 401 | NDP  | C2N-C3N-C7N-O7N |
| 48  | U     | 101 | PEE  | C38-C39-C40-C41 |
| 55  | i     | 402 | CDL  | C31-C32-C33-C34 |
| 48  | l     | 702 | PEE  | O2-C2-C3-O3     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | r     | 501 | PEE  | O2-C2-C3-O3     |
| 49  | i     | 401 | PLX  | O6-C4-C5-O8     |
| 55  | a     | 201 | CDL  | OB6-CB4-CB6-OB8 |
| 55  | a     | 201 | CDL  | CB3-CB4-CB6-OB8 |
| 48  | r     | 501 | PEE  | C31-C30-O3-C3   |
| 48  | r     | 501 | PEE  | C24-C25-C26-C27 |
| 55  | l     | 701 | CDL  | C14-C15-C16-C17 |
| 47  | A     | 503 | NAI  | C5B-O5B-PA-O3   |
| 48  | l     | 703 | PEE  | C1-O3P-P-O1P    |
| 48  | m     | 201 | PEE  | C1-O3P-P-O1P    |
| 48  | r     | 501 | PEE  | C4-O4P-P-O3P    |
| 48  | r     | 501 | PEE  | C4-O4P-P-O1P    |
| 49  | C     | 303 | PLX  | C3-C4-O6-C6     |
| 49  | i     | 401 | PLX  | C3-O4-P1-O2     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O1     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O2     |
| 49  | r     | 502 | PLX  | C3-O4-P1-O3     |
| 49  | r     | 502 | PLX  | C2-O1-P1-O4     |
| 49  | r     | 502 | PLX  | C2-O1-P1-O3     |
| 49  | r     | 503 | PLX  | C3-O4-P1-O2     |
| 49  | r     | 503 | PLX  | C2-O1-P1-O4     |
| 49  | r     | 503 | PLX  | C2-O1-P1-O2     |
| 49  | r     | 503 | PLX  | C2-O1-P1-O3     |
| 51  | J     | 401 | NDP  | C5B-O5B-PA-O2A  |
| 55  | a     | 201 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | a     | 201 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | a     | 201 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | i     | 402 | CDL  | CB2-OB2-PB2-OB3 |
| 55  | i     | 402 | CDL  | CB2-OB2-PB2-OB4 |
| 55  | i     | 402 | CDL  | CB2-OB2-PB2-OB5 |
| 55  | i     | 402 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | l     | 701 | CDL  | CB3-OB5-PB2-OB2 |
| 55  | l     | 701 | CDL  | CB3-OB5-PB2-OB3 |
| 55  | l     | 701 | CDL  | CB3-OB5-PB2-OB4 |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O1A  |
| 57  | w     | 401 | ADP  | C5'-O5'-PA-O3A  |
| 55  | l     | 701 | CDL  | C76-C77-C78-C79 |
| 49  | j     | 201 | PLX  | C26-C27-C28-C29 |
| 48  | U     | 101 | PEE  | C19-C20-C21-C22 |
| 48  | l     | 702 | PEE  | C19-C20-C21-C22 |
| 49  | C     | 303 | PLX  | C15-C16-C17-C18 |
| 49  | a     | 202 | PLX  | C27-C28-C29-C30 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 703 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | C16-C17-C18-C19 |
| 48  | r     | 501 | PEE  | O5-C30-O3-C3    |
| 48  | l     | 702 | PEE  | C34-C35-C36-C37 |
| 49  | r     | 502 | PLX  | C20-C21-C22-C23 |
| 48  | l     | 703 | PEE  | C14-C15-C16-C17 |
| 48  | Q     | 501 | PEE  | C13-C14-C15-C16 |
| 55  | l     | 701 | CDL  | C44-C45-C46-C47 |
| 48  | l     | 702 | PEE  | C13-C14-C15-C16 |
| 49  | r     | 502 | PLX  | O6-C4-C5-O8     |
| 55  | l     | 701 | CDL  | O1-C1-CB2-OB2   |
| 55  | l     | 701 | CDL  | C72-C73-C74-C75 |
| 49  | r     | 503 | PLX  | C9-C10-C11-C12  |
| 48  | Q     | 501 | PEE  | C14-C15-C16-C17 |
| 48  | Q     | 502 | PEE  | C39-C40-C41-C42 |
| 55  | l     | 701 | CDL  | C33-C34-C35-C36 |
| 50  | G     | 201 | 8Q1  | C30-C29-C32-O33 |
| 50  | G     | 201 | 8Q1  | C31-C29-C32-O33 |
| 48  | l     | 702 | PEE  | C1-C2-C3-O3     |
| 48  | C     | 302 | PEE  | C41-C42-C43-C44 |
| 48  | l     | 703 | PEE  | C32-C33-C34-C35 |
| 48  | l     | 703 | PEE  | C15-C16-C17-C18 |
| 48  | l     | 703 | PEE  | C11-C12-C13-C14 |
| 55  | l     | 701 | CDL  | C15-C16-C17-C18 |
| 49  | i     | 401 | PLX  | O8-C24-C25-C26  |
| 49  | r     | 502 | PLX  | O8-C24-C25-C26  |
| 51  | J     | 401 | NDP  | C2B-O2B-P2B-O3X |
| 49  | a     | 202 | PLX  | C16-C17-C18-C19 |
| 48  | r     | 501 | PEE  | C39-C40-C41-C42 |
| 49  | C     | 303 | PLX  | O4-C3-C4-O6     |
| 55  | l     | 701 | CDL  | C12-C13-C14-C15 |
| 48  | Q     | 501 | PEE  | C38-C39-C40-C41 |
| 48  | m     | 201 | PEE  | C16-C17-C18-C19 |
| 49  | j     | 201 | PLX  | C11-C12-C13-C14 |
| 55  | i     | 402 | CDL  | C39-C40-C41-C42 |
| 48  | Q     | 502 | PEE  | C10-C11-C12-C13 |
| 49  | a     | 202 | PLX  | C19-C20-C21-C22 |
| 48  | l     | 703 | PEE  | C1-C2-C3-O3     |
| 48  | r     | 501 | PEE  | C34-C35-C36-C37 |
| 55  | a     | 201 | CDL  | C60-C61-C62-C63 |
| 48  | l     | 702 | PEE  | C1-C2-O2-C10    |
| 48  | l     | 702 | PEE  | C3-C2-O2-C10    |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 48  | l     | 703 | PEE  | O4-C10-O2-C2    |
| 48  | Q     | 501 | PEE  | C2-C1-O3P-P     |
| 55  | i     | 402 | CDL  | C72-C73-C74-C75 |
| 48  | Q     | 501 | PEE  | C18-C19-C20-C21 |
| 48  | l     | 703 | PEE  | O2-C2-C3-O3     |
| 47  | A     | 503 | NAI  | O4D-C1D-N1N-C2N |
| 48  | l     | 702 | PEE  | C38-C39-C40-C41 |
| 55  | i     | 402 | CDL  | C44-C45-C46-C47 |
| 46  | A     | 502 | FMN  | O2'-C2'-C3'-C4' |
| 57  | w     | 401 | ADP  | PB-O3A-PA-O1A   |
| 49  | r     | 503 | PLX  | C16-C17-C18-C19 |
| 56  | s     | 401 | UQ   | C12-C11-C9-C8   |
| 55  | a     | 201 | CDL  | C41-C42-C43-C44 |
| 55  | a     | 201 | CDL  | C59-C60-C61-C62 |
| 49  | i     | 401 | PLX  | O9-C24-C25-C26  |
| 55  | a     | 201 | CDL  | C36-C37-C38-C39 |
| 47  | A     | 503 | NAI  | C2D-C1D-N1N-C2N |
| 49  | i     | 401 | PLX  | C36-C37-C38-C39 |
| 55  | a     | 201 | CDL  | C76-C77-C78-C79 |
| 55  | l     | 701 | CDL  | C31-C32-C33-C34 |
| 55  | l     | 701 | CDL  | C71-C72-C73-C74 |
| 49  | a     | 202 | PLX  | C13-C14-C15-C16 |
| 48  | m     | 201 | PEE  | C13-C14-C15-C16 |
| 55  | a     | 201 | CDL  | C74-C75-C76-C77 |
| 48  | l     | 702 | PEE  | C35-C36-C37-C38 |
| 49  | j     | 201 | PLX  | C4-C5-O8-C24    |
| 48  | m     | 201 | PEE  | C18-C19-C20-C21 |
| 50  | X     | 201 | 8Q1  | C13-C14-C15-C16 |
| 55  | l     | 701 | CDL  | C52-C51-CB5-OB6 |
| 48  | Q     | 502 | PEE  | C15-C16-C17-C18 |
| 55  | i     | 402 | CDL  | C33-C34-C35-C36 |
| 48  | r     | 501 | PEE  | C18-C19-C20-C21 |
| 48  | U     | 101 | PEE  | C22-C23-C24-C25 |
| 48  | l     | 702 | PEE  | C20-C21-C22-C23 |
| 48  | C     | 302 | PEE  | C38-C39-C40-C41 |
| 48  | l     | 702 | PEE  | C16-C17-C18-C19 |
| 48  | l     | 703 | PEE  | C5-C4-O4P-P     |
| 55  | a     | 201 | CDL  | C22-C23-C24-C25 |
| 48  | l     | 703 | PEE  | C11-C10-O2-C2   |
| 48  | U     | 101 | PEE  | C16-C17-C18-C19 |
| 48  | U     | 101 | PEE  | O3-C30-C31-C32  |
| 49  | j     | 201 | PLX  | C7-C6-O6-C4     |

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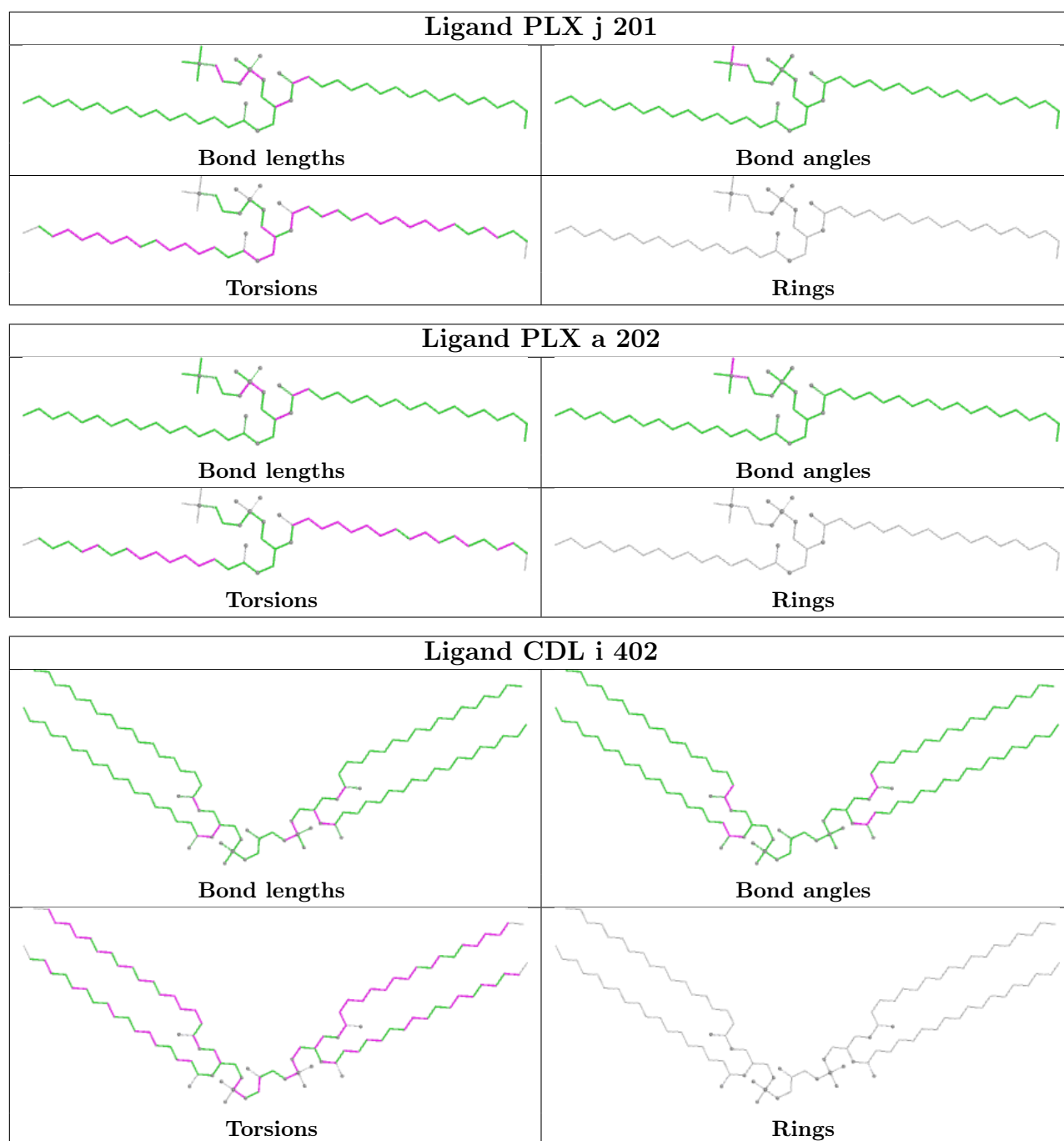
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 55  | i     | 402 | CDL  | C32-C33-C34-C35 |
| 48  | Q     | 501 | PEE  | C36-C37-C38-C39 |
| 48  | l     | 703 | PEE  | C38-C39-C40-C41 |
| 47  | A     | 503 | NAI  | C3D-C4D-C5D-O5D |
| 55  | a     | 201 | CDL  | C43-C44-C45-C46 |
| 49  | j     | 201 | PLX  | C32-C33-C34-C35 |
| 55  | i     | 402 | CDL  | C83-C84-C85-C86 |
| 48  | C     | 302 | PEE  | O3-C30-C31-C32  |
| 48  | C     | 302 | PEE  | C18-C19-C20-C21 |
| 49  | r     | 503 | PLX  | C36-C37-C38-C39 |
| 48  | l     | 702 | PEE  | C10-C11-C12-C13 |
| 48  | Q     | 501 | PEE  | C24-C25-C26-C27 |
| 48  | m     | 201 | PEE  | C10-C11-C12-C13 |
| 49  | a     | 202 | PLX  | C6-C7-C8-C9     |
| 49  | r     | 502 | PLX  | C25-C24-O8-C5   |
| 48  | U     | 101 | PEE  | O2-C10-C11-C12  |
| 55  | i     | 402 | CDL  | C37-C38-C39-C40 |
| 49  | C     | 303 | PLX  | C24-C25-C26-C27 |
| 48  | l     | 703 | PEE  | O3-C30-C31-C32  |
| 50  | G     | 201 | 8Q1  | C9-C10-C11-C12  |
| 49  | r     | 502 | PLX  | C26-C27-C28-C29 |
| 48  | U     | 101 | PEE  | C31-C32-C33-C34 |
| 55  | i     | 402 | CDL  | C76-C77-C78-C79 |
| 49  | r     | 502 | PLX  | C4-C3-O4-P1     |
| 55  | l     | 701 | CDL  | C34-C35-C36-C37 |
| 48  | C     | 302 | PEE  | O5-C30-C31-C32  |
| 48  | m     | 201 | PEE  | O5-C30-C31-C32  |
| 48  | U     | 101 | PEE  | O5-C30-C31-C32  |
| 49  | j     | 201 | PLX  | O9-C24-O8-C5    |
| 48  | C     | 302 | PEE  | C32-C33-C34-C35 |
| 48  | C     | 302 | PEE  | C43-C44-C45-C46 |
| 48  | l     | 703 | PEE  | O5-C30-C31-C32  |
| 48  | U     | 101 | PEE  | O4-C10-C11-C12  |
| 49  | r     | 502 | PLX  | C25-C26-C27-C28 |
| 50  | X     | 201 | 8Q1  | O33-C32-C34-N36 |
| 55  | l     | 701 | CDL  | C32-C31-CA7-OA8 |
| 55  | i     | 402 | CDL  | C72-C71-CB7-OB8 |

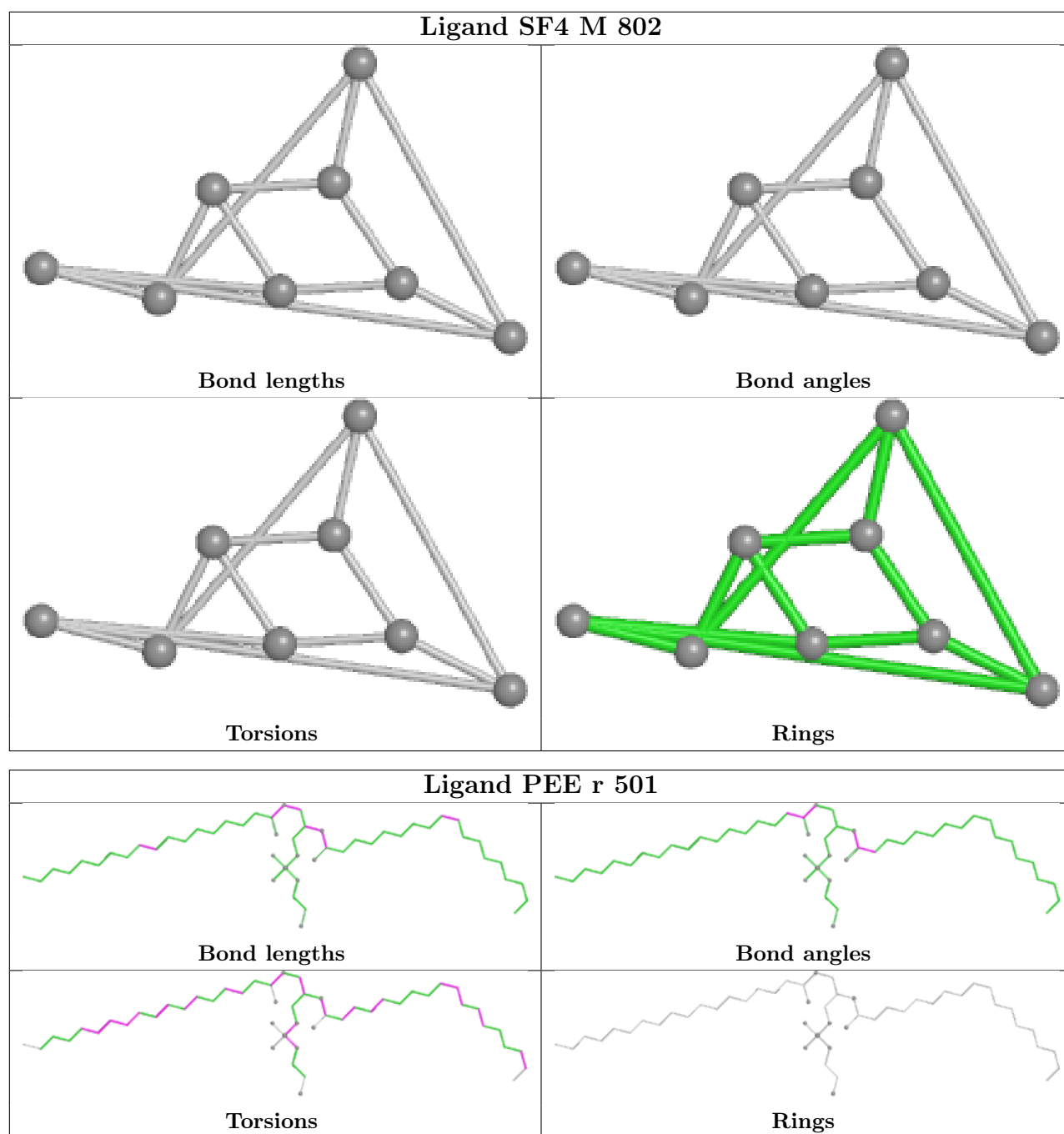
There are no ring outliers.

25 monomers are involved in 88 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 49  | j     | 201 | PLX  | 3       | 0            |
| 49  | a     | 202 | PLX  | 3       | 0            |
| 55  | i     | 402 | CDL  | 8       | 0            |
| 48  | r     | 501 | PEE  | 6       | 0            |
| 47  | A     | 503 | NAI  | 5       | 0            |
| 45  | C     | 301 | SF4  | 1       | 0            |
| 48  | U     | 101 | PEE  | 3       | 0            |
| 55  | a     | 201 | CDL  | 6       | 0            |
| 50  | X     | 201 | 8Q1  | 4       | 0            |
| 48  | l     | 702 | PEE  | 2       | 0            |
| 56  | s     | 401 | UQ   | 5       | 0            |
| 48  | Q     | 501 | PEE  | 3       | 0            |
| 55  | l     | 701 | CDL  | 4       | 0            |
| 48  | l     | 703 | PEE  | 3       | 0            |
| 49  | C     | 303 | PLX  | 2       | 0            |
| 50  | G     | 201 | 8Q1  | 8       | 0            |
| 45  | A     | 501 | SF4  | 1       | 0            |
| 48  | m     | 201 | PEE  | 3       | 0            |
| 49  | r     | 503 | PLX  | 3       | 0            |
| 51  | J     | 401 | NDP  | 1       | 0            |
| 48  | Q     | 502 | PEE  | 5       | 0            |
| 49  | r     | 502 | PLX  | 1       | 0            |
| 57  | w     | 401 | ADP  | 2       | 0            |
| 46  | A     | 502 | FMN  | 6       | 0            |
| 49  | i     | 401 | PLX  | 3       | 0            |

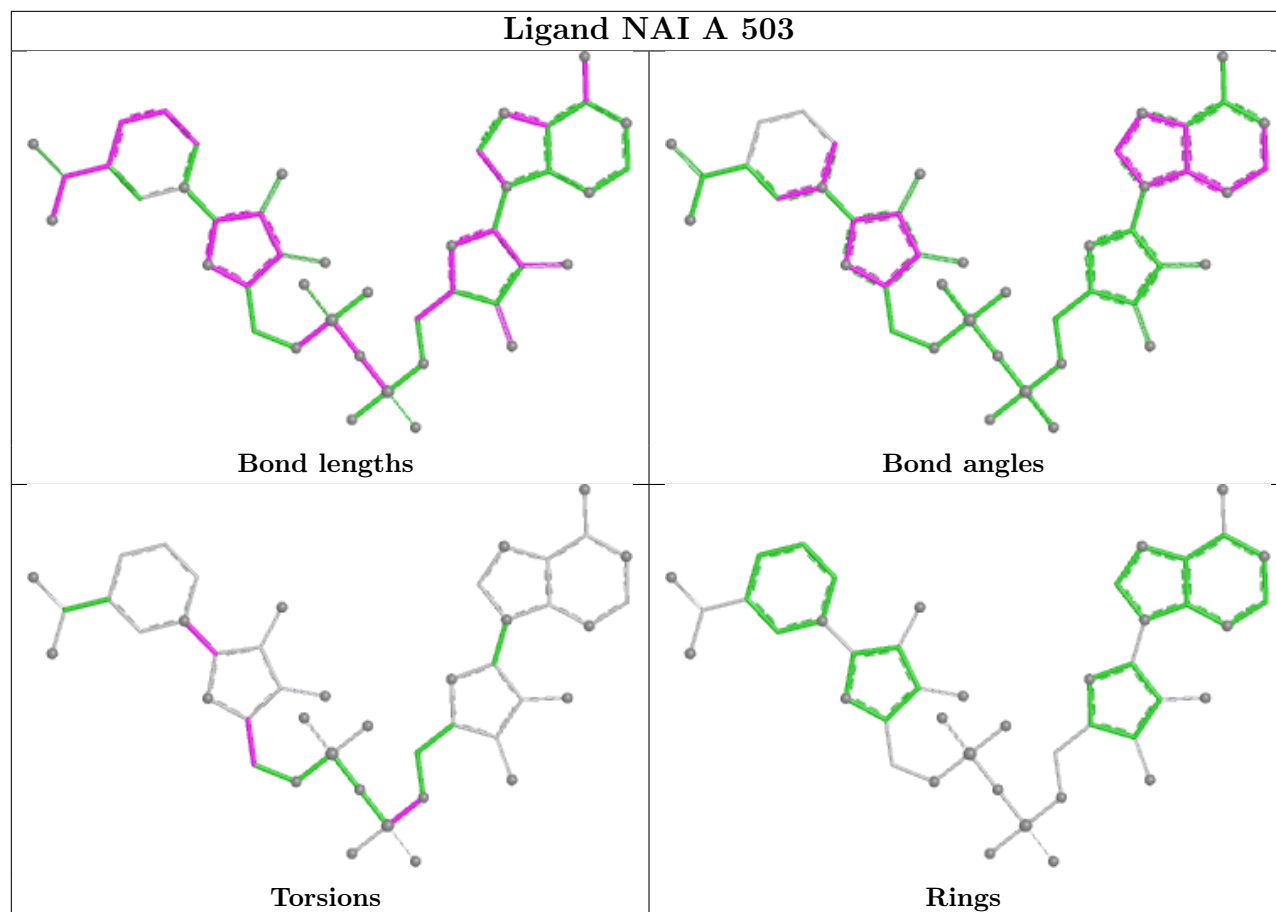
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



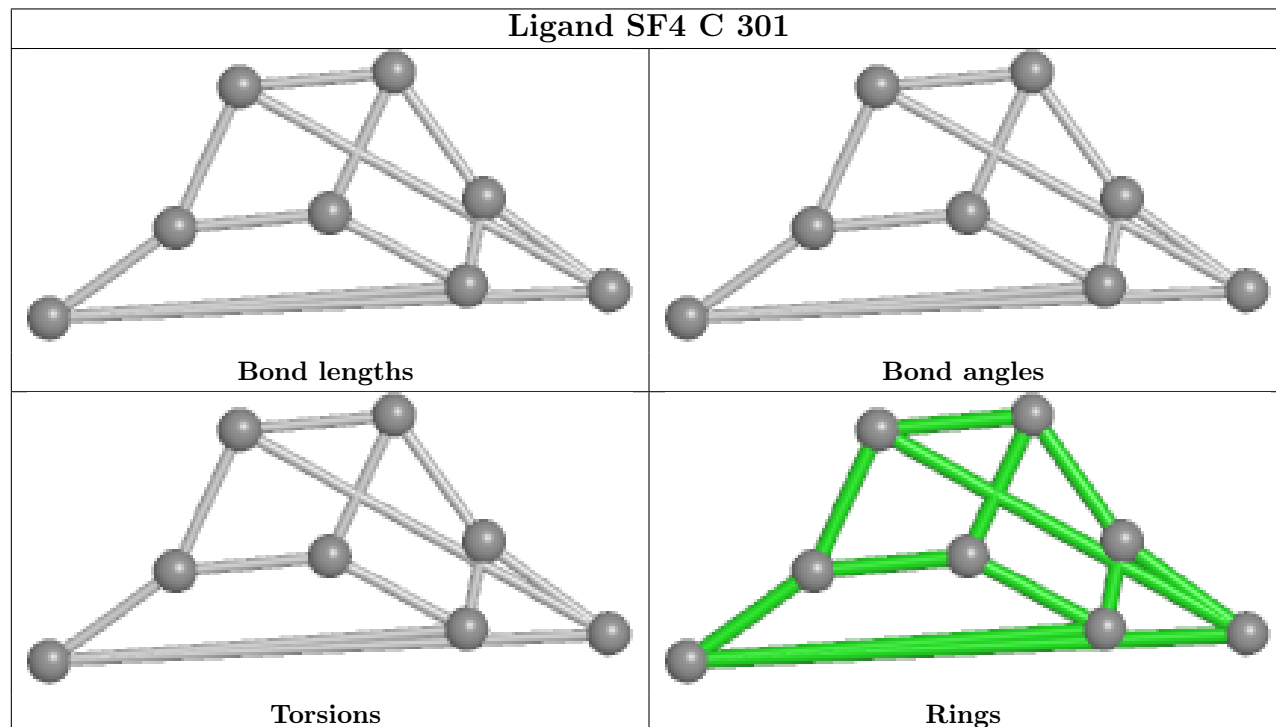


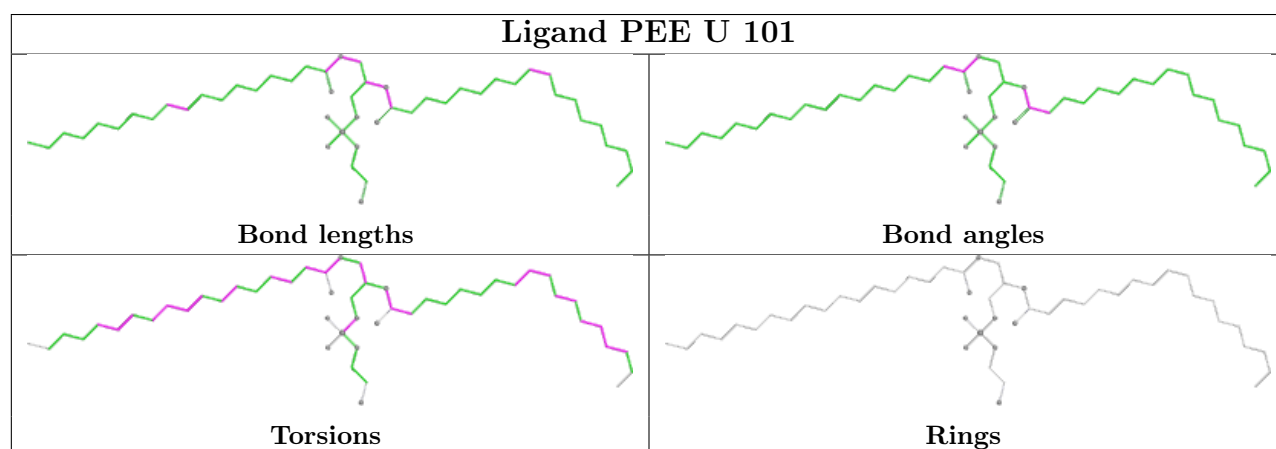
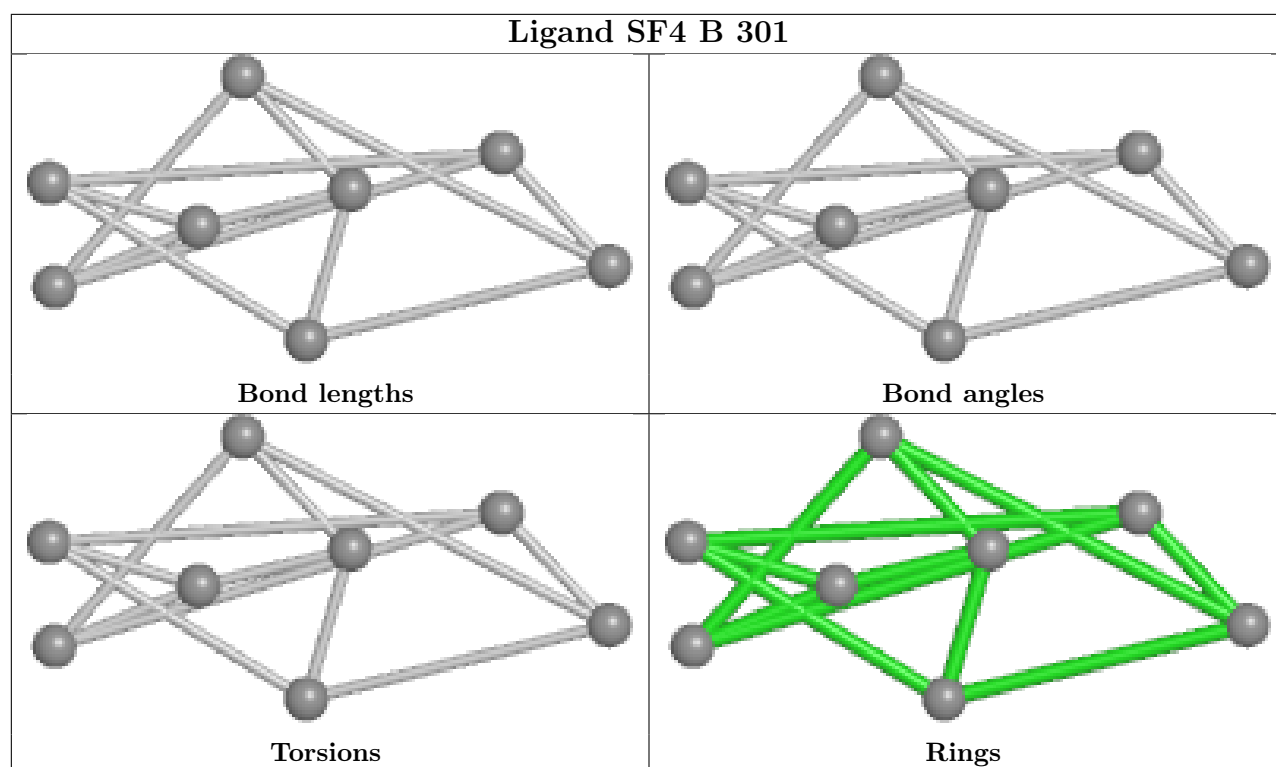


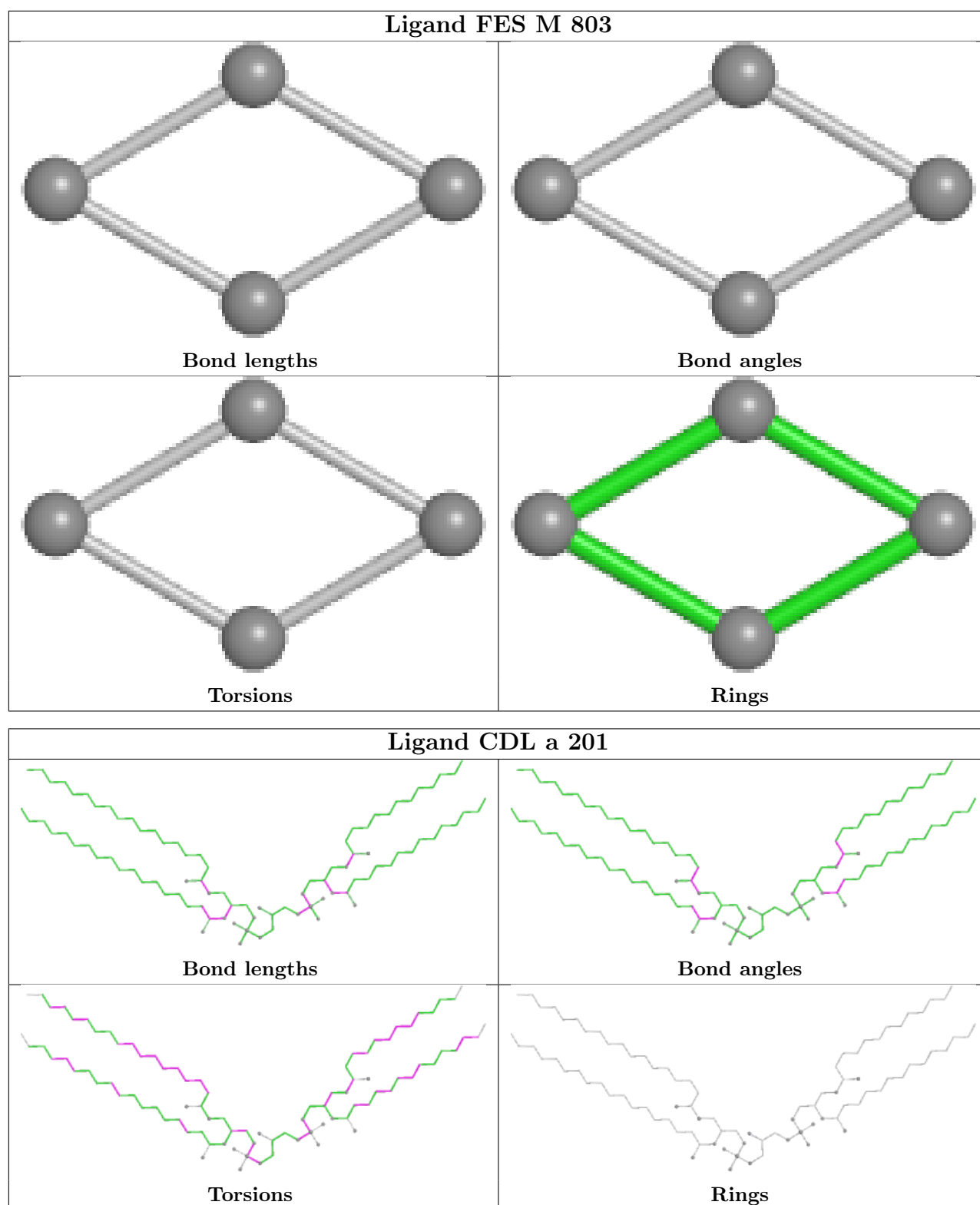
## Ligand NAI A 503

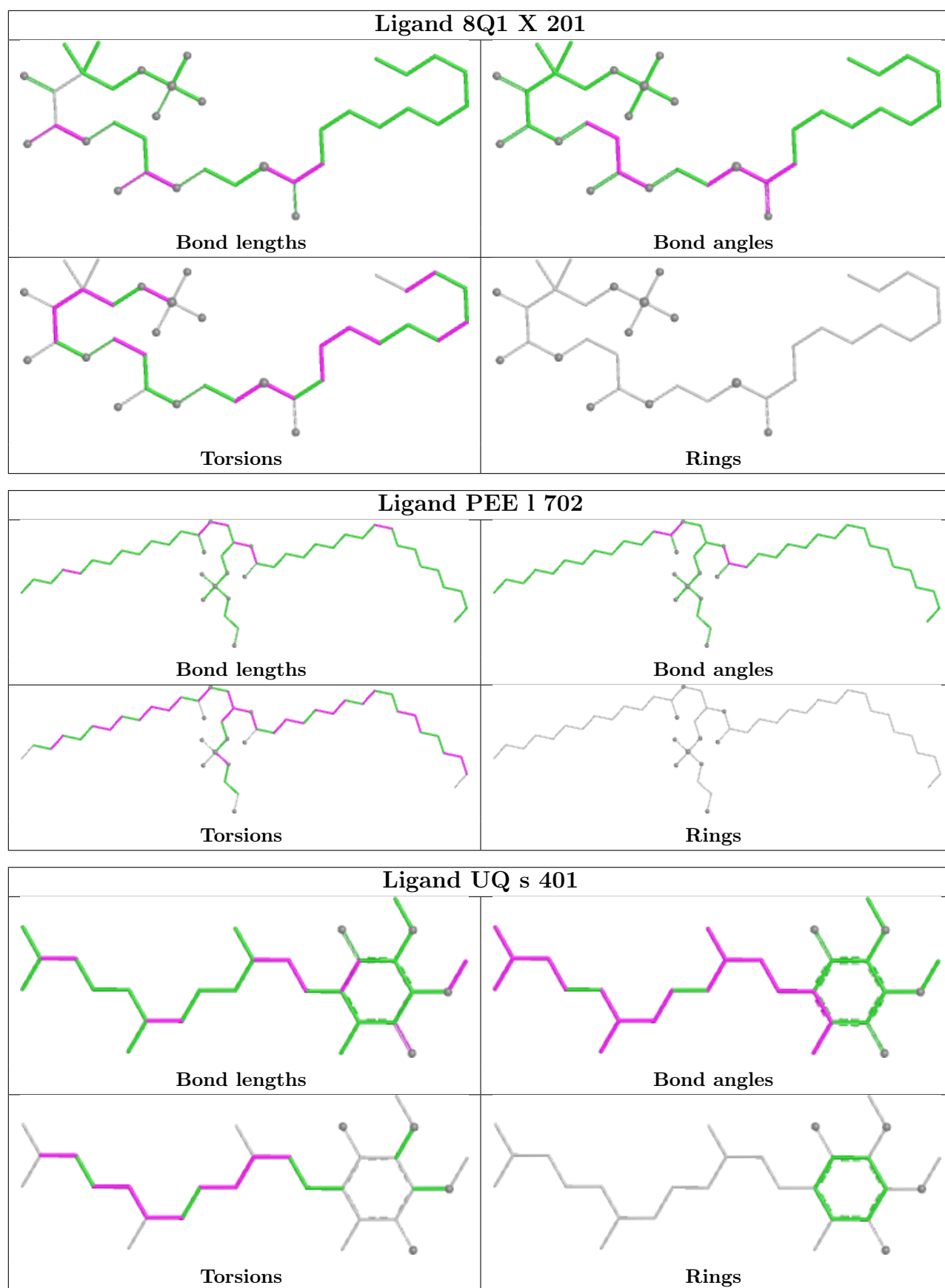


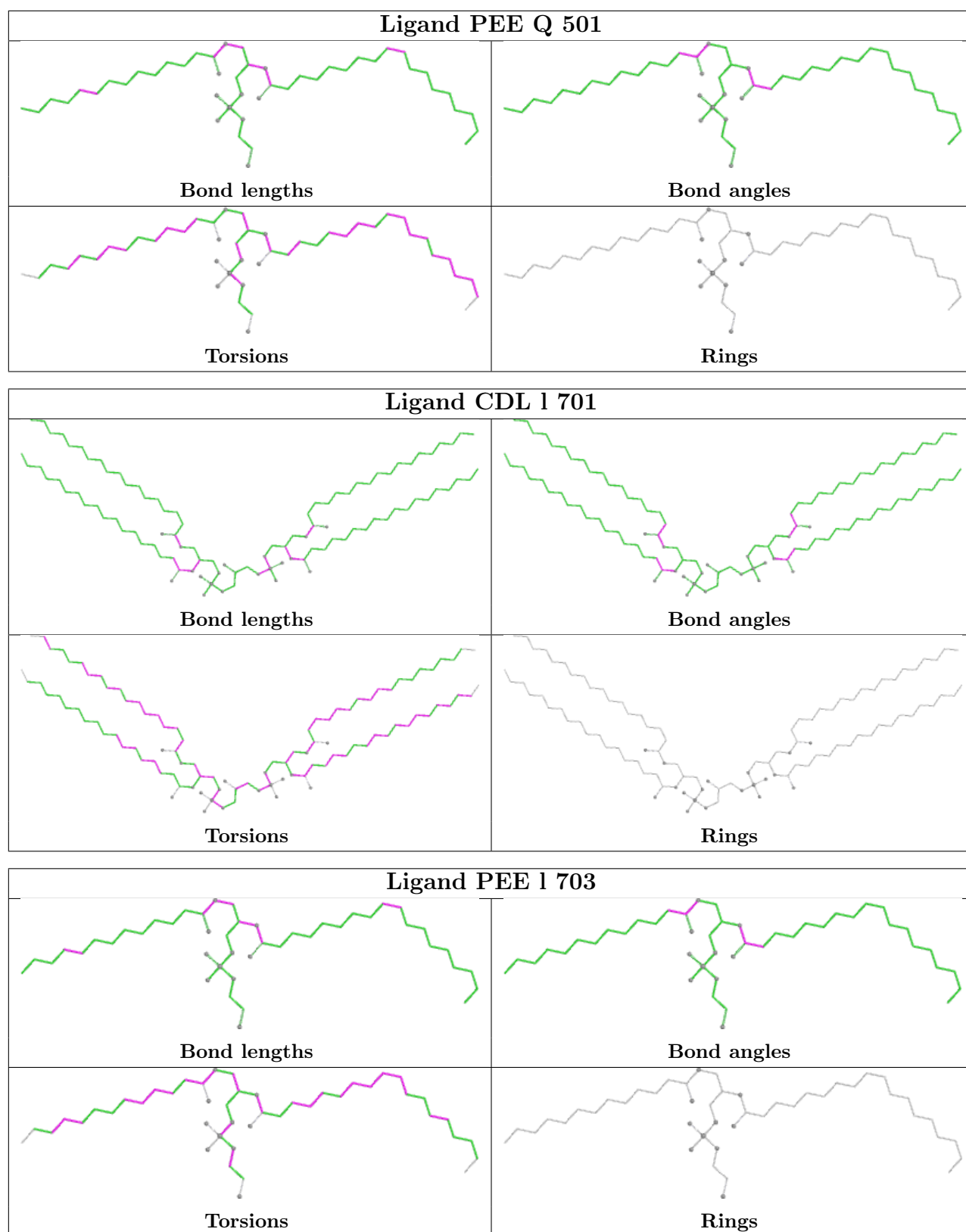
## Ligand SF4 C 301

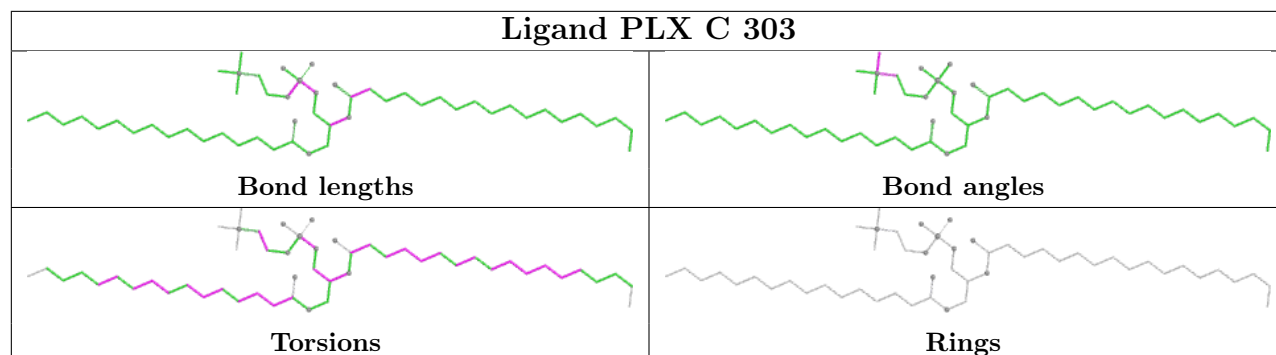
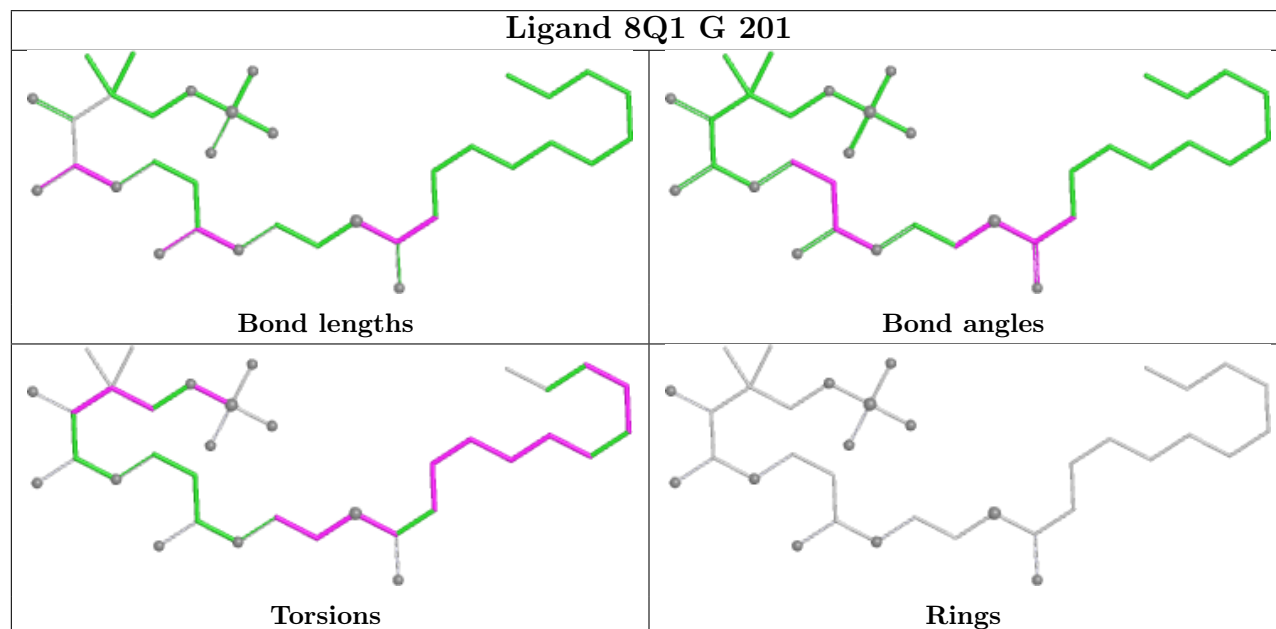
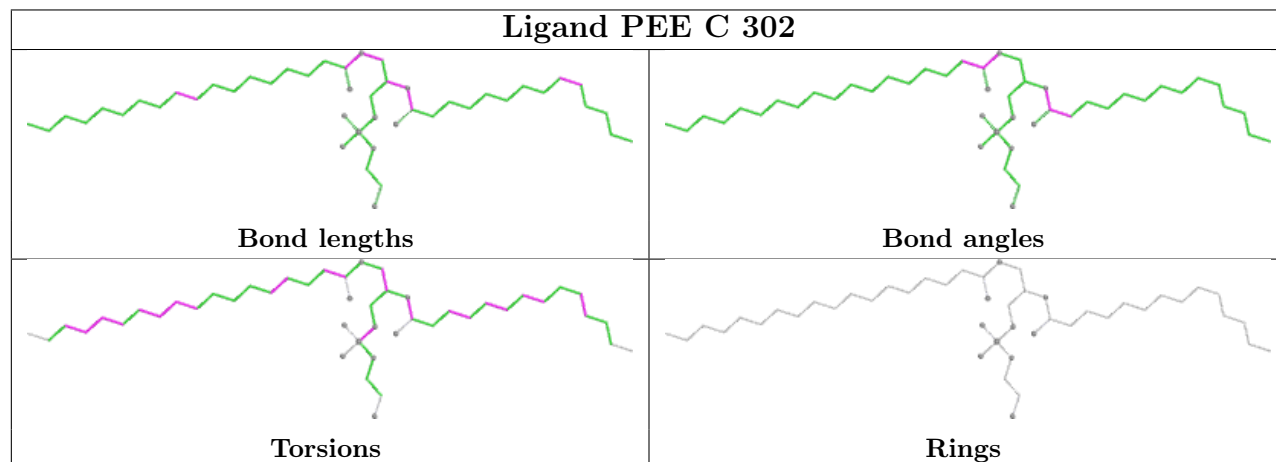


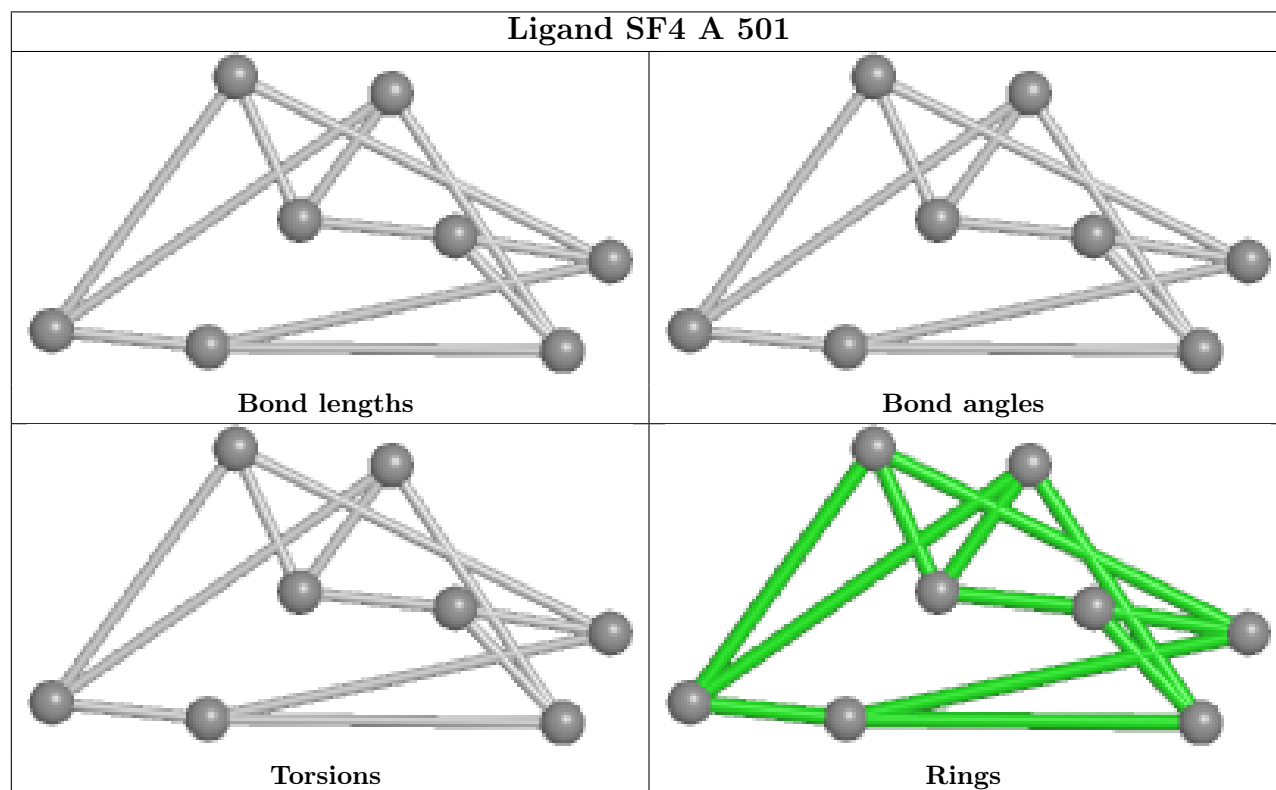
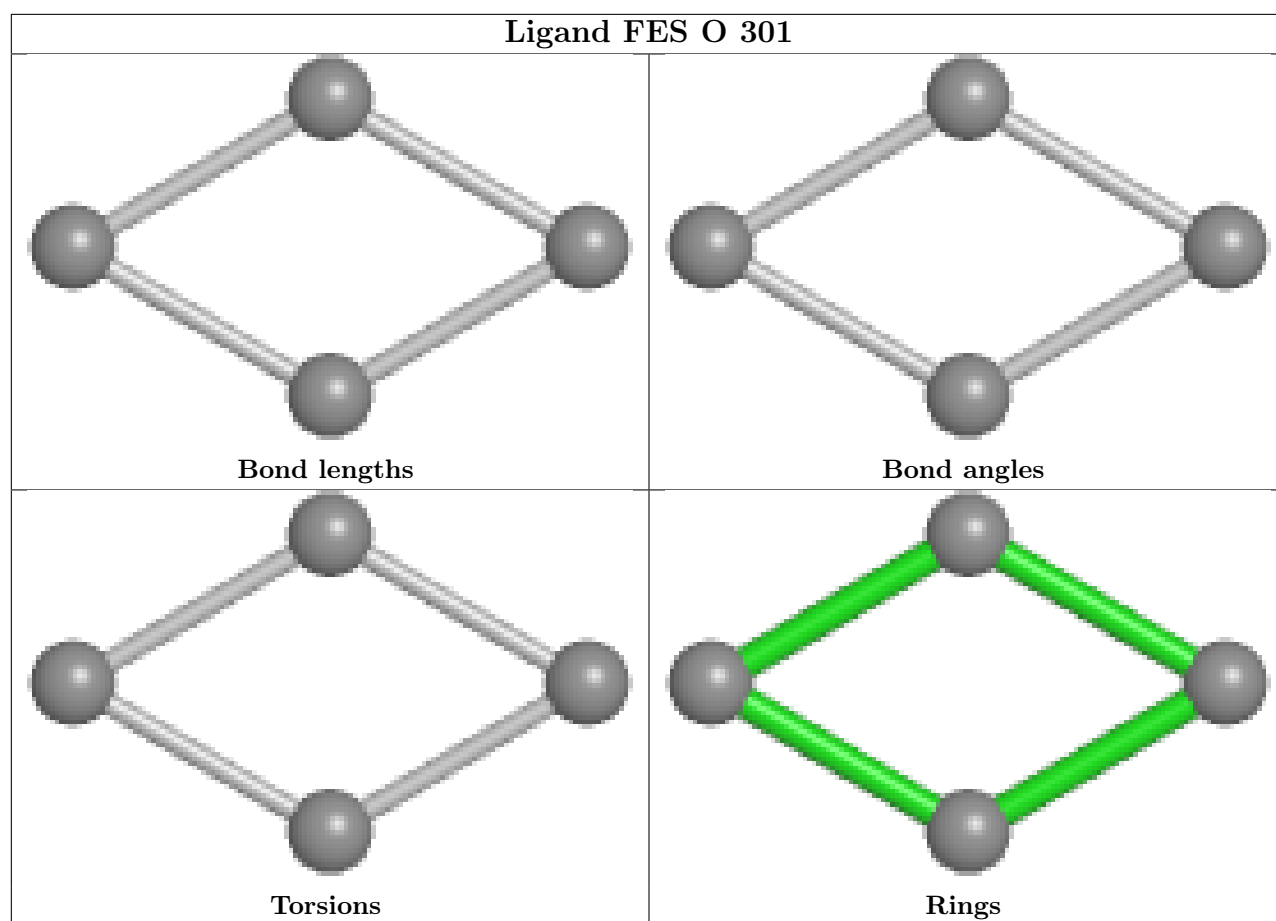


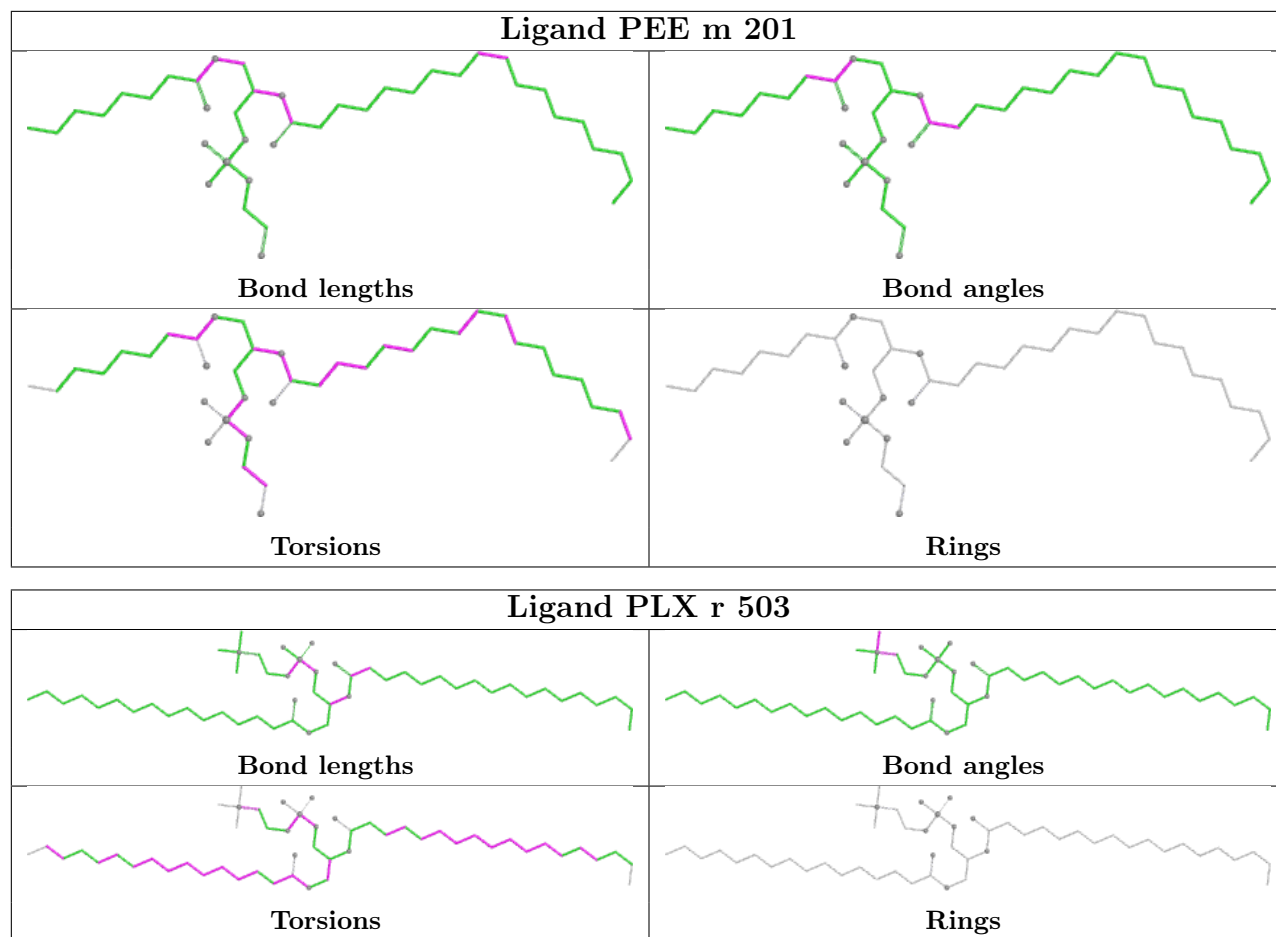






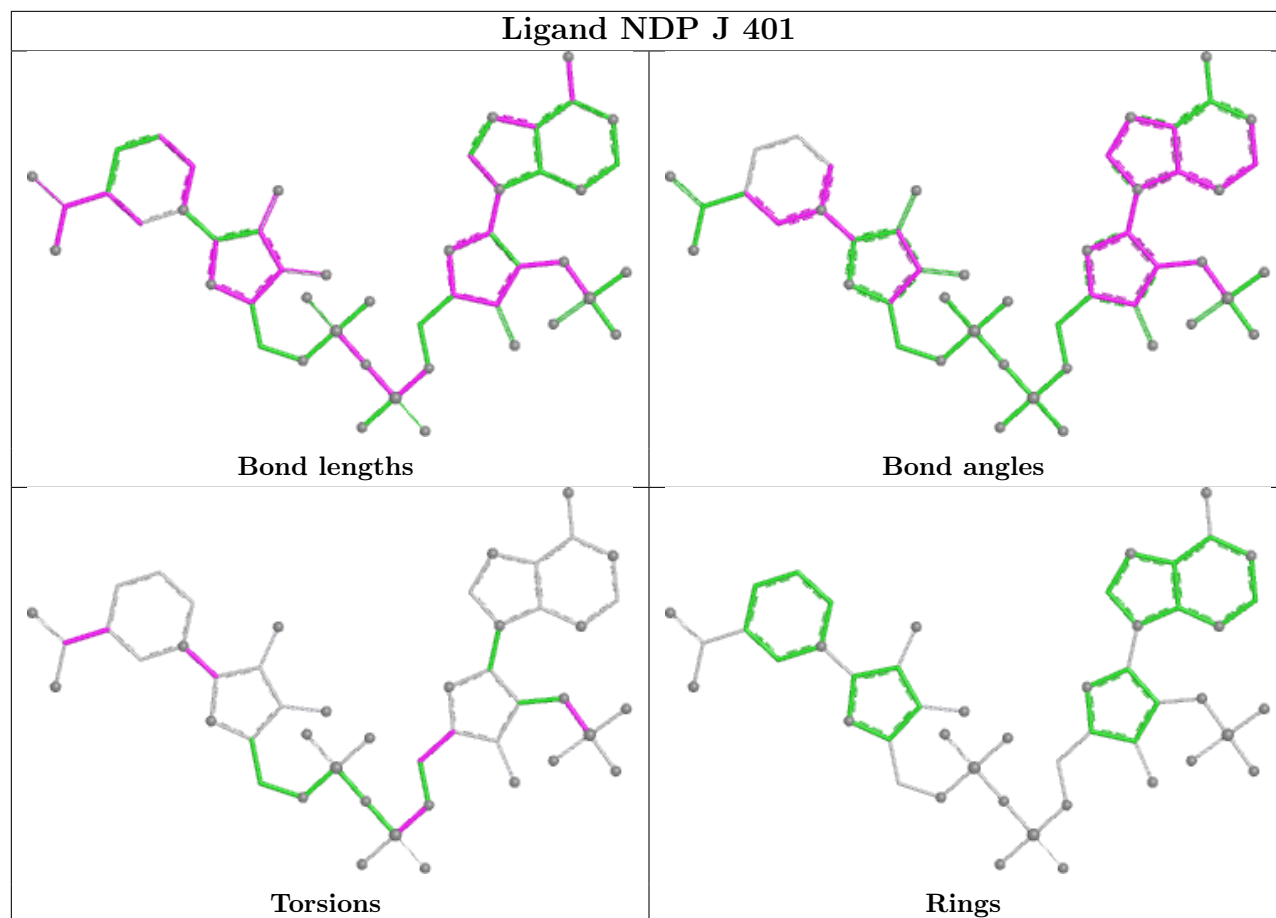
**Ligand PLX C 303****Ligand 8Q1 G 201****Ligand PEE C 302**



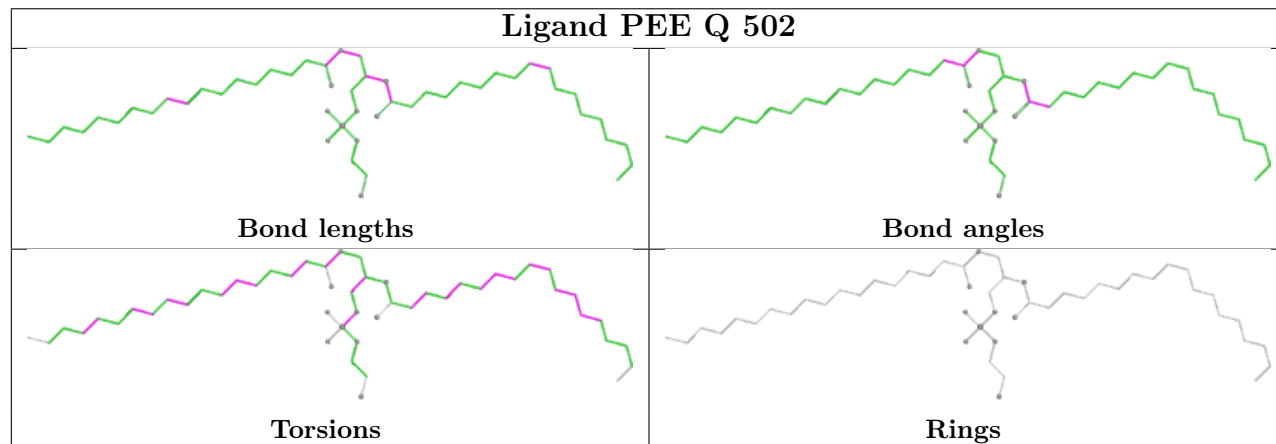


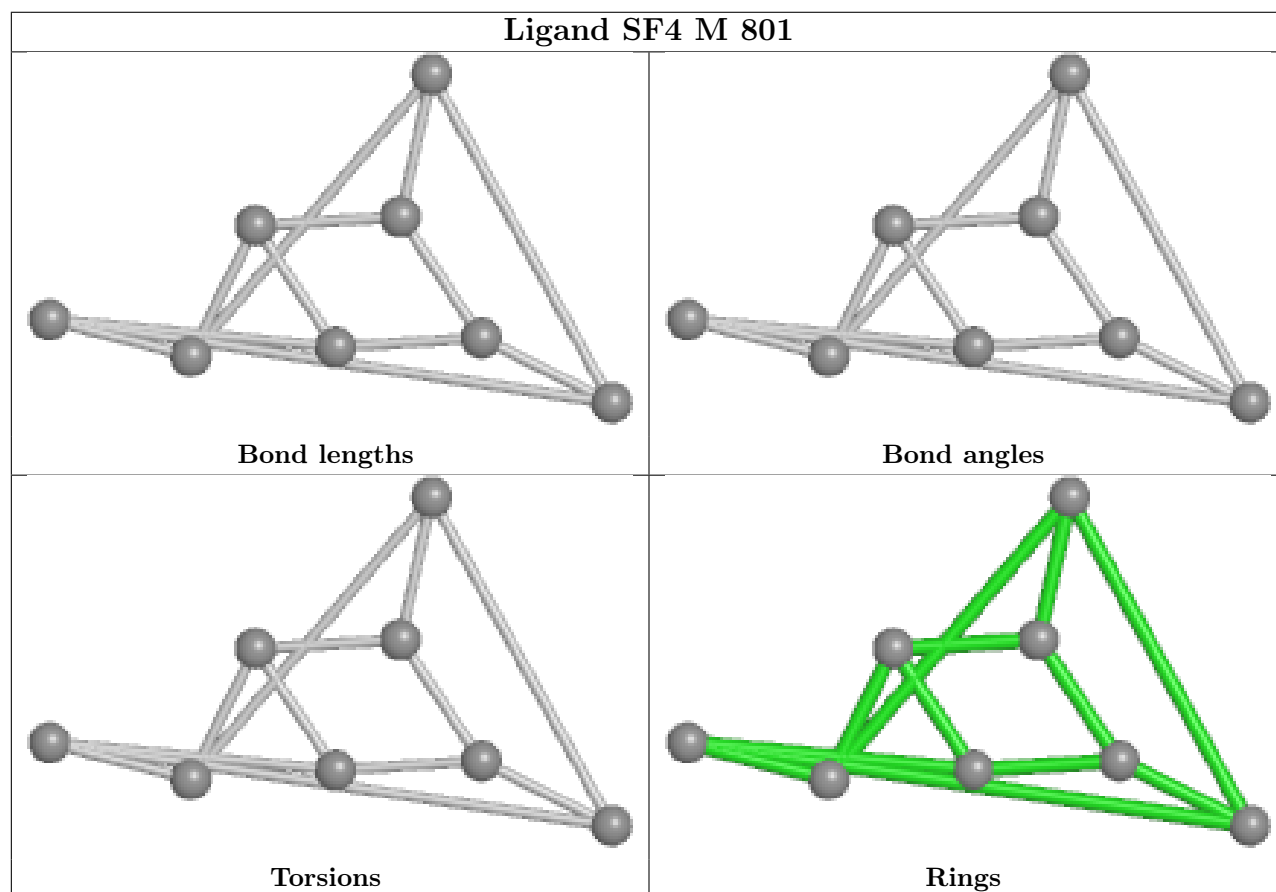
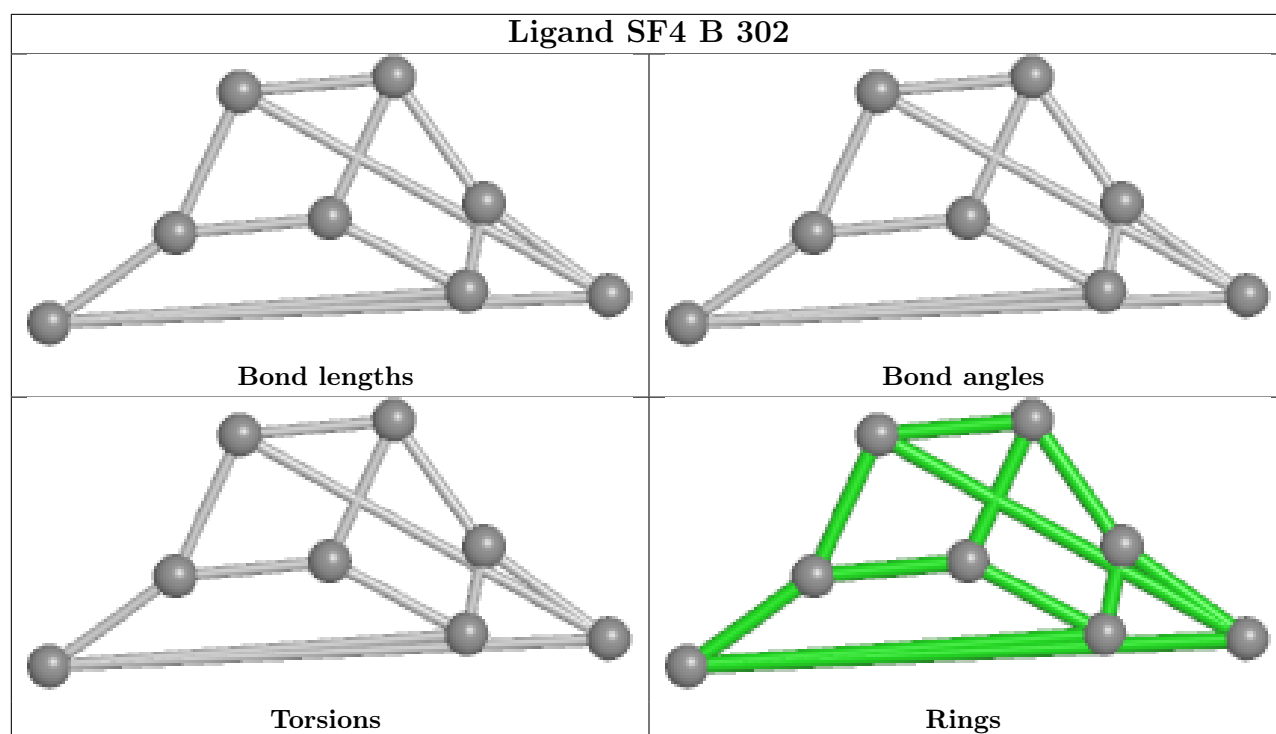


## Ligand NDP J 401

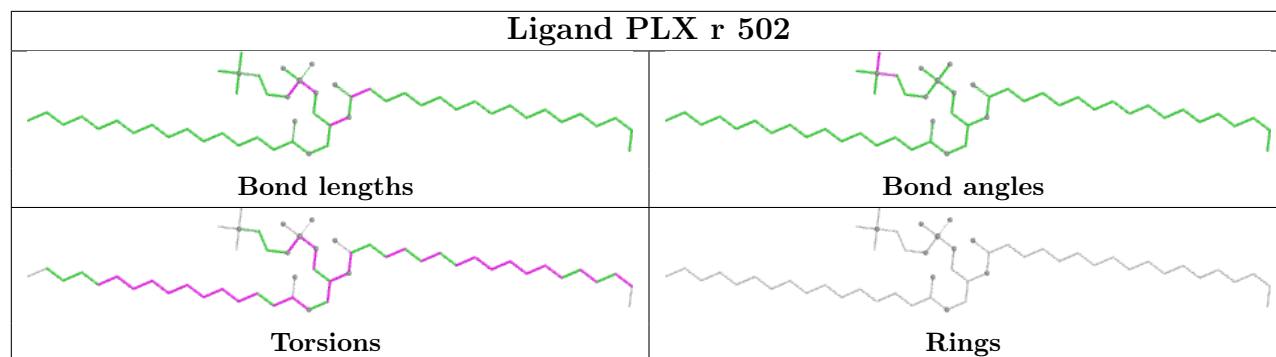


## Ligand PEE Q 502

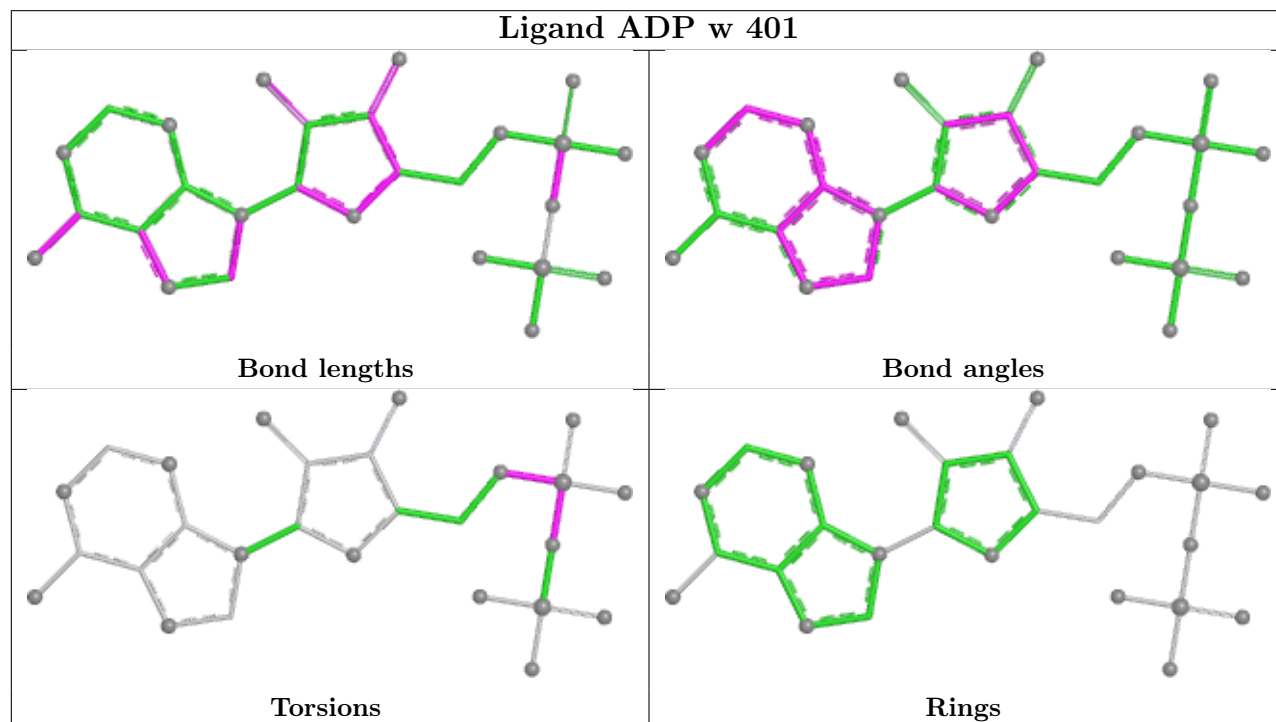


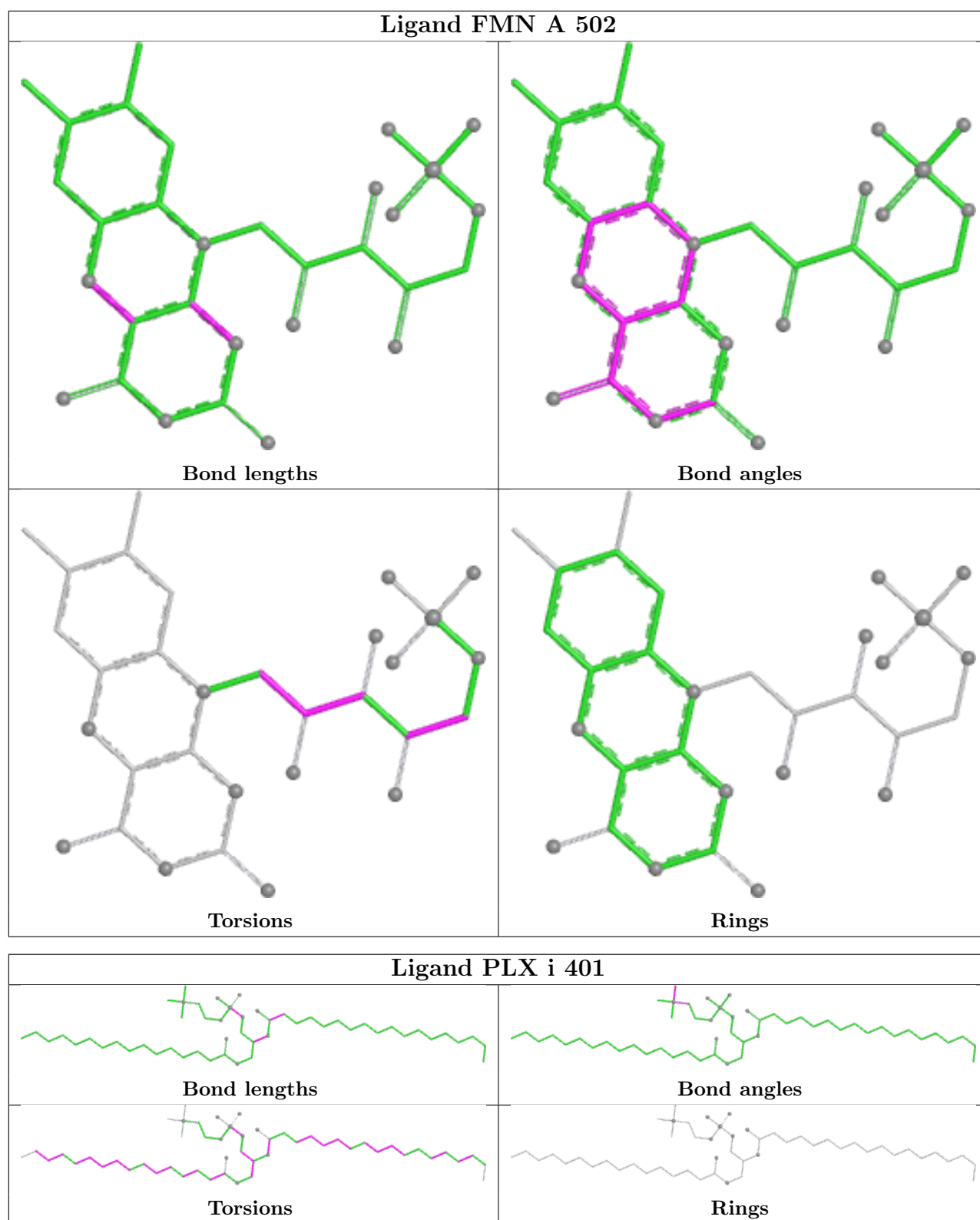


## Ligand PLX r 502



## Ligand ADP w 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

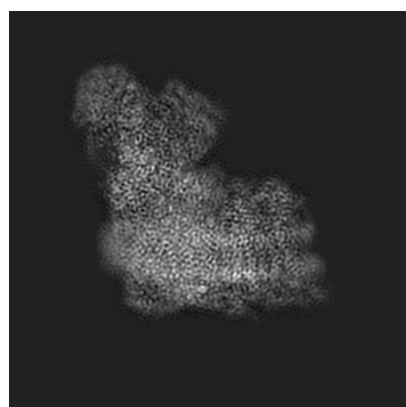
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32306. These allow visual inspection of the internal detail of the map and identification of artifacts.

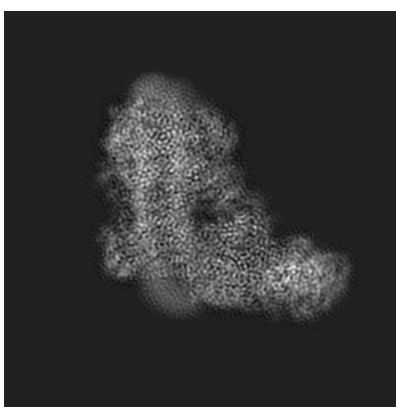
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

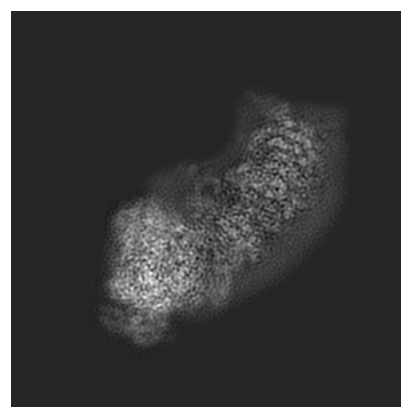
#### 6.1.1 Primary map



X



Y

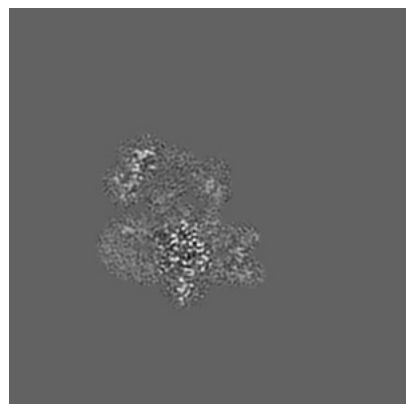


Z

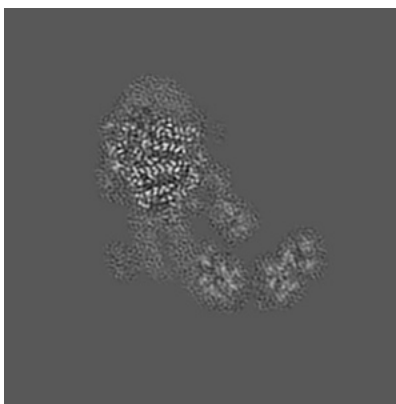
The images above show the map projected in three orthogonal directions.

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

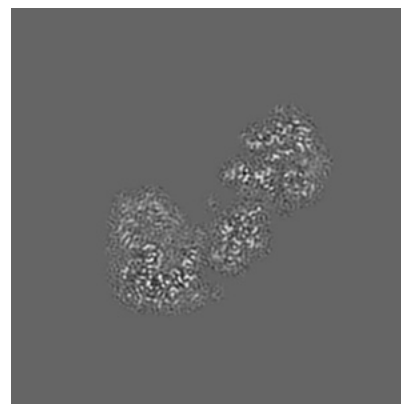
#### 6.2.1 Primary map



X Index: 152



Y Index: 152

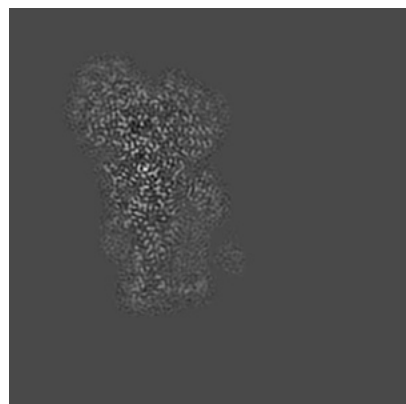


Z Index: 152

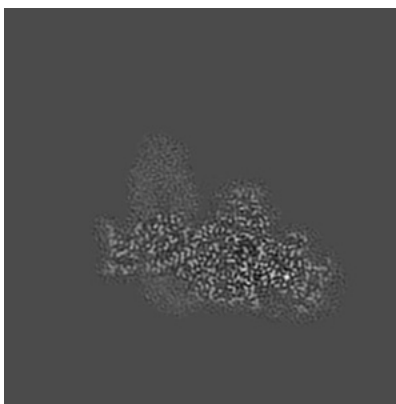
The images above show central slices of the map in three orthogonal directions.

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

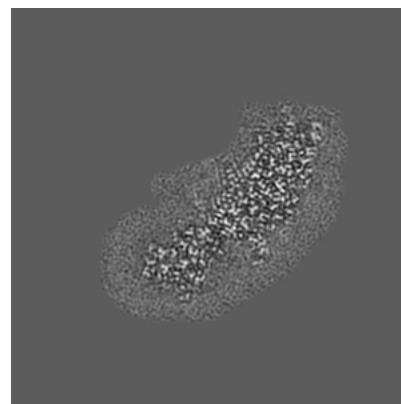
### 6.3.1 Primary map



X Index: 105



Y Index: 98

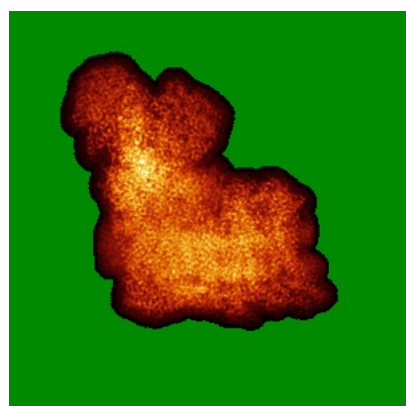


Z Index: 128

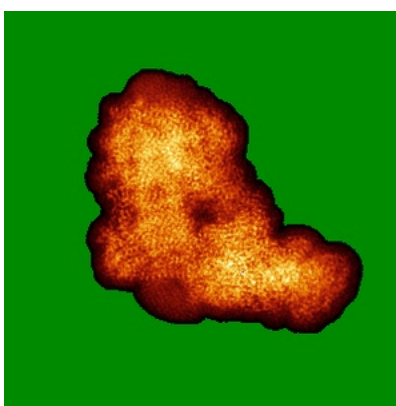
The images above show the largest variance slices of the map in three orthogonal directions.

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

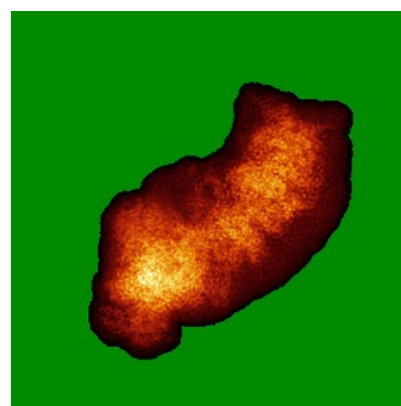
### 6.4.1 Primary map



X



Y

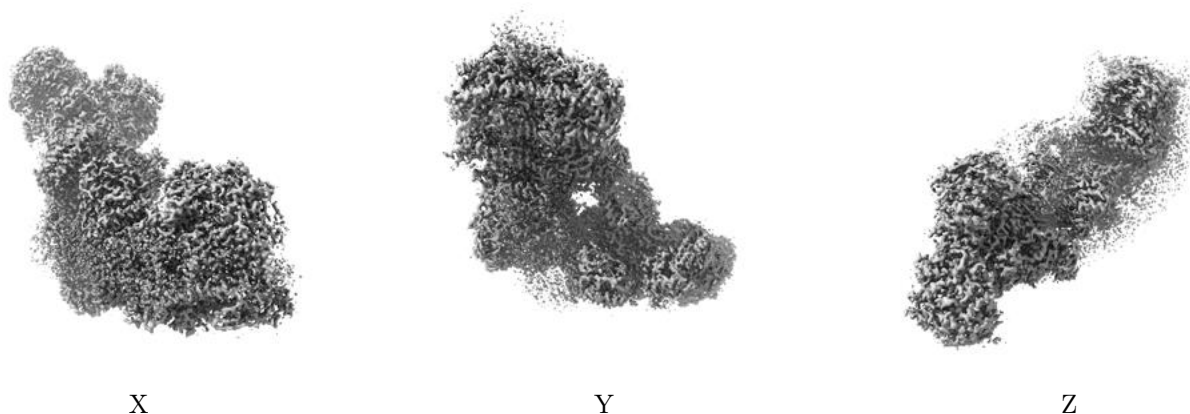


Z

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 0.0282. 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](#)

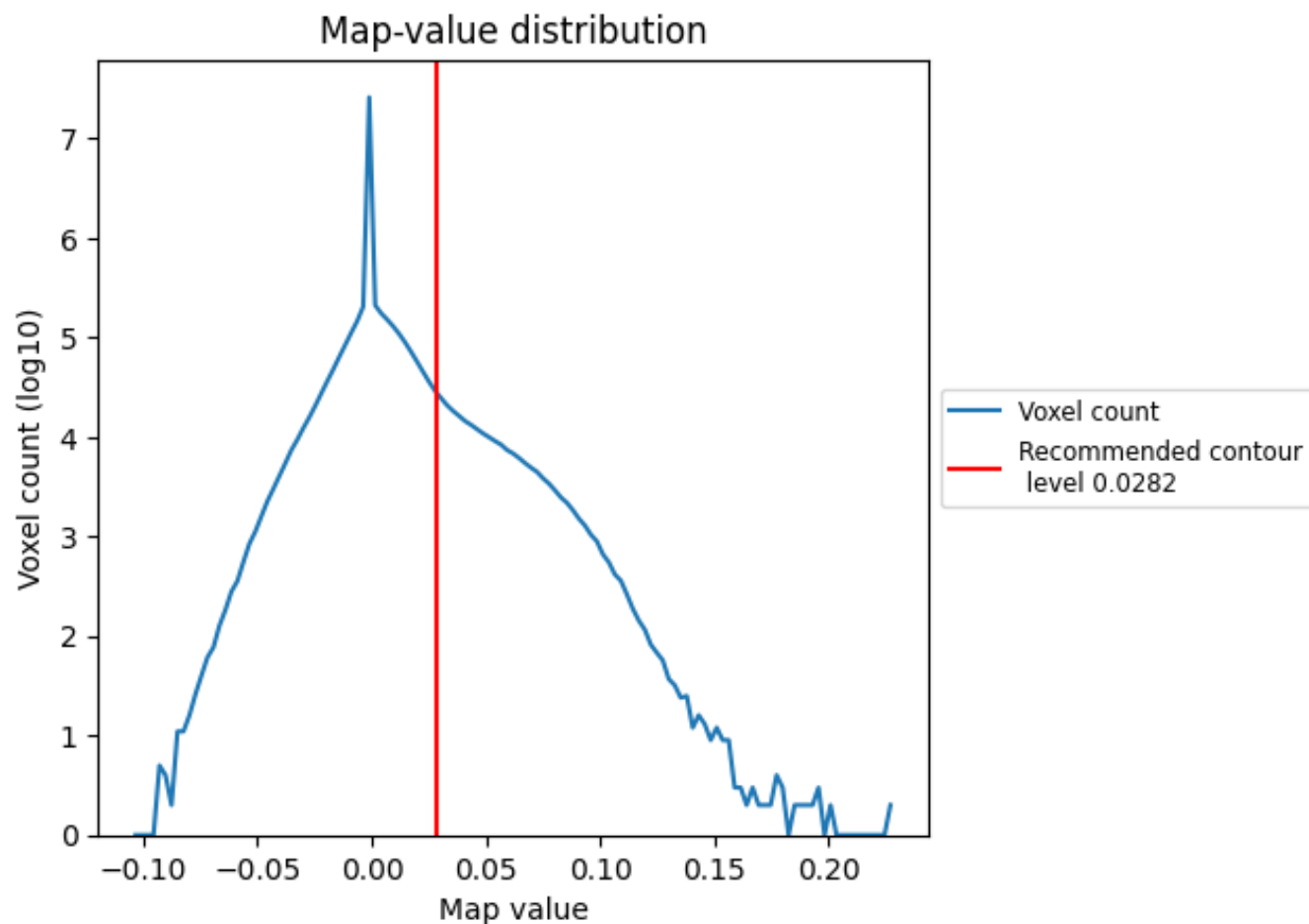
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

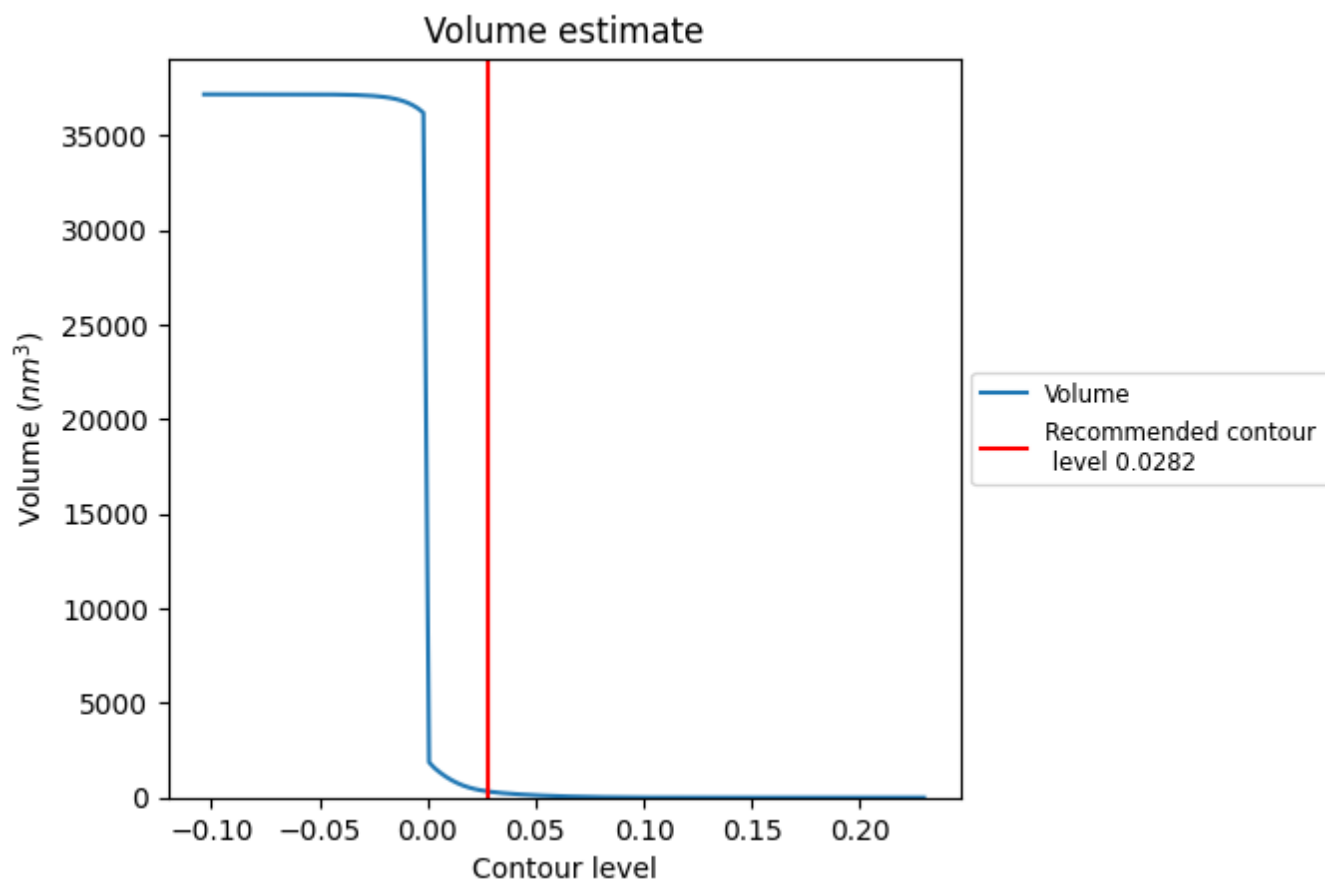
This section contains the results of statistical analysis of the map.

### 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.

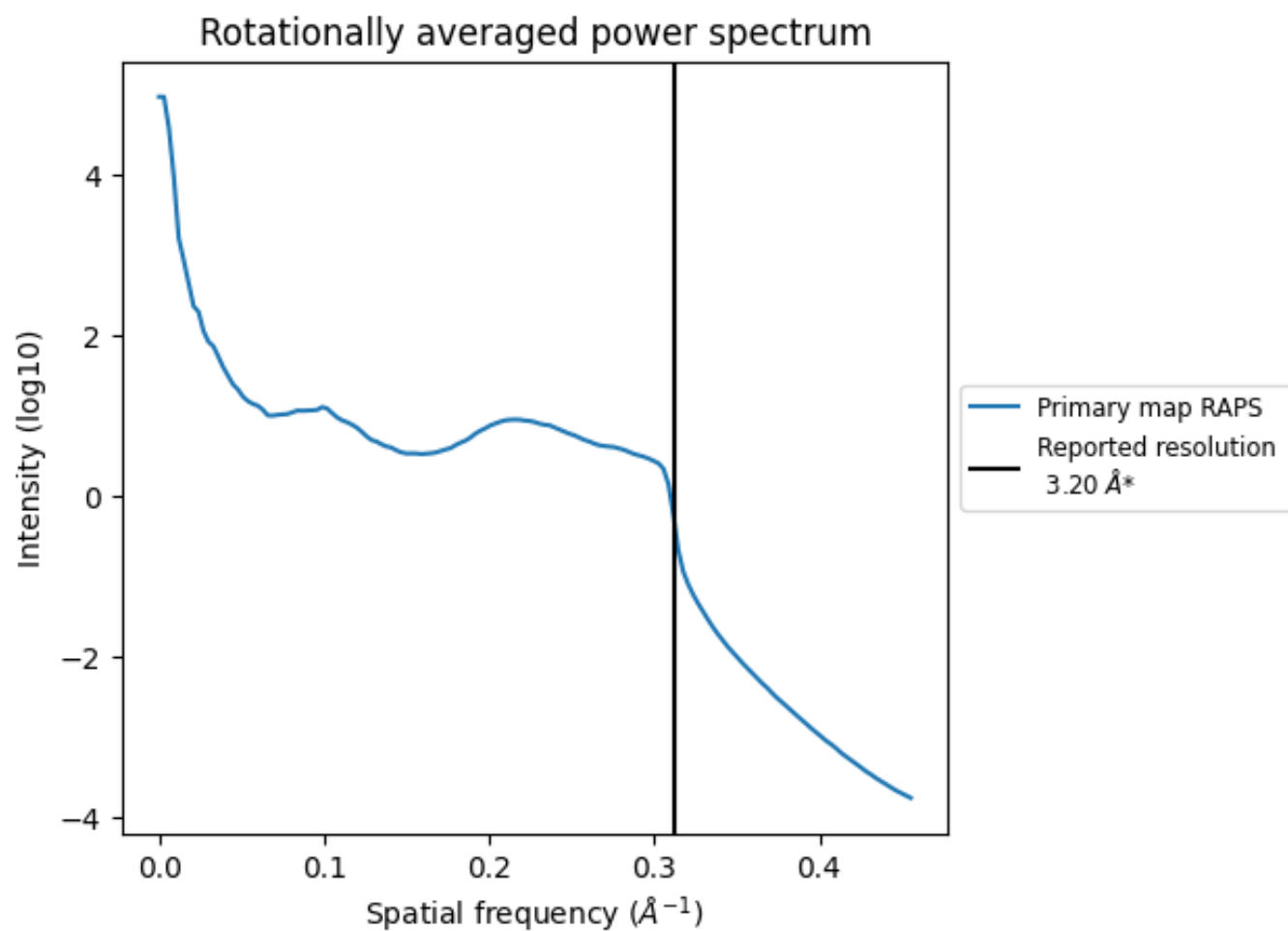
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 321  $\text{nm}^3$ ; this corresponds to an approximate mass of 290 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 0.312  $\text{\AA}^{-1}$

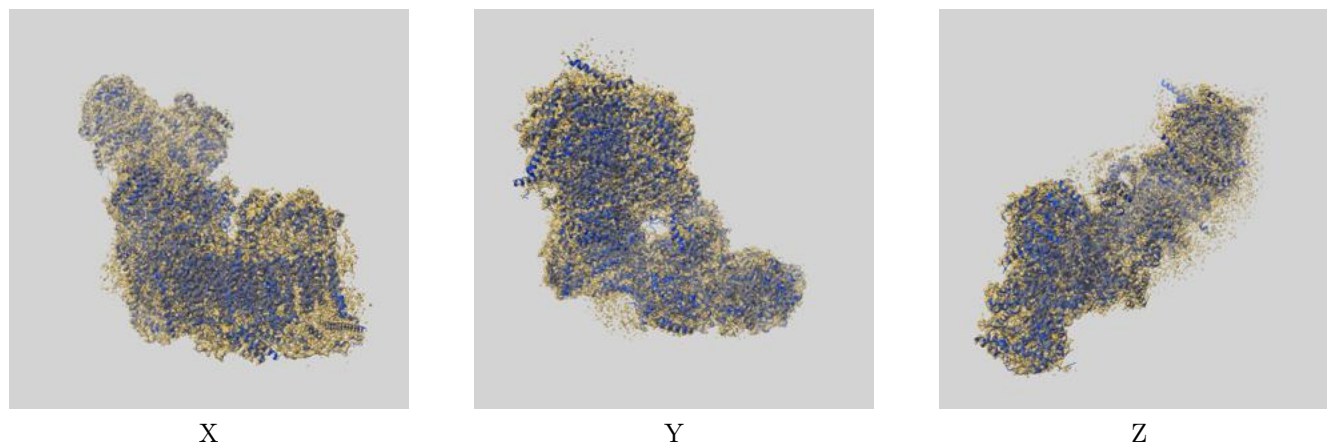
## 8 Fourier-Shell correlation ⓘ

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

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

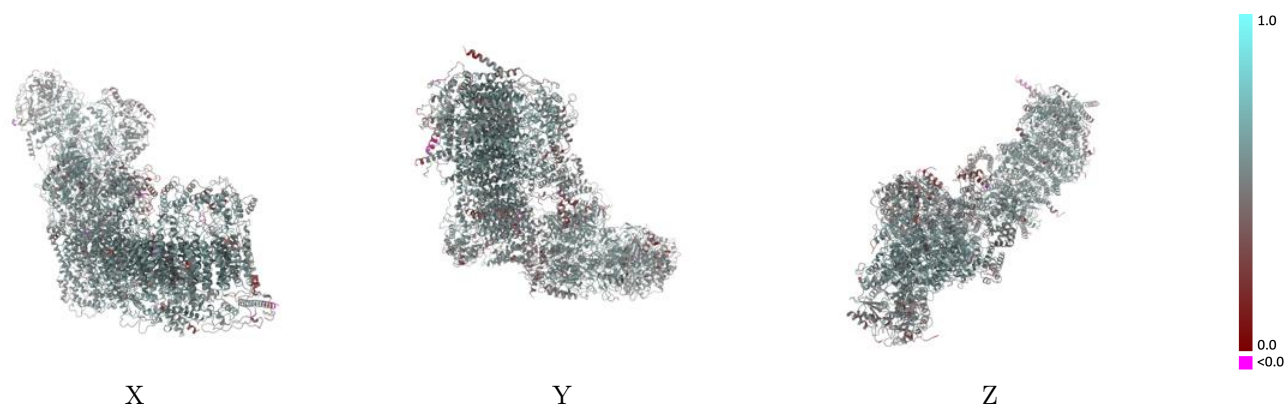
This section contains information regarding the fit between EMDB map EMD-32306 and PDB model 7W4K. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

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



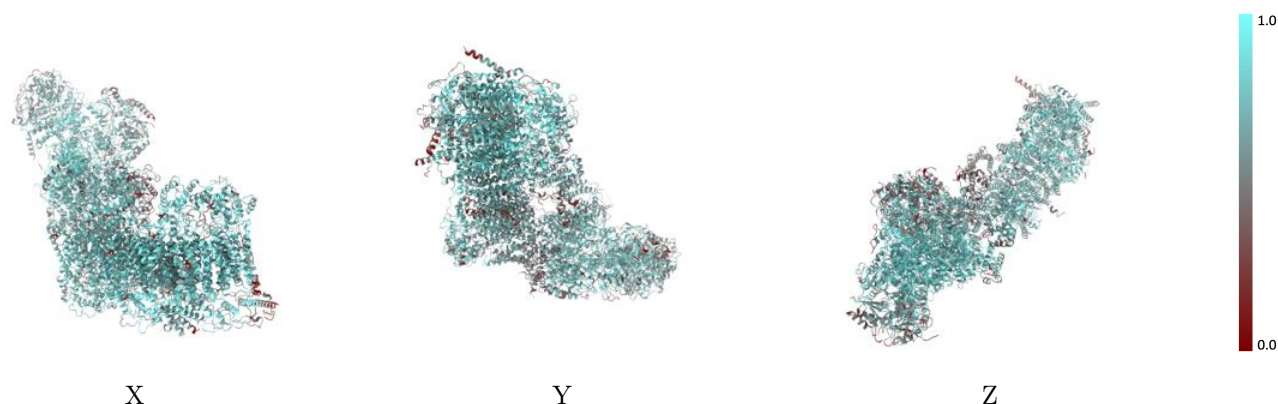
The images above show the 3D surface view of the map at the recommended contour level 0.0282 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



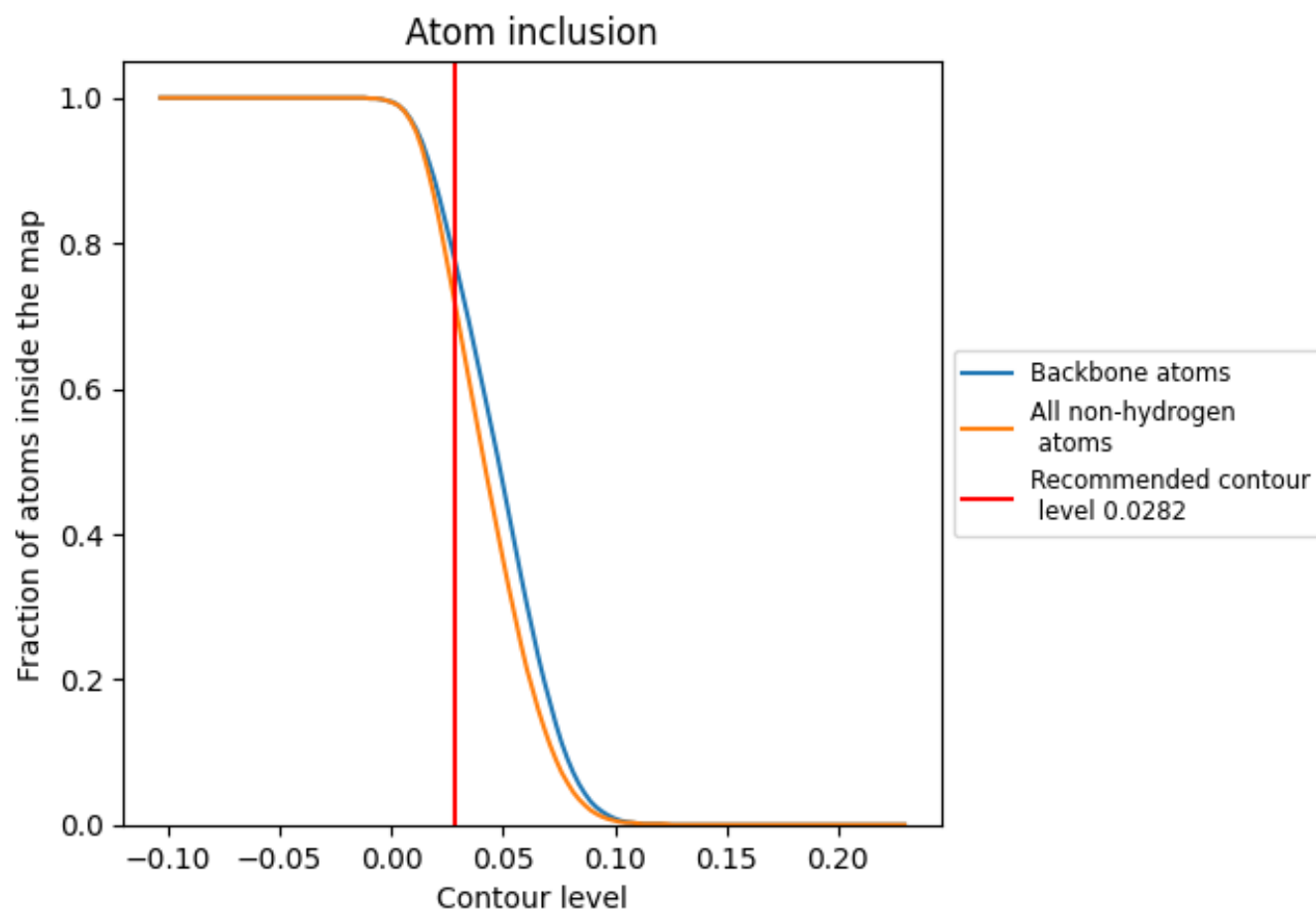
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0282).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.0282) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7210   |  0.5310   |
| A     |  0.6420   |  0.5000   |
| B     |  0.8720   |  0.5840   |
| C     |  0.8040   |  0.5650   |
| E     |  0.6730   |  0.5210   |
| F     |  0.5170   |  0.4330   |
| G     |  0.4060   |  0.3590   |
| H     |  0.6700   |  0.5030   |
| I     |  0.7390   |  0.5420   |
| J     |  0.6040   |  0.4900   |
| K     |  0.5550   |  0.4610   |
| L     |  0.7440   |  0.5530   |
| M     |  0.7190   |  0.5380   |
| N     |  0.7600   |  0.5490   |
| O     |  0.6180  |  0.4960  |
| P     |  0.8390 |  0.5790 |
| Q     |  0.8140 |  0.5760 |
| S     |  0.7850 |  0.5440 |
| T     |  0.7180 |  0.5400 |
| U     |  0.6820 |  0.5020 |
| V     |  0.4510 |  0.4430 |
| W     |  0.7250 |  0.5310 |
| X     |  0.7020 |  0.5020 |
| Y     |  0.6120 |  0.4700 |
| Z     |  0.5610 |  0.4580 |
| a     |  0.7650 |  0.5510 |
| b     |  0.6800 |  0.4870 |
| c     |  0.7540 |  0.5360 |
| d     |  0.7310 |  0.5210 |
| e     |  0.6750 |  0.5140 |
| f     |  0.6350 |  0.4820 |
| g     |  0.8010 |  0.5550 |
| h     |  0.7420 |  0.5310 |
| i     |  0.8020 |  0.5700 |
| j     |  0.6300 |  0.5010 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| k     |  0.6760 |  0.5330 |
| l     |  0.7690 |  0.5560 |
| m     |  0.6440 |  0.5010 |
| n     |  0.6510 |  0.5010 |
| o     |  0.7200 |  0.5290 |
| p     |  0.7540 |  0.5310 |
| r     |  0.8250 |  0.5740 |
| s     |  0.7560 |  0.5430 |
| u     |  0.7340 |  0.5250 |
| v     |  0.6180 |  0.4730 |
| w     |  0.7030 |  0.5210 |