



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:22 PM UTC

PDB ID : 8UGJ / pdb\_00008ugj  
EMDB ID : EMD-42227  
Title : In-situ structure of typeB supercomplex in respiratory chain (composite)  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-05  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

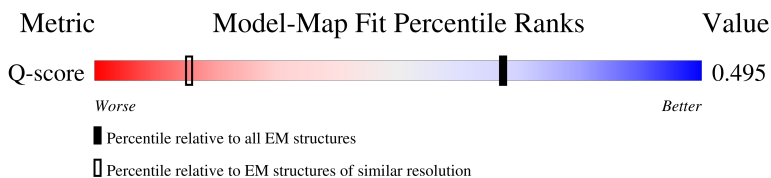
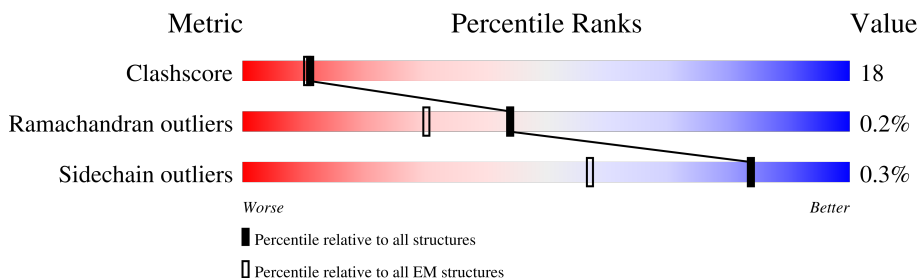
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 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                       | 4254 ( 1.80 - 2.80 )                                     |

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   | 1A    | 115    | <div> <div>12%</div> <div>62%</div> <div>37%</div> <div>.</div> </div> |
| 2   | 1B    | 258    | <div> <div>37%</div> <div>23%</div> <div>40%</div> </div>              |
| 3   | 1C    | 264    | <div> <div>60%</div> <div>19%</div> <div>21%</div> </div>              |
| 4   | 1D    | 476    | <div> <div>58%</div> <div>32%</div> <div>10%</div> </div>              |

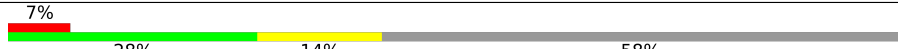
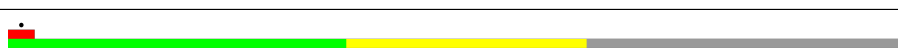
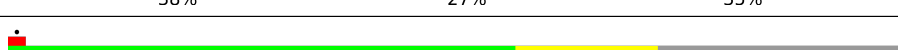
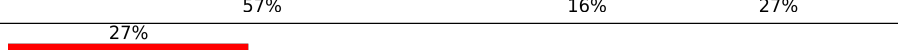
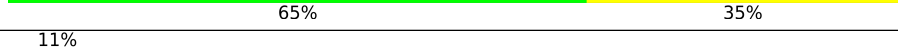
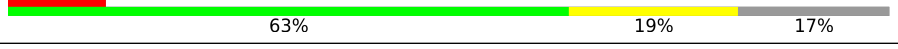
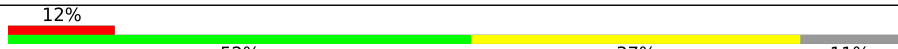
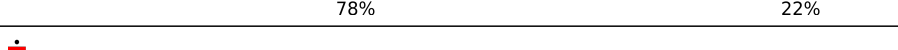
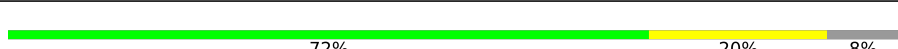
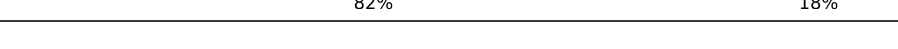
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | 1E    | 249    |                  |
| 6   | 1F    | 464    |                  |
| 7   | 1G    | 727    |                  |
| 8   | 1H    | 318    |                  |
| 9   | 1I    | 239    |                  |
| 10  | 1J    | 175    |                  |
| 11  | 1K    | 98     |                  |
| 12  | 1L    | 606    |                  |
| 13  | 1M    | 459    |                  |
| 14  | 1N    | 347    |                  |
| 15  | 1O    | 357    |                  |
| 16  | 1P    | 377    |                  |
| 17  | 1Q    | 175    |                  |
| 18  | 1R    | 123    |                  |
| 19  | 1S    | 99     |                  |
| 20  | 1T    | 156    |                  |
| 20  | 1U    | 156    |                  |
| 21  | 1V    | 116    |                  |
| 22  | 1W    | 128    |                  |
| 23  | 1X    | 172    |                  |
| 24  | 1Y    | 141    |                  |
| 25  | 1Z    | 144    |                  |
| 26  | 1a    | 70     |                  |
| 27  | 1b    | 84     |                  |
| 28  | 1c    | 76     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | 1d    | 122    |    |
| 30  | 1e    | 106    |    |
| 31  | 1f    | 135    |    |
| 32  | 1g    | 154    |    |
| 33  | 1h    | 189    |    |
| 34  | 1i    | 128    |    |
| 35  | 1j    | 105    |    |
| 36  | 1k    | 98     |    |
| 37  | 1l    | 186    |    |
| 38  | 1m    | 129    |    |
| 39  | 1n    | 179    |    |
| 40  | 1o    | 137    |    |
| 41  | 1p    | 176    |   |
| 42  | 1q    | 145    |  |
| 43  | 1r    | 113    |  |
| 44  | 1s    | 471    |  |
| 45  | 3A    | 480    |  |
| 45  | 3N    | 480    |  |
| 46  | 3B    | 453    |  |
| 46  | 3O    | 453    |  |
| 47  | 3C    | 379    |  |
| 47  | 3P    | 379    |  |
| 48  | 3D    | 326    |  |
| 48  | 3Q    | 326    |  |
| 49  | 3E    | 274    |  |

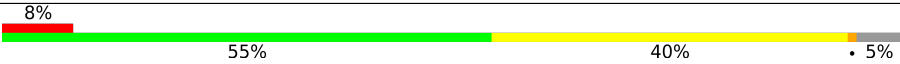
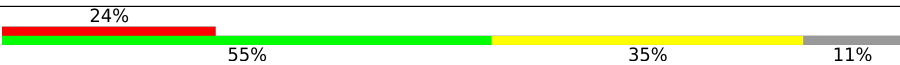
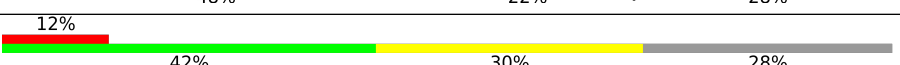
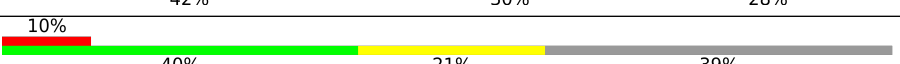
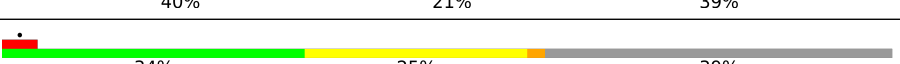
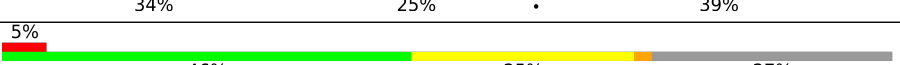
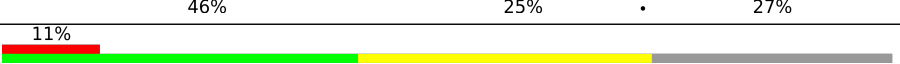
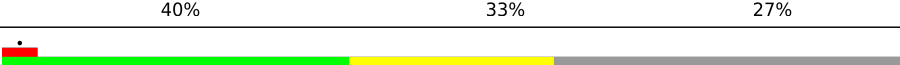
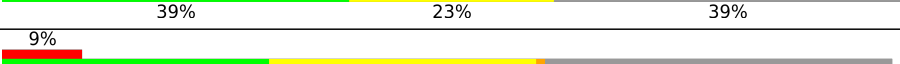
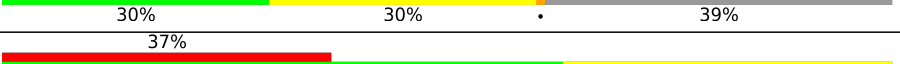
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 49  | 3I    | 274    |                  |
| 49  | 3R    | 274    |                  |
| 49  | 3V    | 274    |                  |
| 50  | 3F    | 111    |                  |
| 50  | 3S    | 111    |                  |
| 51  | 3G    | 82     |                  |
| 51  | 3T    | 82     |                  |
| 52  | 3H    | 91     |                  |
| 52  | 3U    | 91     |                  |
| 53  | 3J    | 60     |                  |
| 53  | 3W    | 60     |                  |
| 54  | 3X    | 56     |                  |
| 54  | 3Y    | 56     |                  |
| 55  | 4A    | 514    |                  |
| 55  | 8A    | 514    |                  |
| 56  | 4B    | 229    |                  |
| 56  | 8B    | 229    |                  |
| 57  | 4C    | 261    |                  |
| 57  | 8C    | 261    |                  |
| 58  | 4D    | 169    |                  |
| 58  | 8D    | 169    |                  |
| 59  | 4E    | 152    |                  |
| 59  | 8E    | 152    |                  |
| 60  | 4F    | 128    |                  |
| 60  | 8F    | 128    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 61  | 4G    | 97     |    |
| 61  | 8G    | 97     |    |
| 62  | 4H    | 86     |    |
| 62  | 8H    | 86     |    |
| 63  | 4I    | 75     |    |
| 63  | 8I    | 75     |    |
| 64  | 4J    | 80     |    |
| 64  | 8J    | 80     |    |
| 65  | 4K    | 80     |    |
| 65  | 8K    | 80     |    |
| 66  | 4L    | 63     |    |
| 66  | 8L    | 63     |    |
| 67  | 4M    | 70     |   |
| 67  | 8M    | 70     |  |
| 68  | 4N    | 82     |  |
| 68  | 8N    | 82     |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 71  | SF4  | 1B    | 201 | -         | -        | X       | -                |
| 71  | SF4  | 1F    | 502 | -         | -        | X       | -                |
| 71  | SF4  | 1G    | 801 | -         | -        | X       | -                |
| 72  | FES  | 1G    | 803 | -         | -        | X       | -                |
| 72  | FES  | 3E    | 301 | -         | -        | X       | -                |
| 72  | FES  | 3R    | 301 | -         | -        | X       | -                |
| 91  | CUA  | 4B    | 304 | -         | -        | X       | -                |
| 91  | CUA  | 8B    | 304 | -         | -        | X       | -                |

## 2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 134346 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 1A    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 916   | 616 | 134 | 159 | 7 |         |       |

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | 1B    | 155      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1242  | 791 | 226 | 211 | 14 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | 1C    | 209      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1740  | 1125 | 297 | 316 | 2 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| 1C    | 104     | GLN      | ARG    | conflict | UNP A0A286ZNN4 |
| 1C    | 154     | GLY      | ASP    | conflict | UNP A0A286ZNN4 |

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | 1D    | 429      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3452  | 2207 | 593 | 628 | 24 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| 1D    | 0       | GLY      | GLU    | conflict | UNP A0A8D0QM68 |

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 5   | 1E    | 214      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1658  | 1058 | 278 | 312 | 10 |         |       |

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | 1F    | 432      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3325  | 2100 | 592 | 613 | 20 |         |       |

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 7   | 1G    | 699      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5362  | 3360 | 933 | 1029 | 40 |         |       |

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | 1H    | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2504  | 1673 | 385 | 425 | 21 |         |       |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 9   | 1I    | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1412  | 887 | 243 | 269 | 13 |         |       |

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 10  | 1J    | 174      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1329  | 892 | 189 | 236 | 12 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 11  | 1K    | 98       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 750   | 494 | 113 | 129 | 14 |         |       |

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | 1L    | 606      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4818  | 3195 | 746 | 826 | 51 |         |       |

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 13  | 1M    | 459      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3632  | 2411 | 572 | 610 | 39 |         |       |

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | 1N    | 347      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2712  | 1783 | 420 | 463 | 46 |         |       |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | 1O    | 320      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2590  | 1649 | 440 | 491 | 10 |         |       |

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | 1P    | 342      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2751  | 1783 | 481 | 478 | 9 |         |       |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | 1Q    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 659 | 186 | 199 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | 1R    | 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 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | 1S    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 440 | 131 | 127 | 2 |         |       |

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | 1T    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 689   | 445 | 101 | 138 | 5 |         |       |
| 20  | 1U    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 694   | 448 | 102 | 139 | 5 |         |       |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | 1V    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 927   | 599 | 157 | 168 | 3 |         |       |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | 1W    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 971   | 619 | 179 | 168 | 5 |         |       |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 23  | 1X    | 171      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1398  | 887 | 250 | 251 | 10 |         |       |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | 1Y    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 648 | 173 | 189 | 6 |         |       |

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | 1Z    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1168  | 752 | 202 | 205 | 9 |         |       |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 26  | 1a    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 562   | 361 | 101 | 94 | 6 |         |       |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | 1b    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 643   | 417 | 110 | 115 | 1 |         |       |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 28  | 1c    | 49       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 417   | 276 | 71 | 70 |         |       |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | 1d    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 641 | 171 | 168 | 5 |         |       |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | 1e    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 816   | 519 | 151 | 140 | 6 |         |       |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

1 [Sus scrofa].

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 31  | 1f    | 57       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 487   | 316 | 89 | 80 | 2 |         |       |

There are 29 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference      |
|-------|---------|----------|--------|-----------------------|----------------|
| 1f    | -77     | MET      | -      | initiating methionine | UNP A0A8D1IZ33 |
| 1f    | -76     | ALA      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -75     | ALA      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -74     | ALA      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -73     | ILE      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -72     | LEU      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -71     | LYS      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -70     | LEU      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -69     | GLU      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -68     | GLU      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -67     | THR      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -66     | ARG      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -65     | GLY      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -64     | GLY      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -63     | GLY      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -62     | GLU      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -61     | LYS      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -60     | CYS      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -59     | ASP      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -58     | LYS      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -57     | ASN      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -56     | GLN      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -55     | GLY      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -54     | VAL      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -53     | LYS      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -52     | GLY      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -51     | ARG      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -50     | ARG      | -      | expression tag        | UNP A0A8D1IZ33 |
| 1f    | -49     | PHE      | -      | expression tag        | UNP A0A8D1IZ33 |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | 1g    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 835   | 535 | 138 | 158 | 4 |         |       |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | 1h    | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1151  | 754 | 195 | 199 | 3 |         |       |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | 1i    | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 723 | 194 | 181 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference      |
|-------|---------|----------|--------|-------------|----------------|
| 1i    | 0       | ACE      | -      | acetylation | UNP A0A4X1UIV8 |

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 35  | 1j    | 71       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 601   | 394 | 99 | 107 | 1 |         |       |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | 1k    | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 649   | 422 | 110 | 116 | 1 |         |       |

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | 1l    | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1310  | 847 | 213 | 242 | 8 |         |       |

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

4.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 38  | 1m    | 128      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1062  | 691 | 182 | 189 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | 1n    | 172      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1495  | 956 | 273 | 258 | 8 |         |       |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 40  | 1o    | 122      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1045  | 650 | 198 | 187 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| 1o    | 0       | MYR      | -      | insertion | UNP F1SCH1 |

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | 1p    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1449  | 908 | 263 | 270 | 8 |         |       |

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | 1q    | 145      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1212  | 775 | 219 | 213 | 5 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | 1r    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 759   | 478 | 143 | 135 | 3 |         |       |

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | 1s    | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 382   | 238 | 70 | 73 | 1 |         |       |

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 45  | 3A    | 440      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3411  | 2131 | 599 | 662 | 19 |         |       |
| 45  | 3N    | 445      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 3424  | 2162 | 606 | 637 | 19 |         |       |

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | 3B    | 418      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3138  | 1965 | 555 | 610 | 8 |         |       |
| 46  | 3O    | 417      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3124  | 1960 | 554 | 602 | 8 |         |       |

- Molecule 47 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47  | 3C    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3025  | 2031 | 471 | 502 | 21 |         |       |
| 47  | 3P    | 379      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3024  | 2031 | 471 | 501 | 21 |         |       |

- Molecule 48 is a protein called Cytochrome c1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | 3D    | 237      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1888  | 1205 | 325 | 342 | 16 |         |       |
| 48  | 3Q    | 239      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1904  | 1215 | 327 | 346 | 16 |         |       |

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | 3E    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 955 | 265 | 291 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | 3I    | 47       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 340   | 211 | 65  | 63  | 1 |         |       |
| 49  | 3R    | 196      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 955 | 265 | 291 | 7 |         |       |
| 49  | 3V    | 31       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 224   | 136 | 48  | 39  | 1 |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| 3E    | 34      | VAL      | LEU    | conflict | UNP A0A4X1TWD8 |
| 3E    | 45      | LEU      | ALA    | conflict | UNP A0A4X1TWD8 |
| 3E    | 49      | VAL      | PHE    | conflict | UNP A0A4X1TWD8 |
| 3E    | 56      | ARG      | SER    | conflict | UNP A0A4X1TWD8 |
| 3I    | 34      | VAL      | LEU    | conflict | UNP A0A4X1TWD8 |
| 3I    | 45      | LEU      | ALA    | conflict | UNP A0A4X1TWD8 |
| 3I    | 49      | VAL      | PHE    | conflict | UNP A0A4X1TWD8 |
| 3I    | 56      | ARG      | SER    | conflict | UNP A0A4X1TWD8 |
| 3R    | 34      | VAL      | LEU    | conflict | UNP A0A4X1TWD8 |
| 3R    | 45      | LEU      | ALA    | conflict | UNP A0A4X1TWD8 |
| 3R    | 49      | VAL      | PHE    | conflict | UNP A0A4X1TWD8 |
| 3R    | 56      | ARG      | SER    | conflict | UNP A0A4X1TWD8 |
| 3V    | 34      | VAL      | LEU    | conflict | UNP A0A4X1TWD8 |
| 3V    | 45      | LEU      | ALA    | conflict | UNP A0A4X1TWD8 |
| 3V    | 49      | VAL      | PHE    | conflict | UNP A0A4X1TWD8 |
| 3V    | 56      | ARG      | SER    | conflict | UNP A0A4X1TWD8 |

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | 3F    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 557 | 152 | 157 | 2 |         |       |
| 50  | 3S    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 557 | 152 | 157 | 2 |         |       |

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 51  | 3G    | 74       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 628   | 411 | 116 | 99 | 2 |         |       |
| 51  | 3T    | 74       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 628   | 411 | 116 | 99 | 2 |         |       |

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 52  | 3H    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 533   | 325 | 97 | 106 | 5 |         |       |
| 52  | 3U    | 65       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 533   | 325 | 97 | 106 | 5 |         |       |

- Molecule 53 is a protein called Complex III subunit 9.

| Mol | Chain | Residues | Atoms |     |    |    |  | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|--|---------|-------|
| 53  | 3J    | 56       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 464   | 305 | 82 | 77 |  |         |       |
| 53  | 3W    | 56       | Total | C   | N  | O  |  | 0       | 0     |
|     |       |          | 464   | 305 | 82 | 77 |  |         |       |

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 54  | 3X    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 286 | 75 | 66 | 2 |         |       |
| 54  | 3Y    | 51       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 421   | 281 | 74 | 65 | 1 |         |       |

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | 4A    | 514      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4026  | 2693 | 625 | 676 | 32 |         |       |
| 55  | 8A    | 514      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4026  | 2693 | 625 | 676 | 32 |         |       |

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | 4B    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1828  | 1190 | 281 | 339 | 18 |         |       |
| 56  | 8B    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1828  | 1190 | 281 | 339 | 18 |         |       |

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 57  | 4C    | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2096  | 1399 | 336 | 351 | 10 |         |       |
| 57  | 8C    | 259      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2096  | 1399 | 336 | 351 | 10 |         |       |

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | 4D    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 757 | 190 | 212 | 4 |         |       |
| 58  | 8D    | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 757 | 190 | 212 | 4 |         |       |

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | 4E    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 852   | 544 | 144 | 162 | 2 |         |       |
| 59  | 8E    | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 852   | 544 | 144 | 162 | 2 |         |       |

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | 4F    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 455 | 130 | 143 | 6 |         |       |
| 60  | 8F    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 455 | 130 | 143 | 6 |         |       |

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | 4G    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 398 | 118 | 100 | 1 |         |       |
| 61  | 8G    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 398 | 118 | 100 | 1 |         |       |

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | 4H    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 434 | 125 | 123 | 5 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | 8H    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 687   | 434 | 125 | 123 | 5 |         |       |

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 63  | 4I    | 67       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 550   | 359 | 97 | 91 | 3 |         |       |
| 63  | 8I    | 67       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 550   | 359 | 97 | 91 | 3 |         |       |

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 64  | 4J    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 456   | 293 | 78 | 82 | 3 |         |       |
| 64  | 8J    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 456   | 293 | 78 | 82 | 3 |         |       |

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 65  | 4K    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 383   | 249 | 65 | 68 | 1 |         |       |
| 65  | 8K    | 49       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 383   | 249 | 65 | 68 | 1 |         |       |

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 66  | 4L    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 381   | 254 | 64 | 61 | 2 |         |       |
| 66  | 8L    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 381   | 254 | 64 | 61 | 2 |         |       |

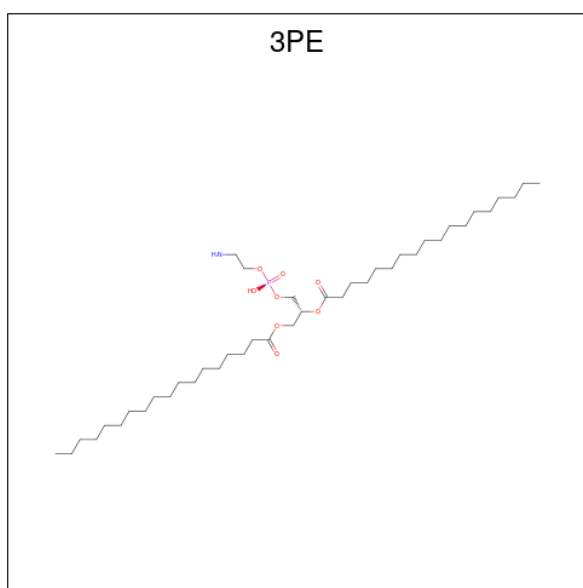
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 67  | 4M    | 43       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 338   | 222 | 57 | 59 |         |       |
| 67  | 8M    | 43       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 338   | 222 | 57 | 59 |         |       |

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUF4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | 4N    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 660   | 432 | 112 | 114 | 2 |         |       |
| 68  | 8N    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 660   | 432 | 112 | 114 | 2 |         |       |

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



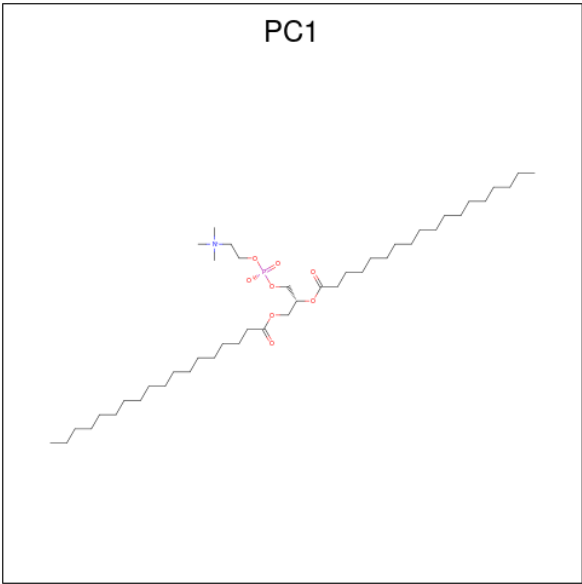
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 69  | 1A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 69  | 1K    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 69  | 1L    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 69  | 1L    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 69  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 69  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 69  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 69  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 50    | 40 | 1 | 8 | 1 |         |

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| Mol | Chain | Residues | Atoms       |         |        |        |        | AltConf |
|-----|-------|----------|-------------|---------|--------|--------|--------|---------|
| 69  | 1N    | 1        | Total<br>49 | C<br>39 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1P    | 1        | Total<br>35 | C<br>25 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1Y    | 1        | Total<br>31 | C<br>21 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1Y    | 1        | Total<br>40 | C<br>30 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1Y    | 1        | Total<br>30 | C<br>20 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1Y    | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1Y    | 1        | Total<br>27 | C<br>17 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1d    | 1        | Total<br>49 | C<br>39 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1j    | 1        | Total<br>44 | C<br>34 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 1m    | 1        | Total<br>41 | C<br>31 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3A    | 1        | Total<br>27 | C<br>17 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3A    | 1        | Total<br>32 | C<br>22 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3C    | 1        | Total<br>35 | C<br>25 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3C    | 1        | Total<br>34 | C<br>24 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3D    | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3G    | 1        | Total<br>29 | C<br>19 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3N    | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3N    | 1        | Total<br>25 | C<br>15 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3P    | 1        | Total<br>33 | C<br>23 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3R    | 1        | Total<br>47 | C<br>37 | N<br>1 | O<br>8 | P<br>1 | 0       |
| 69  | 3Y    | 1        | Total<br>30 | C<br>20 | N<br>1 | O<br>8 | P<br>1 | 0       |

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



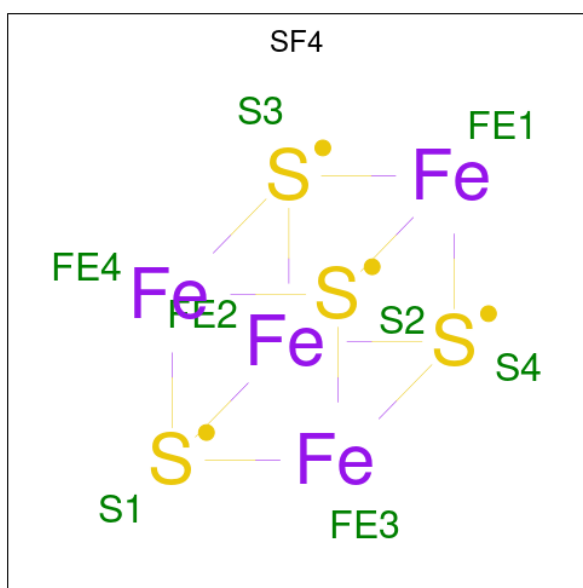
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 70  | 1A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 70  | 1A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 70  | 1B    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 70  | 1B    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 70  | 1H    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 70  | 1H    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 48    | 38 | 1 | 8 | 1 |         |
| 70  | 1I    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 70  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 70  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 70  | 1P    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 33    | 23 | 1 | 8 | 1 |         |
| 70  | 1Y    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 70  | 1d    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 39    | 29 | 1 | 8 | 1 |         |

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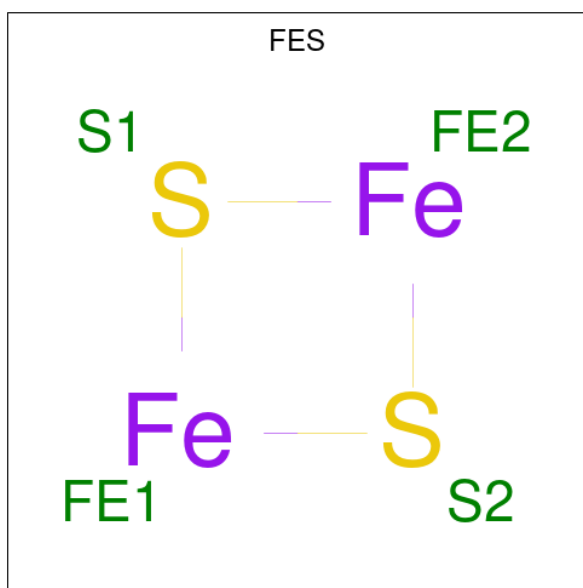
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 70  | 1h    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 70  | 1q    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 49    | 39 | 1 | 8 | 1 |         |
| 70  | 3J    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 70  | 3R    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 45    | 35 | 1 | 8 | 1 |         |
| 70  | 3X    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 29    | 19 | 1 | 8 | 1 |         |

- Molecule 71 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



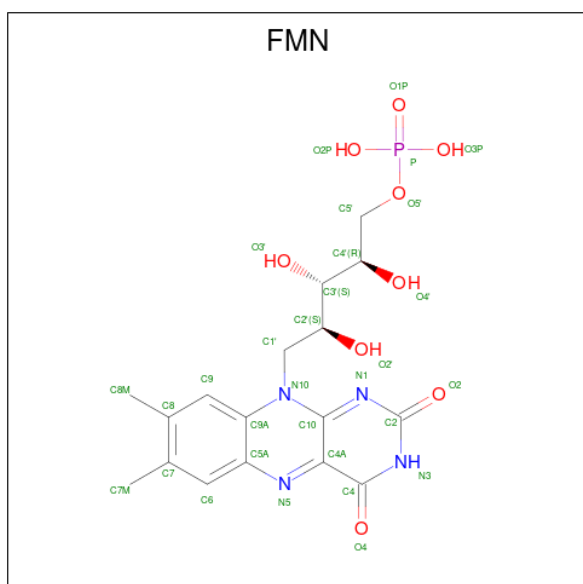
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 71  | 1B    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 71  | 1F    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 71  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 71  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 71  | 1I    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 71  | 1I    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 72  | 1E    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 72  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 72  | 3E    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 72  | 3R    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula:  $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$ ).

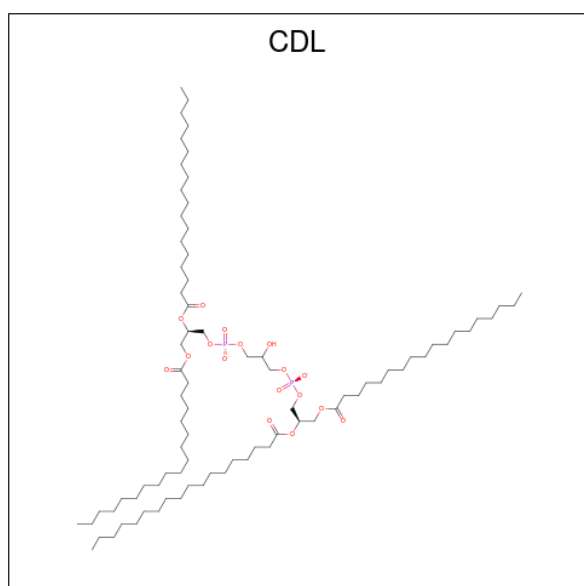


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 73  | 1F    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 74  | 1G    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



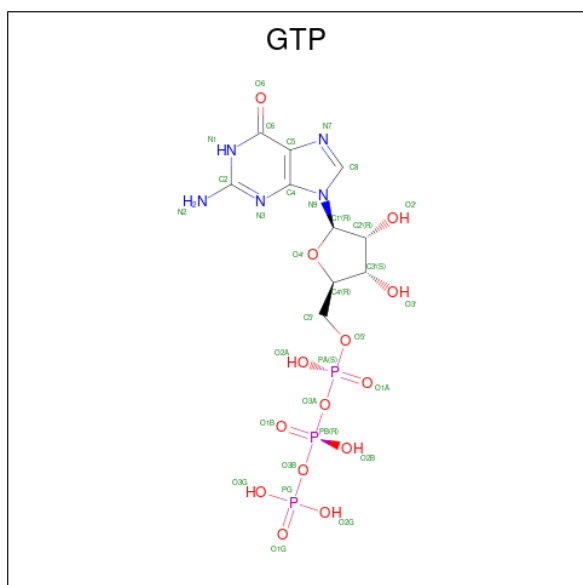
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 75  | 1H    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 32 | 17 | 2 |         |
| 75  | 1L    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 76    | 57 | 17 | 2 |         |
| 75  | 1N    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 62    | 43 | 17 | 2 |         |
| 75  | 1X    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 86    | 67 | 17 | 2 |         |
| 75  | 1d    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 65    | 46 | 17 | 2 |         |
| 75  | 1h    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 80    | 61 | 17 | 2 |         |
| 75  | 1q    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 61    | 42 | 17 | 2 |         |
| 75  | 3A    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 58    | 39 | 17 | 2 |         |

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| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 75  | 3G    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 52    | 33 | 17 | 2 |         |
| 75  | 3G    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 56    | 37 | 17 | 2 |         |
| 75  | 3N    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 24 | 17 | 2 |         |
| 75  | 3P    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 56    | 37 | 17 | 2 |         |
| 75  | 3T    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 57    | 38 | 17 | 2 |         |
| 75  | 4B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 75  | 4C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 75  | 4D    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 75  | 8B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 75  | 8C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |
| 75  | 8D    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 100   | 81 | 17 | 2 |         |

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).

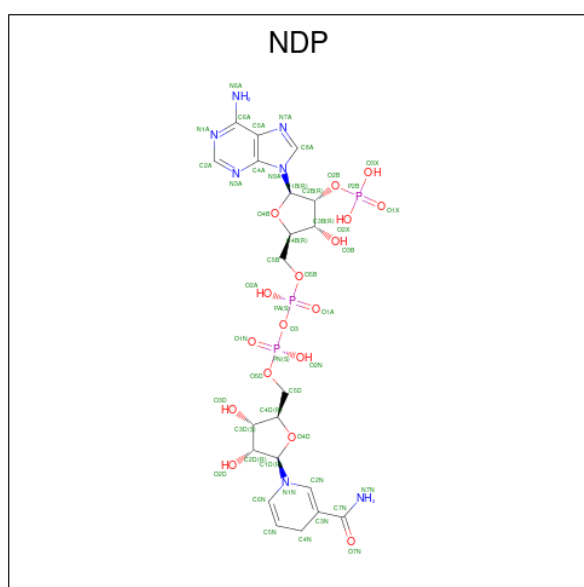


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 76  | 1O    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 77  | 1O    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 77  | 4A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 77  | 8A    | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 78  | 1P    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 79 is ZINC ION (CCD ID: ZN) (formula: Zn).

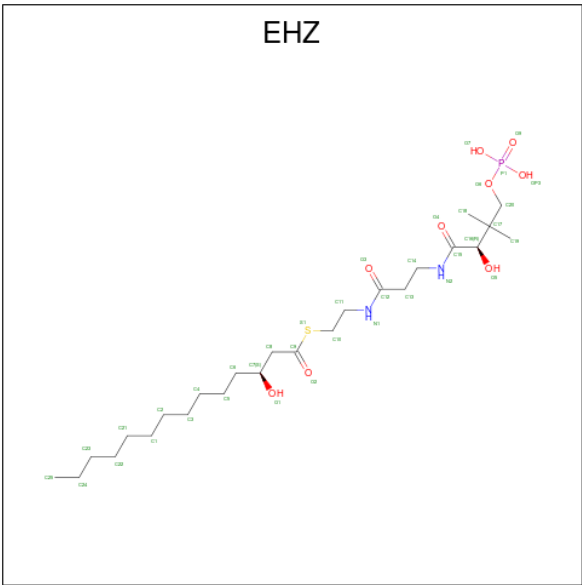
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 79  | 1R    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 79  | 4F    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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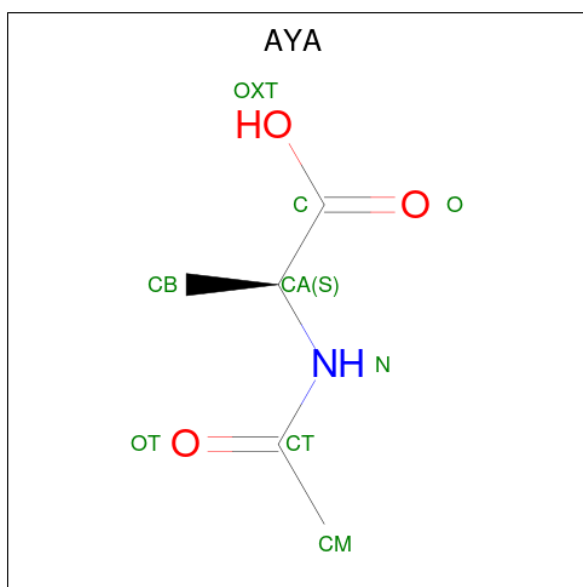
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 79  | 8F    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 80 is {S}-[2-[3-[[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>9</sub>PS).



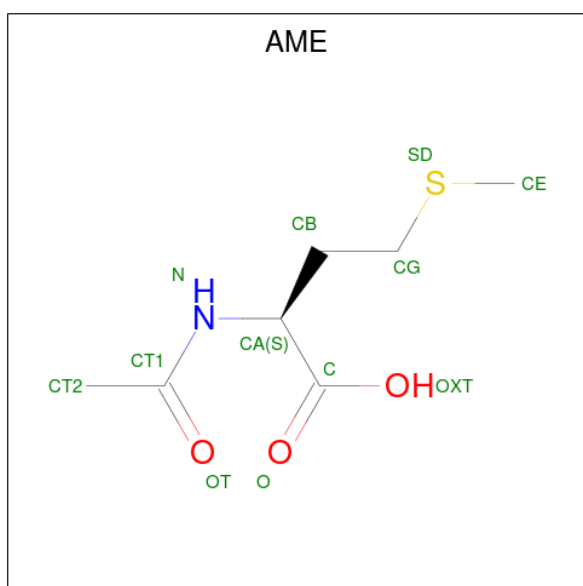
| Mol | Chain | Residues | Atoms |    |   |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---|---------|
| 80  | 1T    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |
| 80  | 1n    | 1        | Total | C  | N | O | P | S | 0       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1 |         |

- Molecule 81 is N-ACETYLALANINE (CCD ID: AYA) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>).



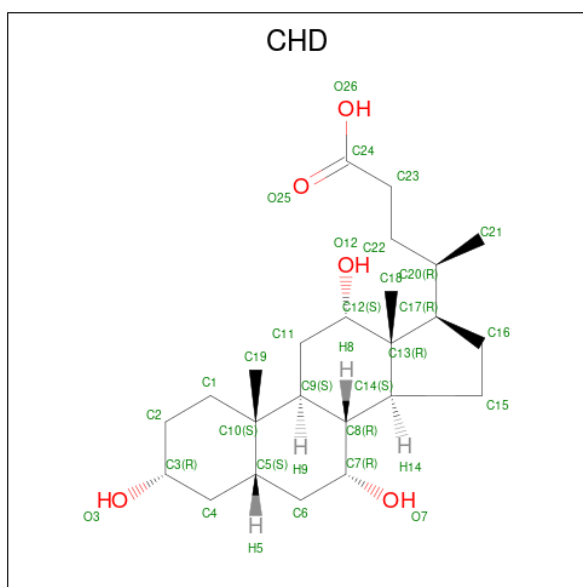
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 81  | 1Y    | 1        | Total | C | N | O | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |
| 81  | 1q    | 1        | Total | C | N | O | 0       |
|     |       |          | 8     | 5 | 1 | 2 |         |

- Molecule 82 is N-ACETYL METHIONINE (CCD ID: AME) (formula:  $C_7H_{13}NO_3S$ ).



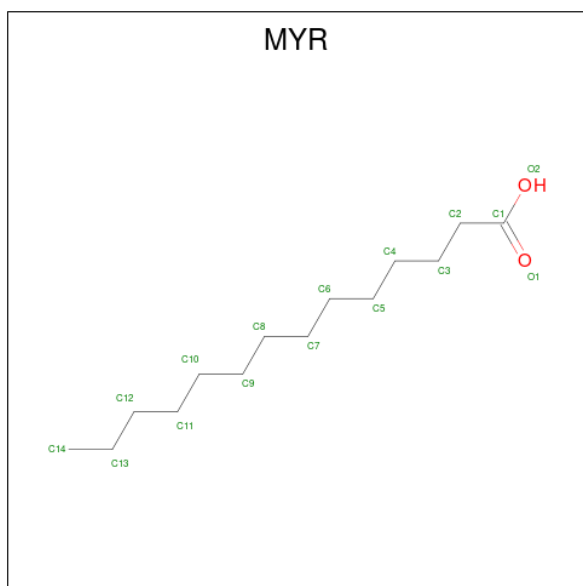
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 82  | 1h    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 11    | 7 | 1 | 2 | 1 |         |

- Molecule 83 is CHOLIC ACID (CCD ID: CHD) (formula:  $C_{24}H_{40}O_5$ ).



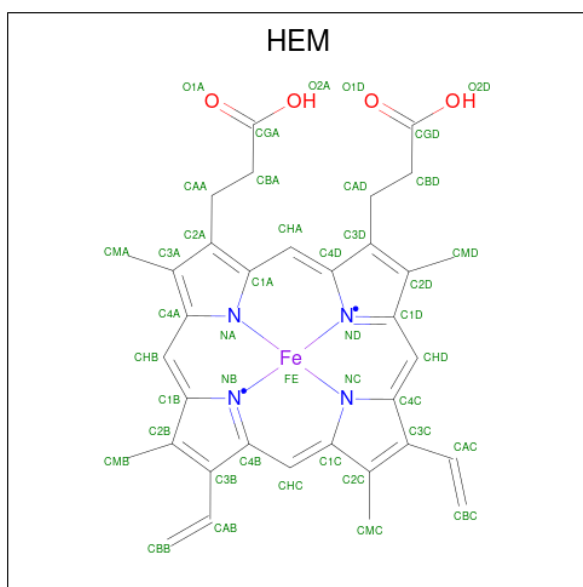
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 83  | 1i    | 1        | Total | C  | O | 0       |
|     |       |          | 29    | 24 | 5 |         |

- Molecule 84 is MYRISTIC ACID (CCD ID: MYR) (formula:  $C_{14}H_{28}O_2$ ).



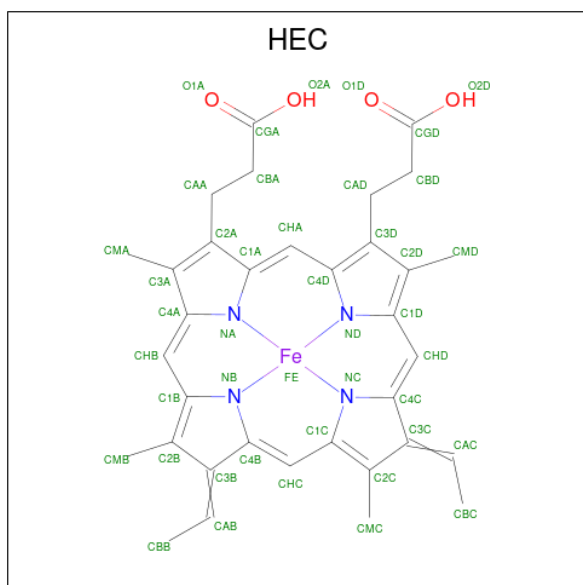
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 84  | 1l    | 1        | Total | C  | O | 0       |
|     |       |          | 15    | 14 | 1 |         |

- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



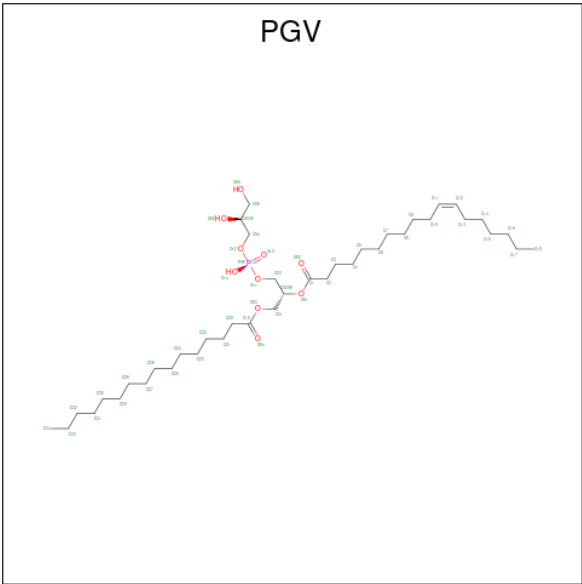
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 85  | 3C    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 85  | 3C    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 85  | 3P    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 85  | 3P    | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

- Molecule 86 is HEME C (CCD ID: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 86  | 3D    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 42    | 34 | 1  | 4 | 3 |         |
| 86  | 3Q    | 1        | Total | C  | Fe | N | O | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |

- Molecule 87 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



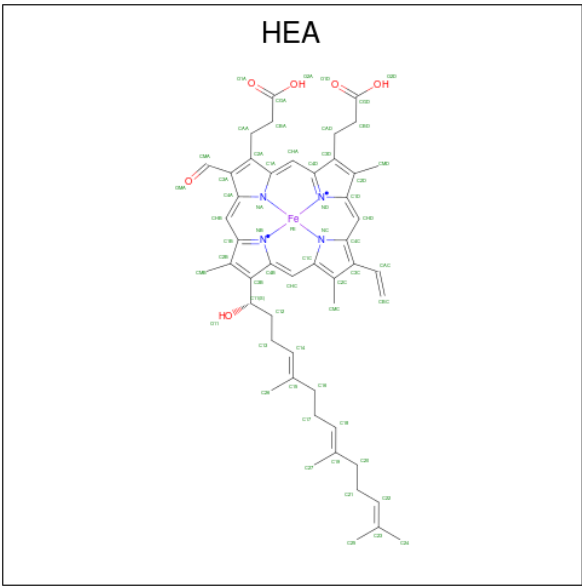
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 87  | 4A    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4A    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4A    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4B    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |
| 87  | 4C    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|
| 87  | 4C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 4G    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 4J    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 4K    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 4L    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 4M    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8A    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8A    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8A    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8B    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8B    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8C    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8G    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8J    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8K    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |
| 87  | 8L    | 1        | Total<br>51 | C<br>40 | O<br>10 | P<br>1 | 0       |

- Molecule 88 is HEME-A (CCD ID: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 88  | 4A    | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       |
| 88  | 4A    | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       |
| 88  | 8A    | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       |
| 88  | 8A    | 1        | Total<br>60 | C<br>49 | Fe<br>1 | N<br>4 | O<br>6 | 0       |

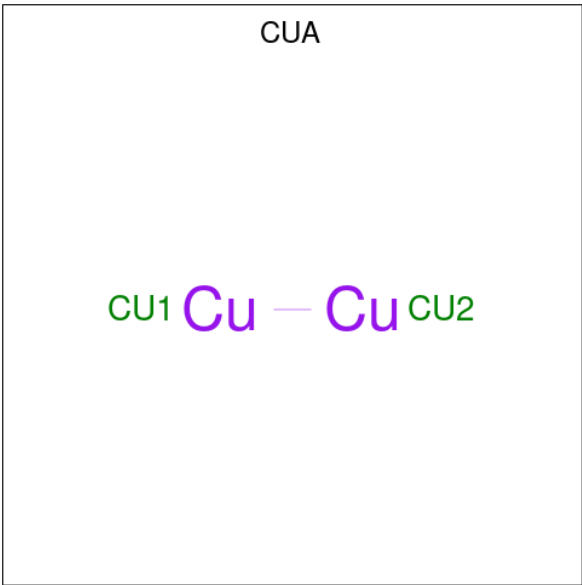
- Molecule 89 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 89  | 4A    | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |
| 89  | 8A    | 1        | Total | Cu | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

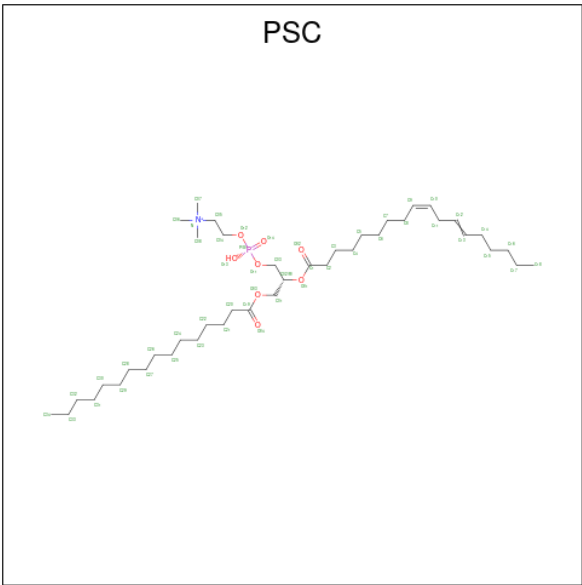
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 90  | 4A    | 1        | Total | Na | 0       |
|     |       |          | 1     | 1  |         |
| 90  | 8A    | 1        | Total | Na | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 91 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 91  | 4B    | 1        | Total | Cu | 0       |
|     |       |          | 2     | 2  |         |
| 91  | 8B    | 1        | Total | Cu | 0       |
|     |       |          | 2     | 2  |         |

- Molecule 92 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



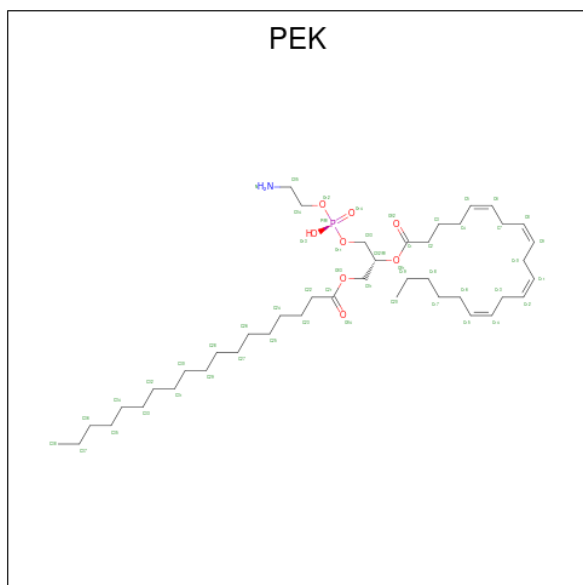
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 92  | 4B    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

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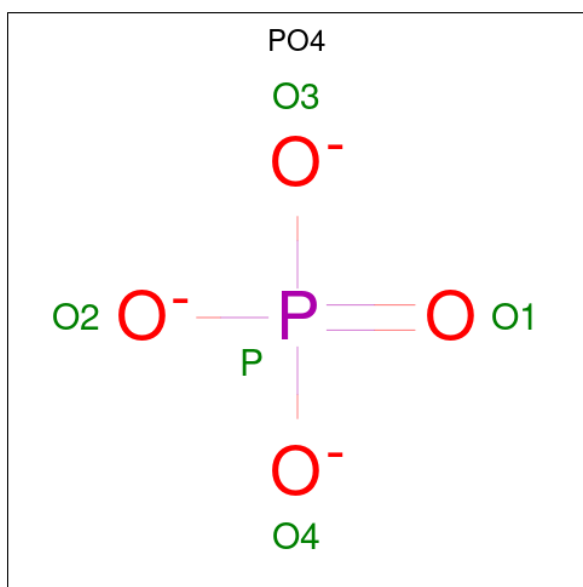
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 92  | 8B    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |

- Molecule 93 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



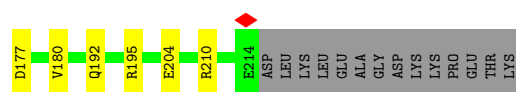
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 93  | 4C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 93  | 4G    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |
| 93  | 8C    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 52    | 42 | 1 | 8 | 1 |         |
| 93  | 8G    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 53    | 43 | 1 | 8 | 1 |         |

- Molecule 94 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).

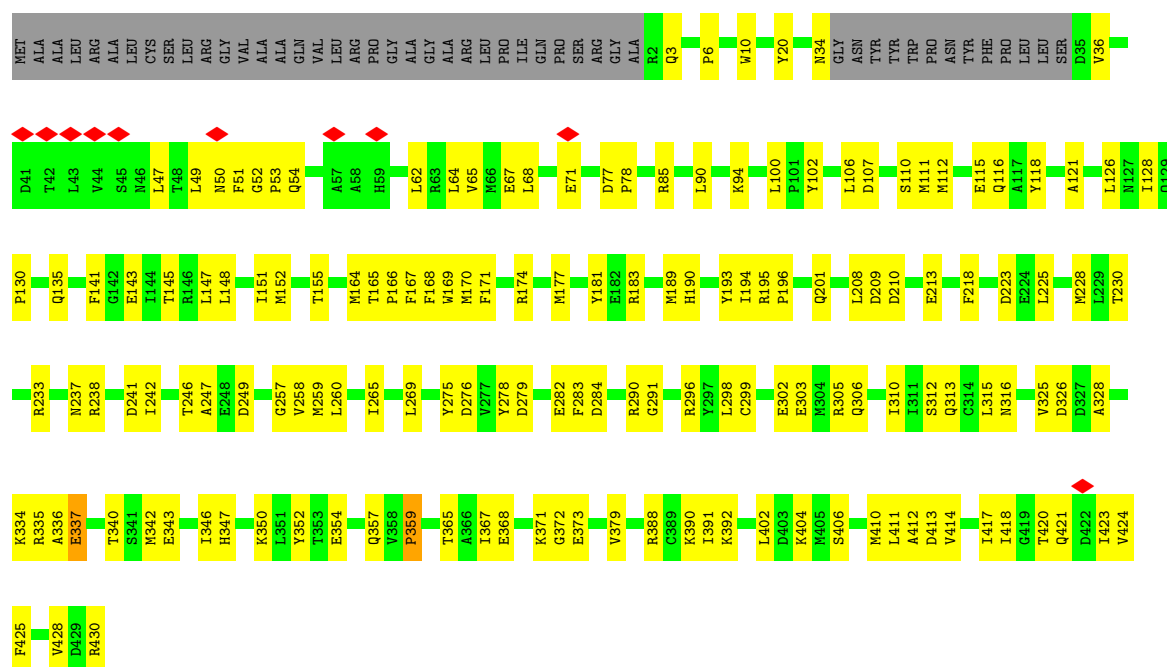


| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 94  | 4H    | 1        | Total | O | P | 0       |
|     |       |          | 5     | 4 | 1 |         |
| 94  | 8H    | 1        | Total | O | P | 0       |
|     |       |          | 5     | 4 | 1 |         |

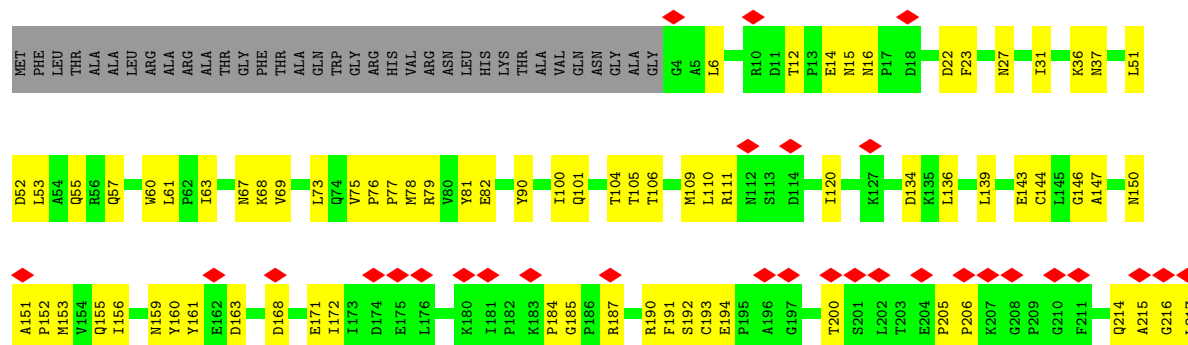




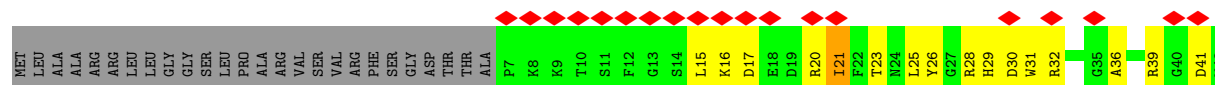
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

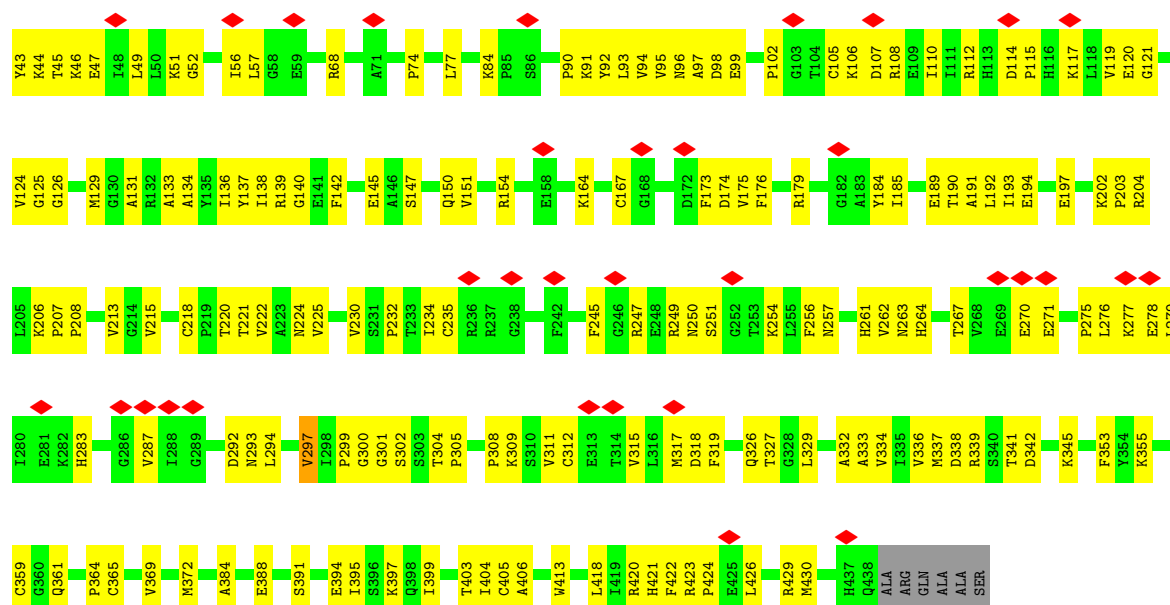


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



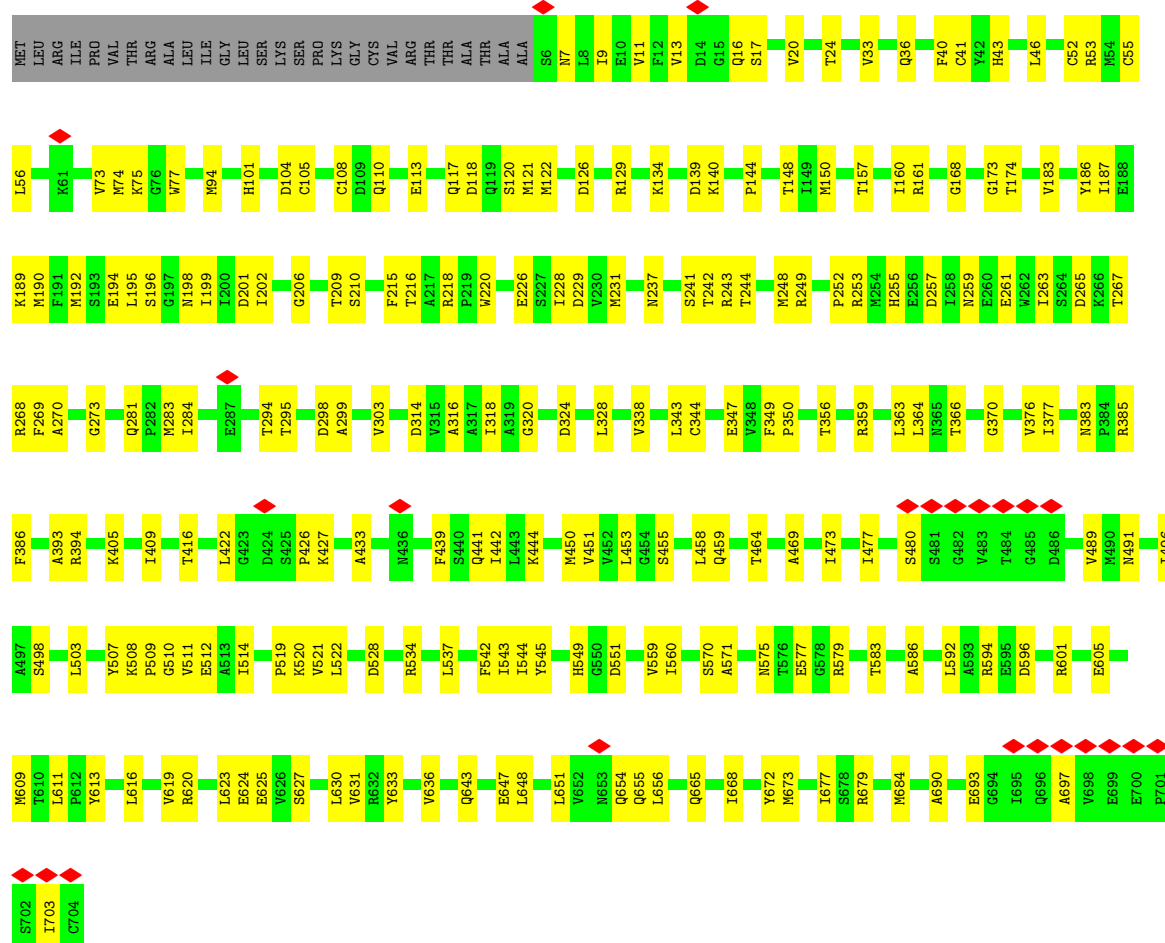
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



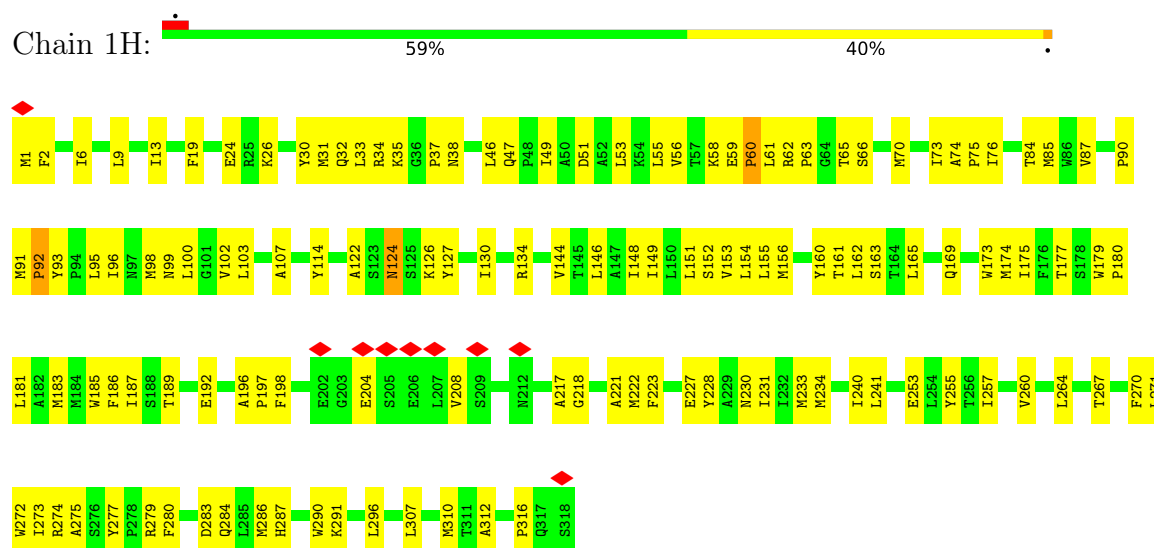


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

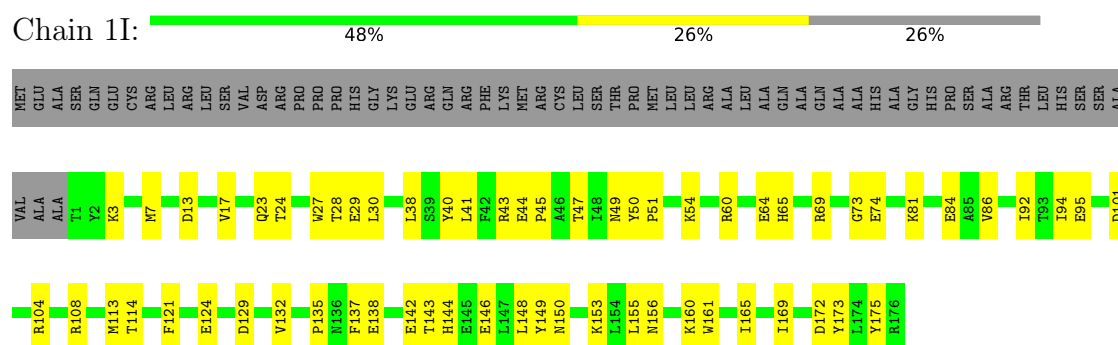
Chain 1G: 66% 30%



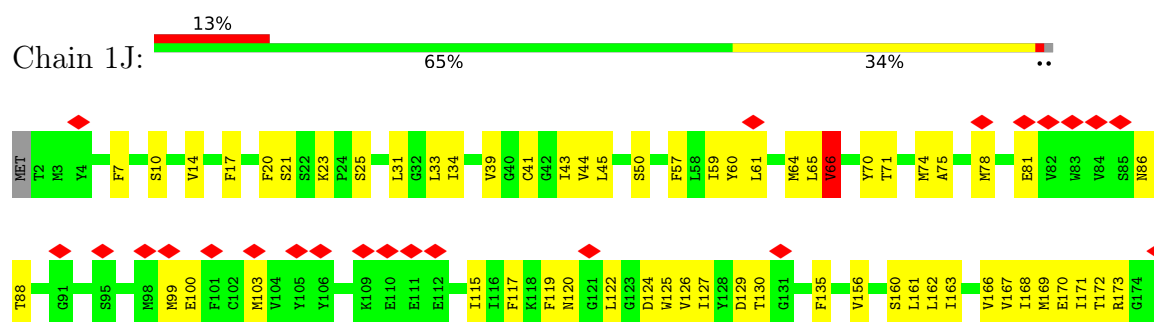
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1



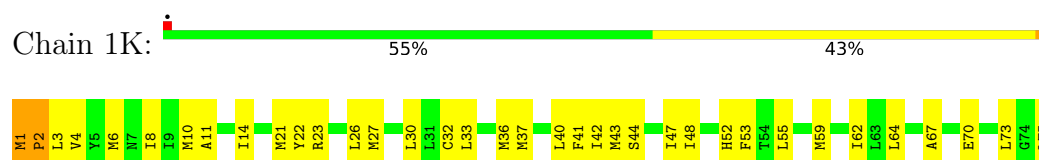
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

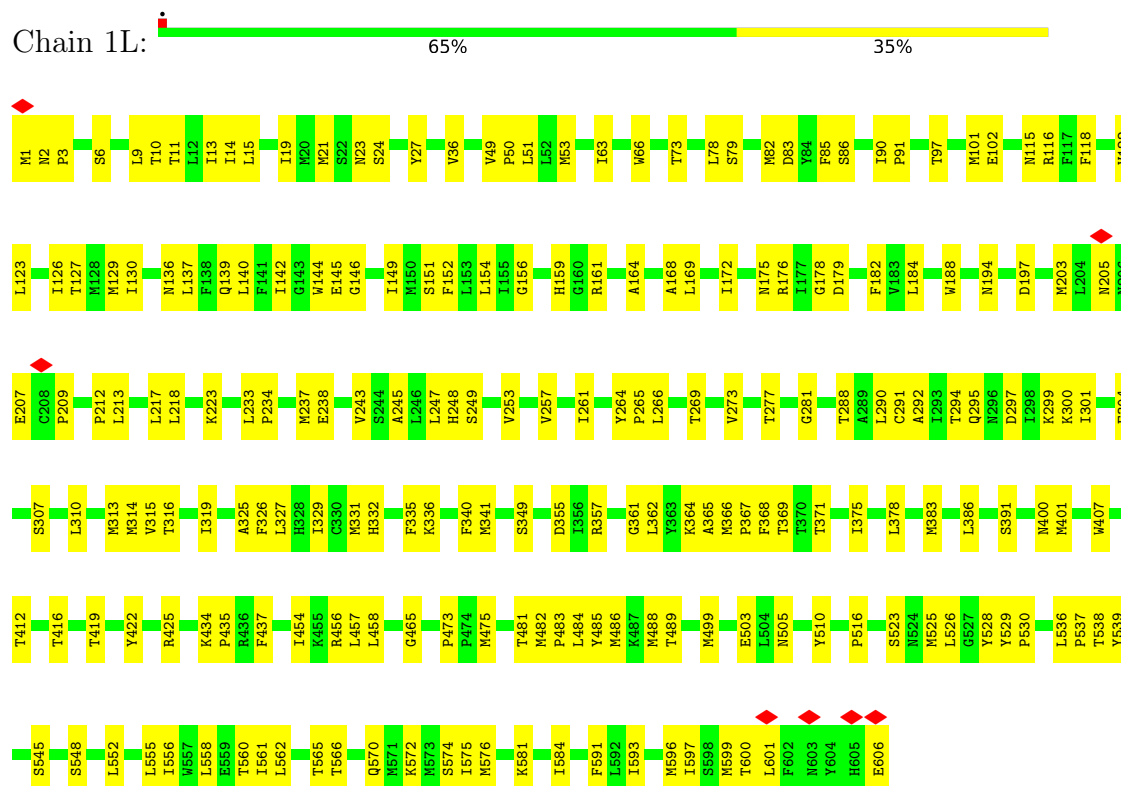


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

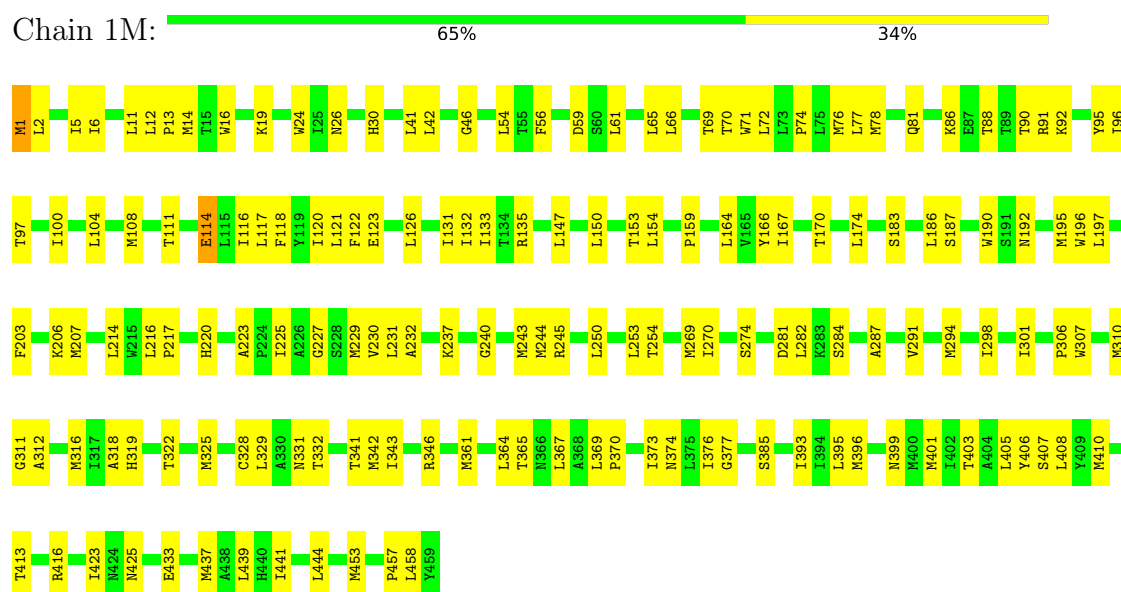




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

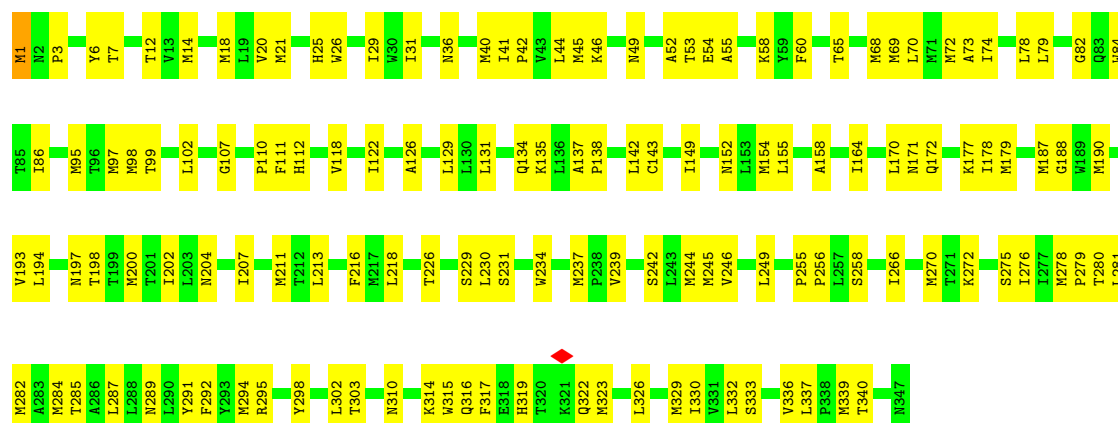


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



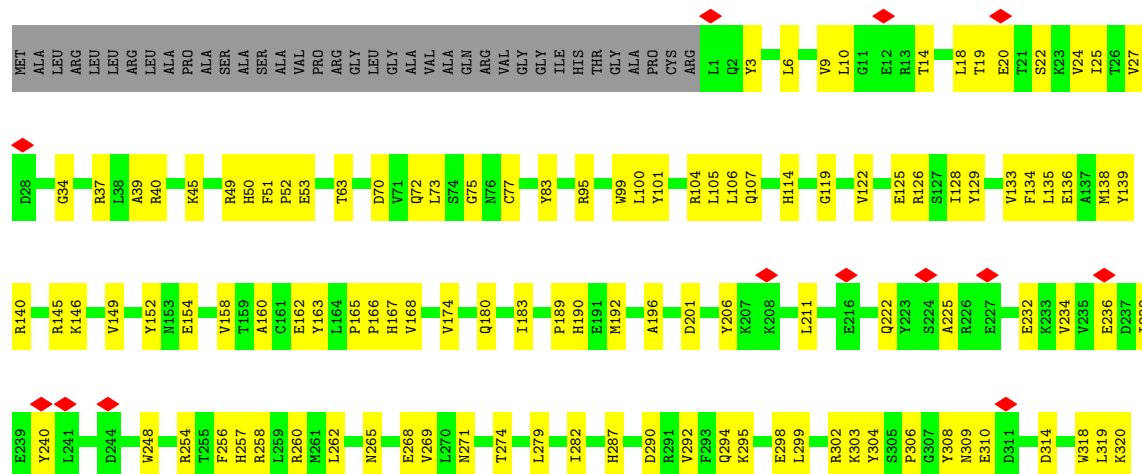
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:  60% 40%



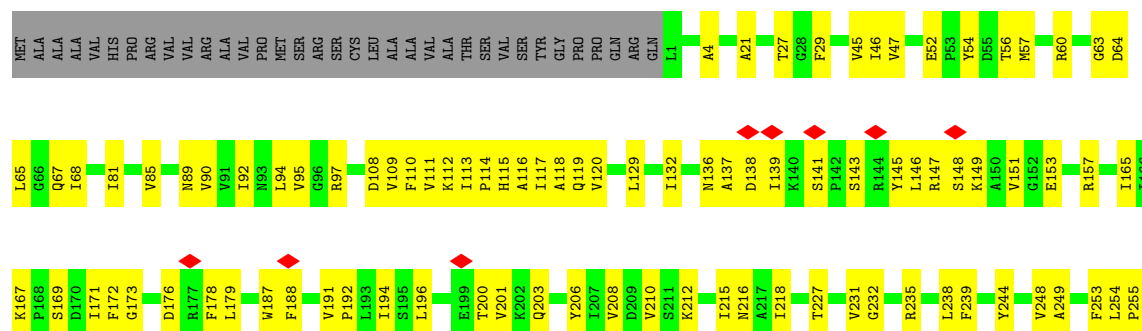
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:  58% 32% 10%



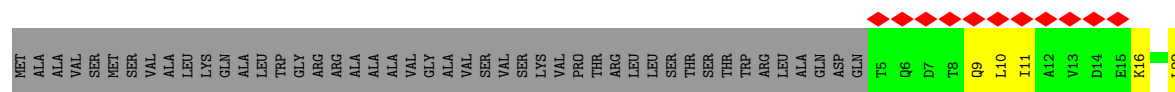
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:  60% 31% 9%





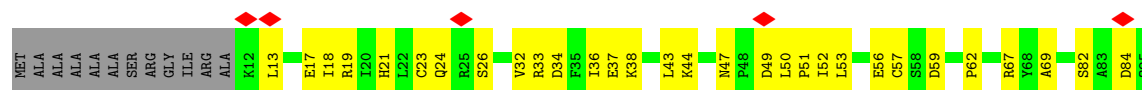
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



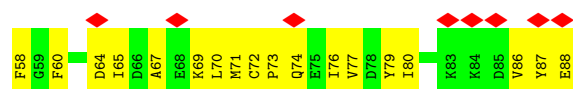
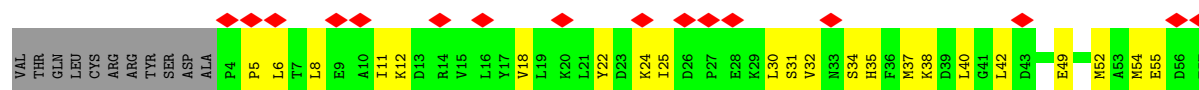
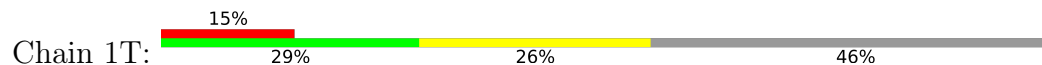
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



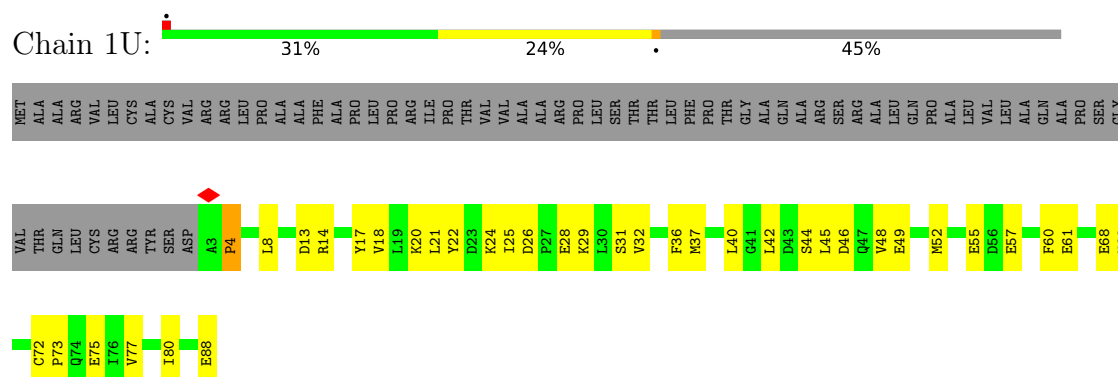
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



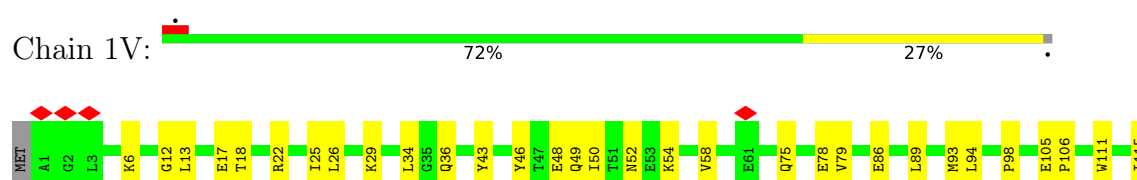
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



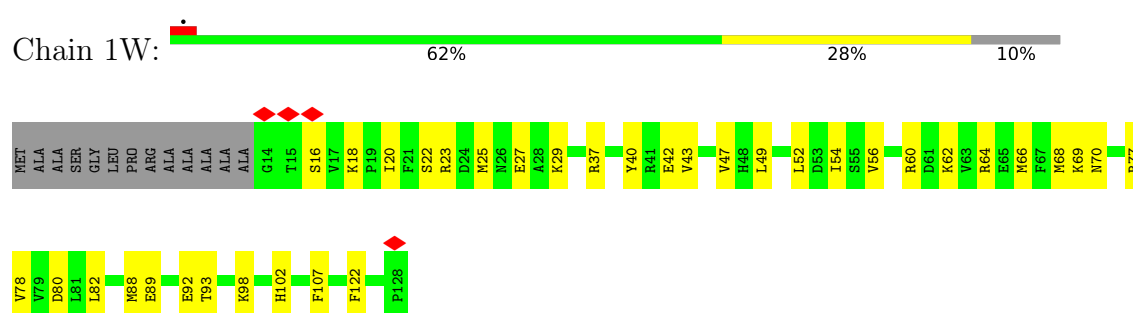
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



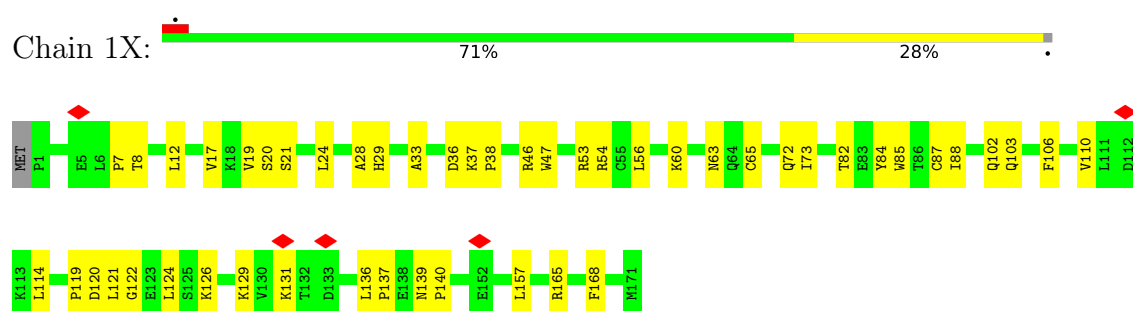
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



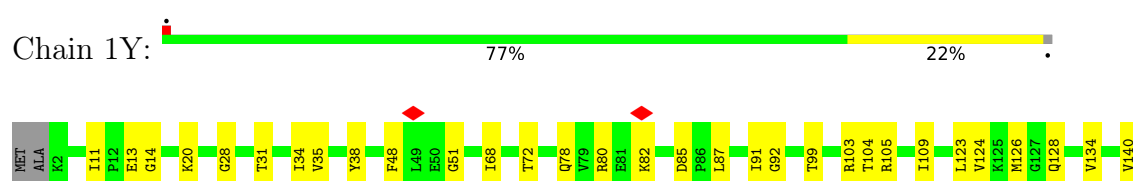
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



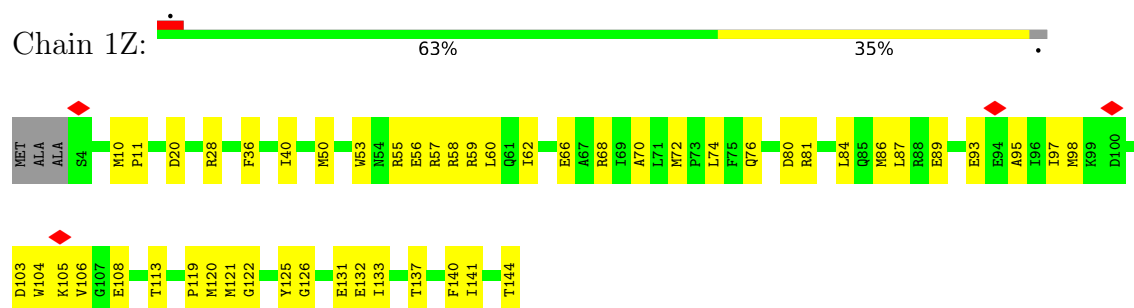
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



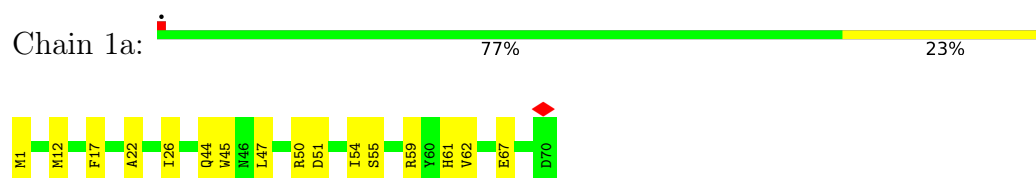
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



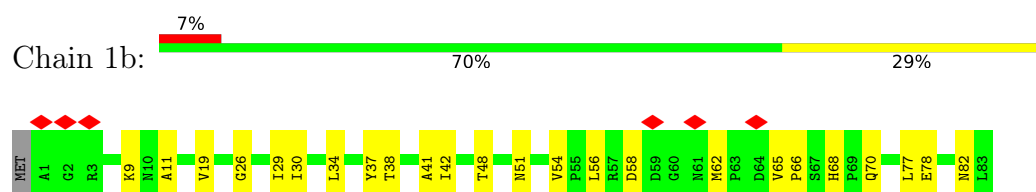
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



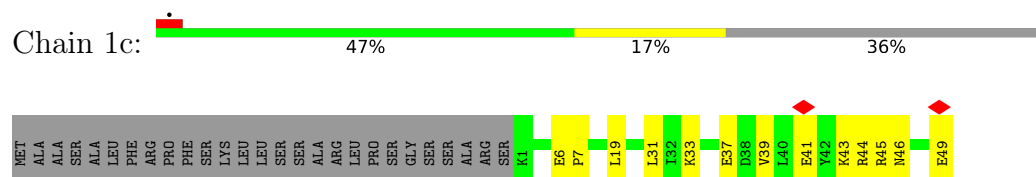
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



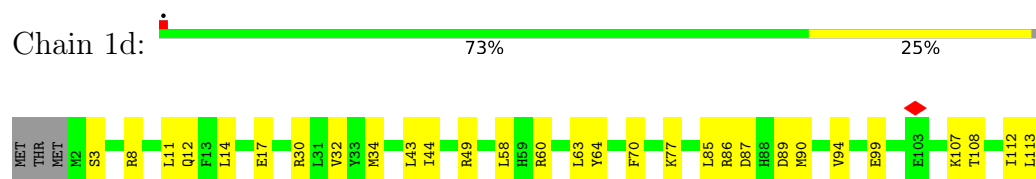
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



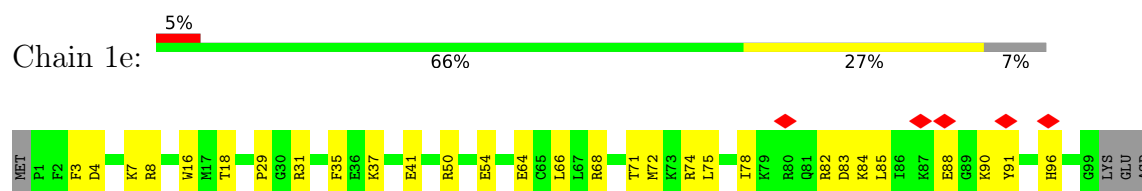
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

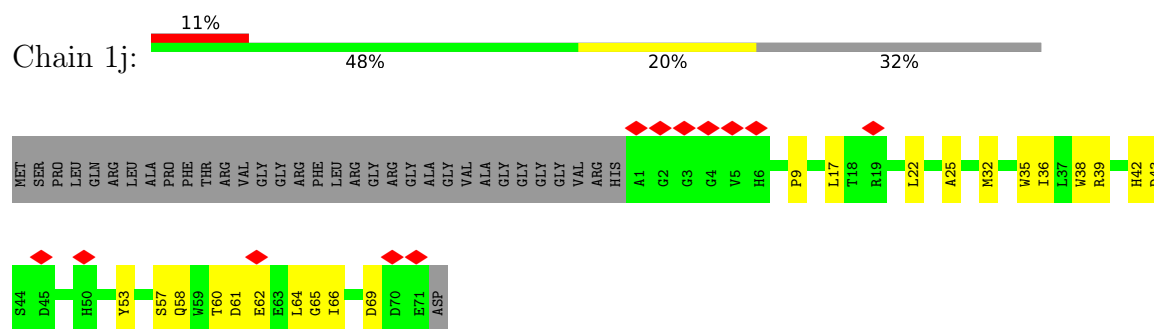


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

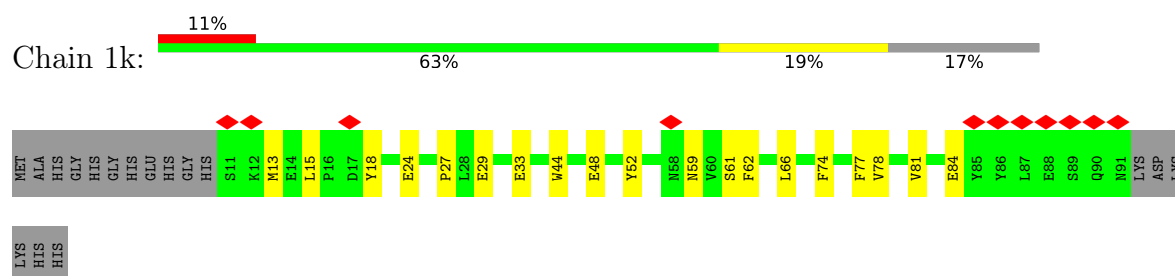




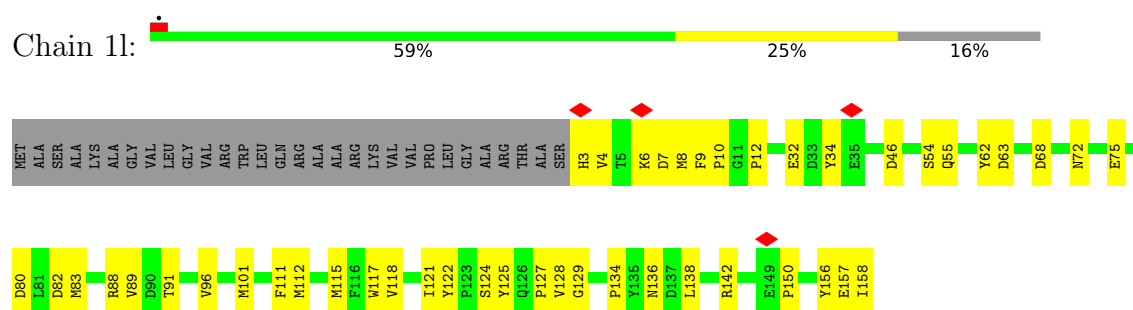
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



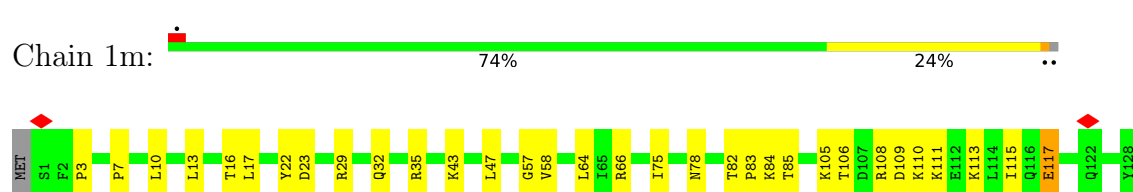
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



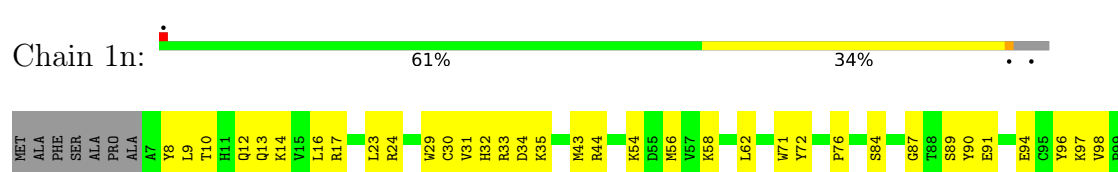
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

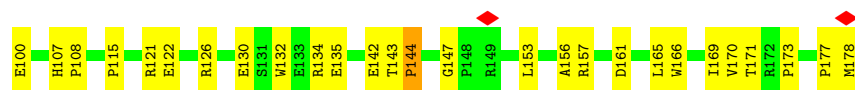


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

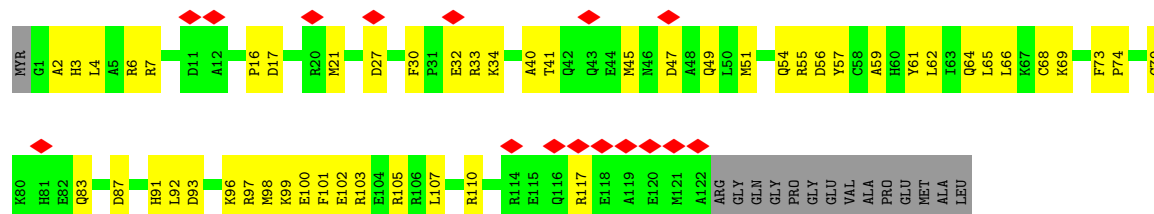


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

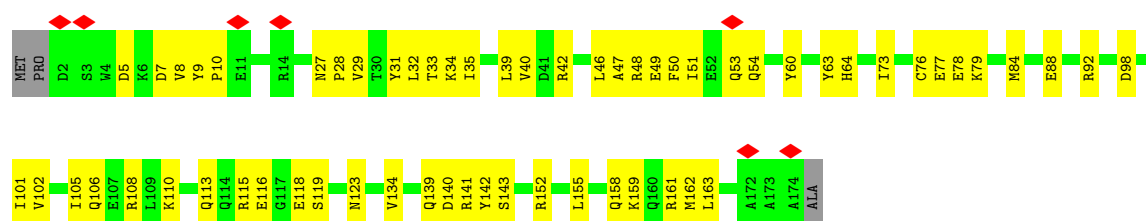




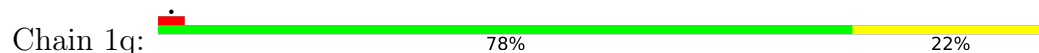
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



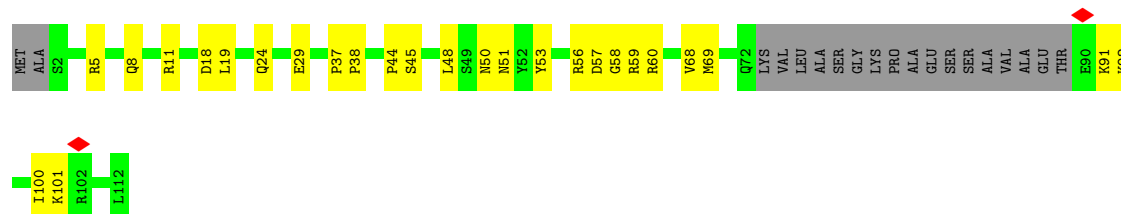
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

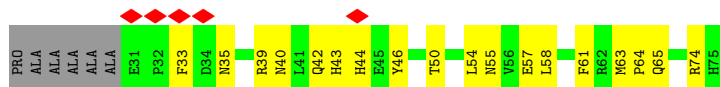


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

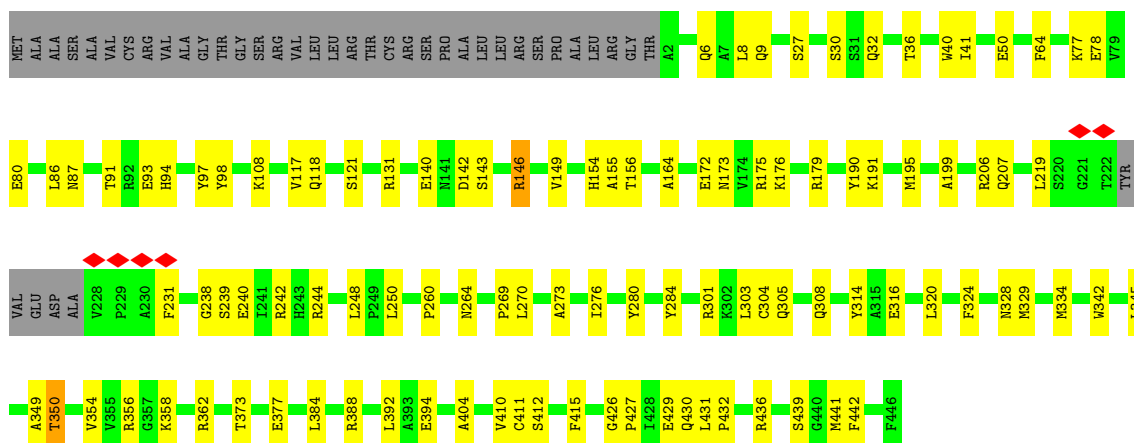


- Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

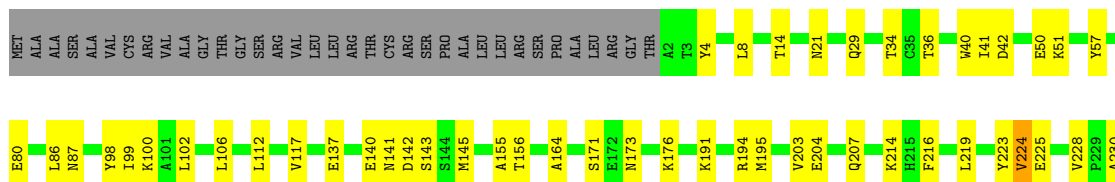


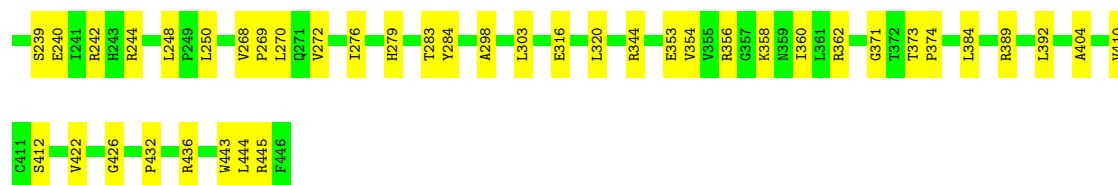


- Chain 3A:  70% 21% 8%



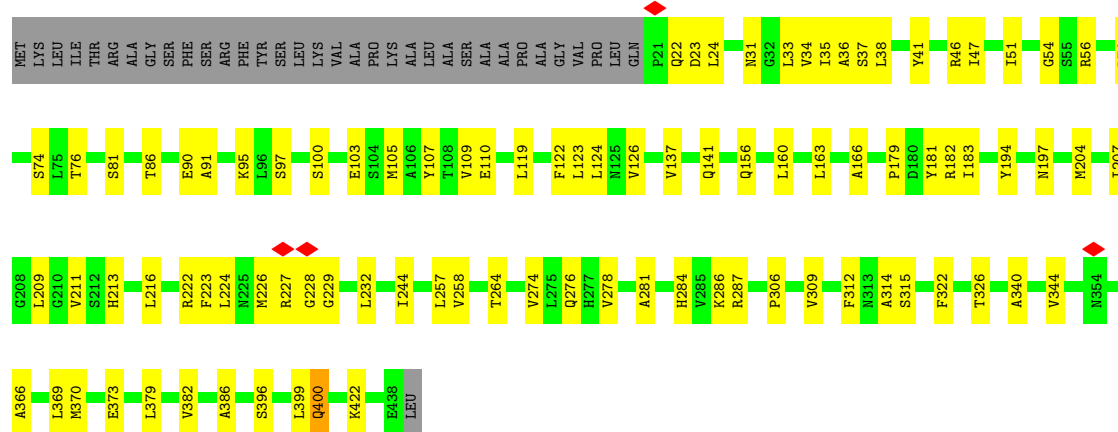
- Chain 3N:  74% 19% 7%





- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 72% 21% 8%



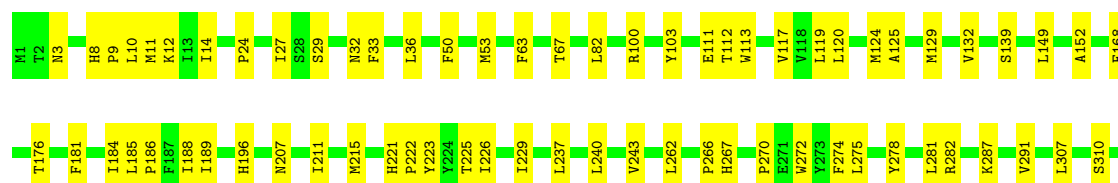
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O: 72% 20% 8%



- Molecule 47: Cytochrome b

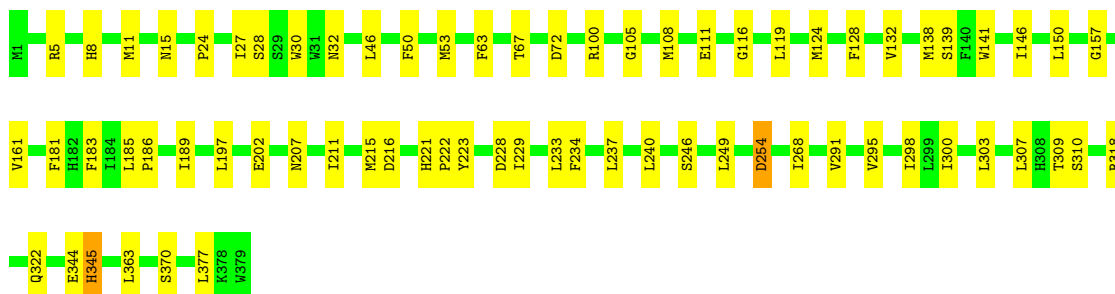
Chain 3C: 79% 21%





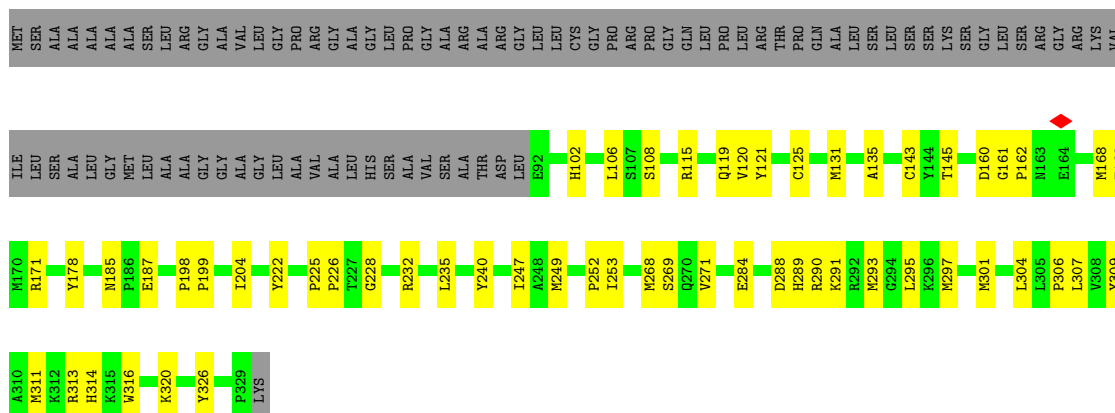
• Molecule 47: Cytochrome b

Chain 3P: 82% 18%



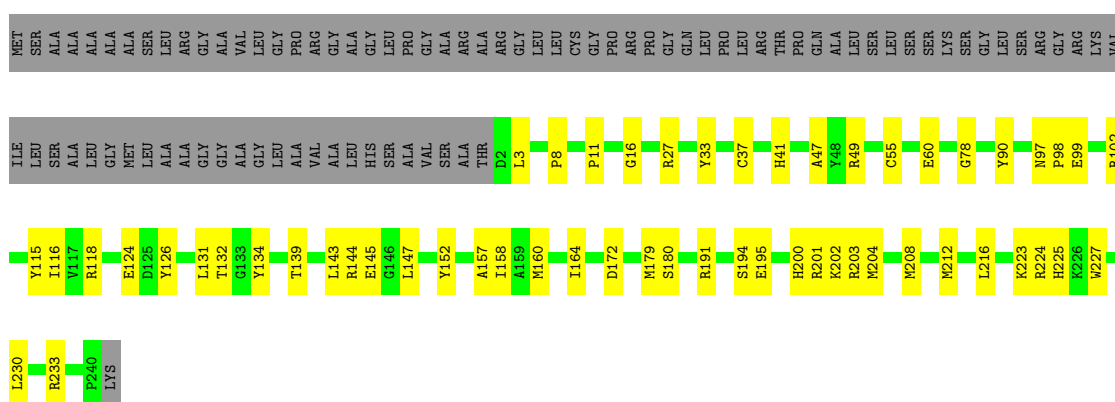
• Molecule 48: Cytochrome c1

Chain 3D: 55% 17% 27%

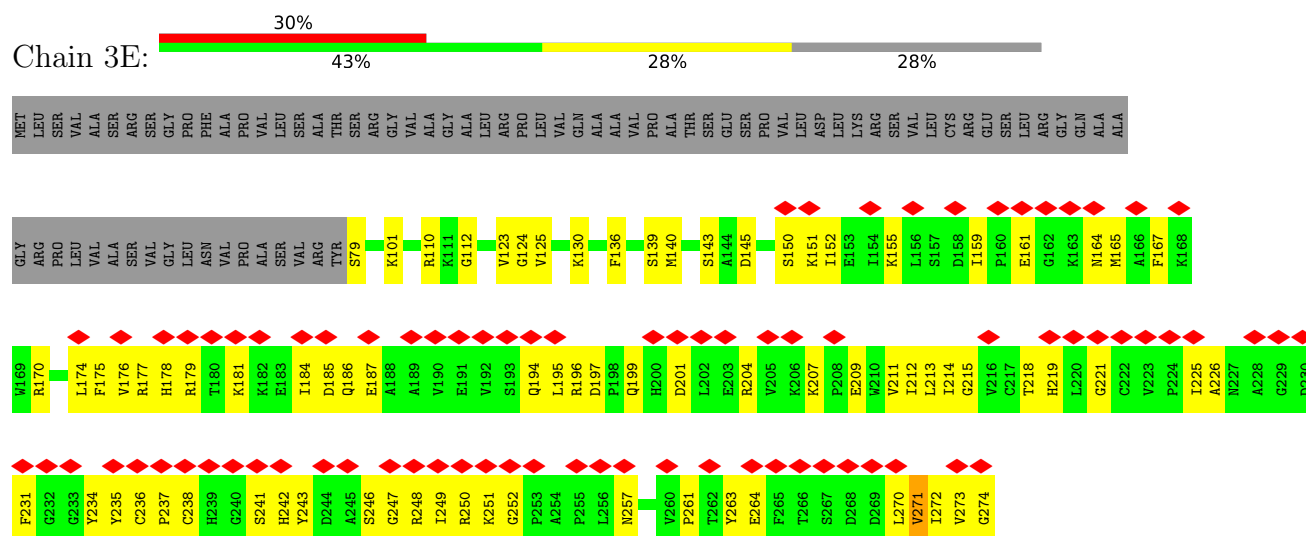


• Molecule 48: Cytochrome c1

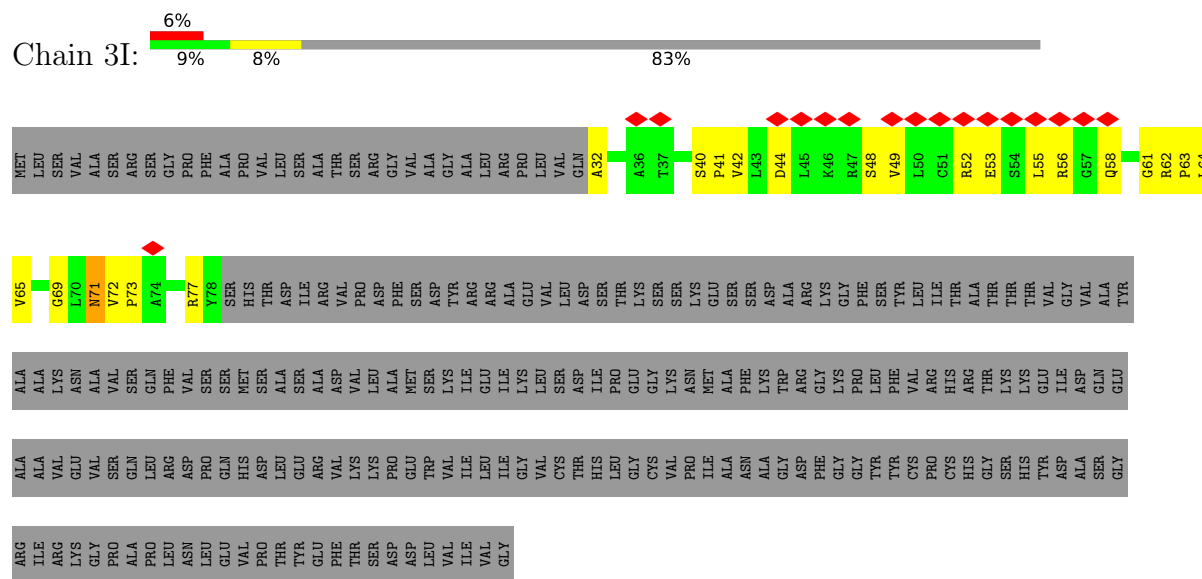
Chain 3Q: 56% 17% 27%



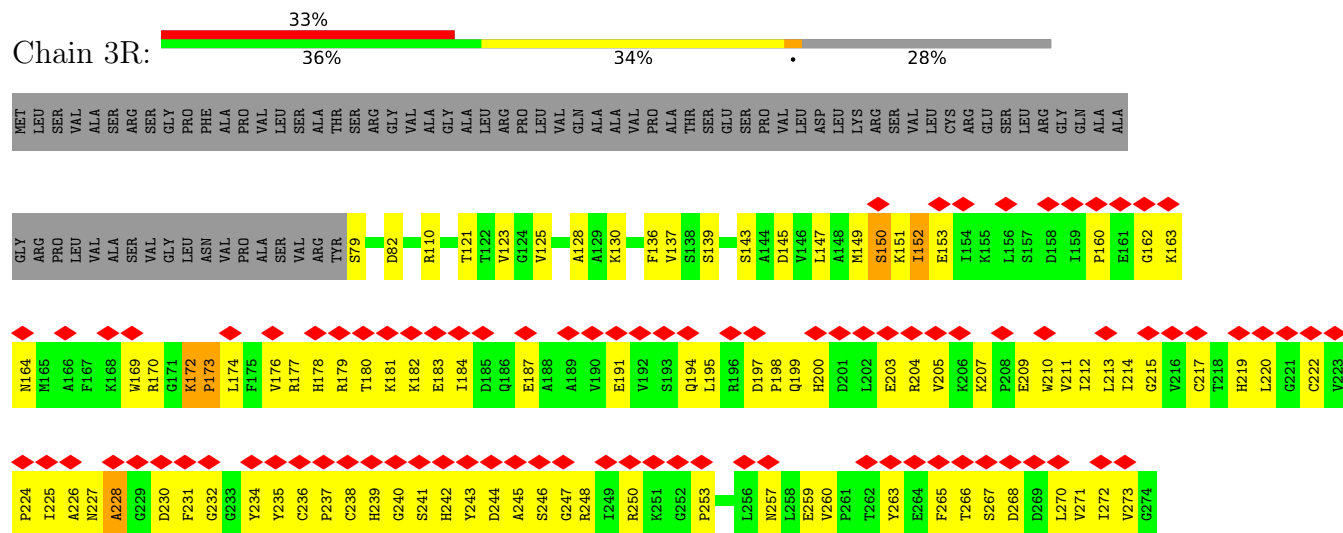
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



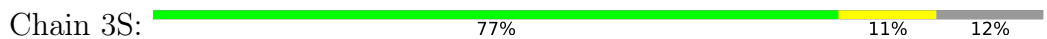
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

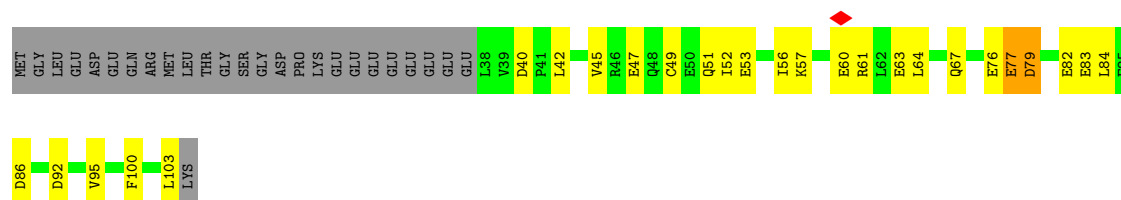


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



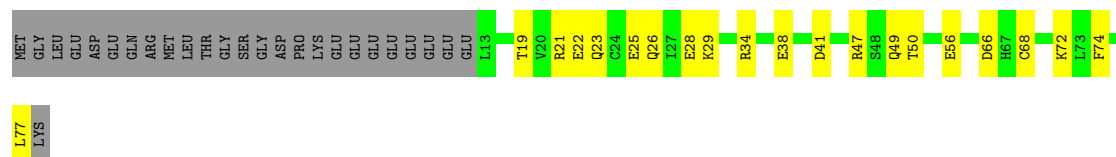
- Chain 3V:  5% 5% 89%





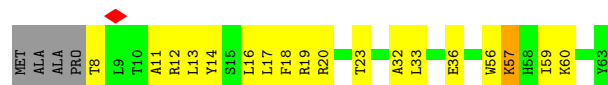
- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U: 49% 22% 29%



- Molecule 53: Complex III subunit 9

Chain 3J: 63% 28% 7%



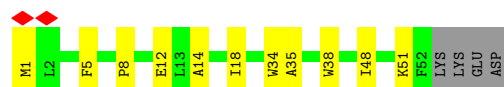
- Molecule 53: Complex III subunit 9

Chain 3W: 72% 22% 7%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X: 73% 20% 7%



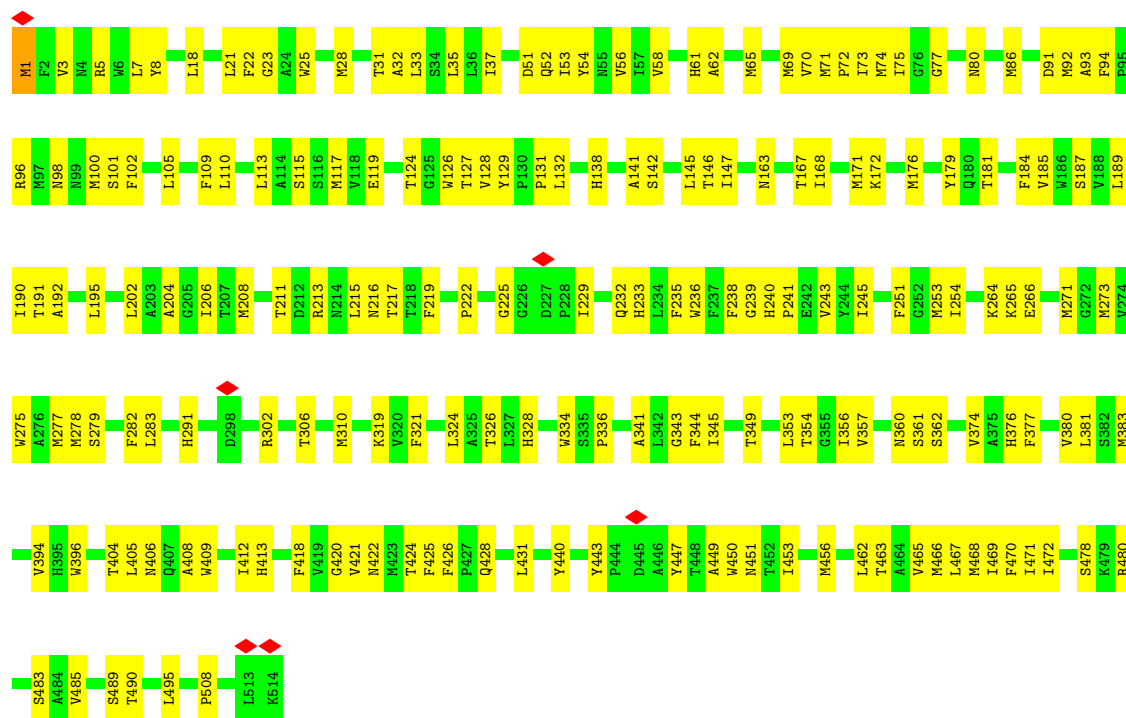
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y: 64% 27% 9%

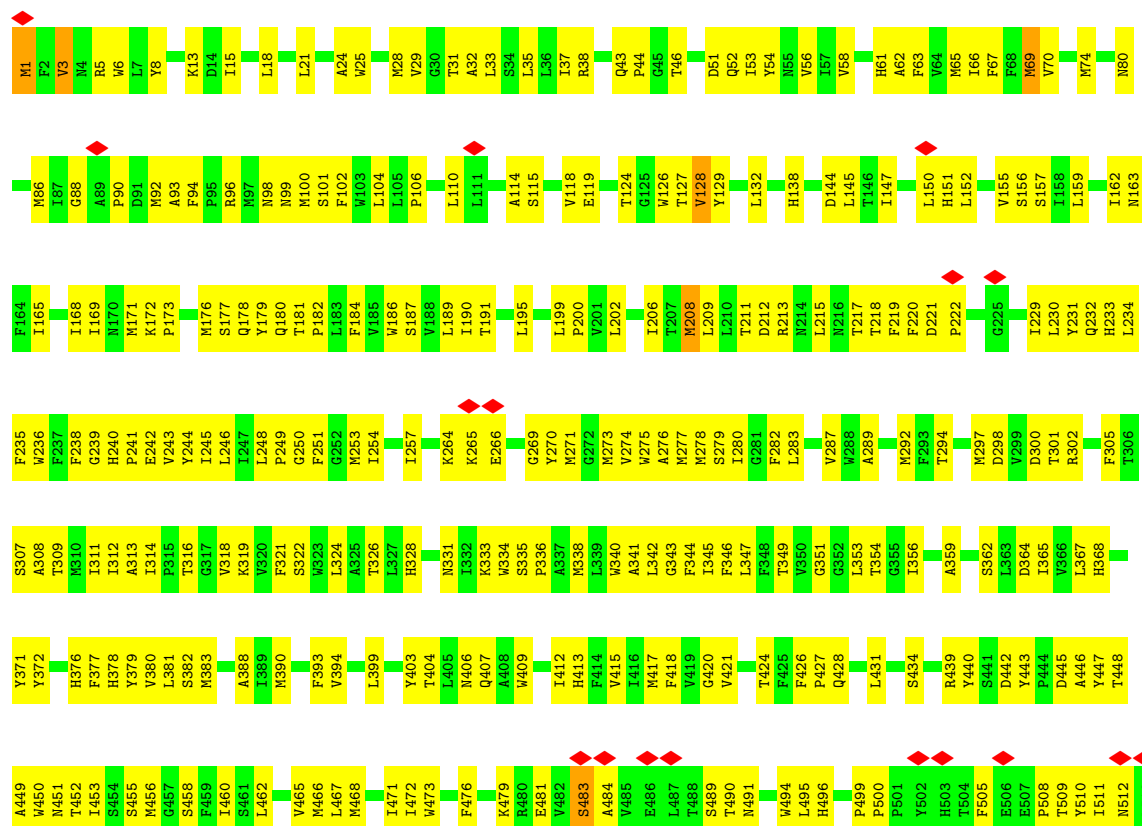


- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A: 63% 37%



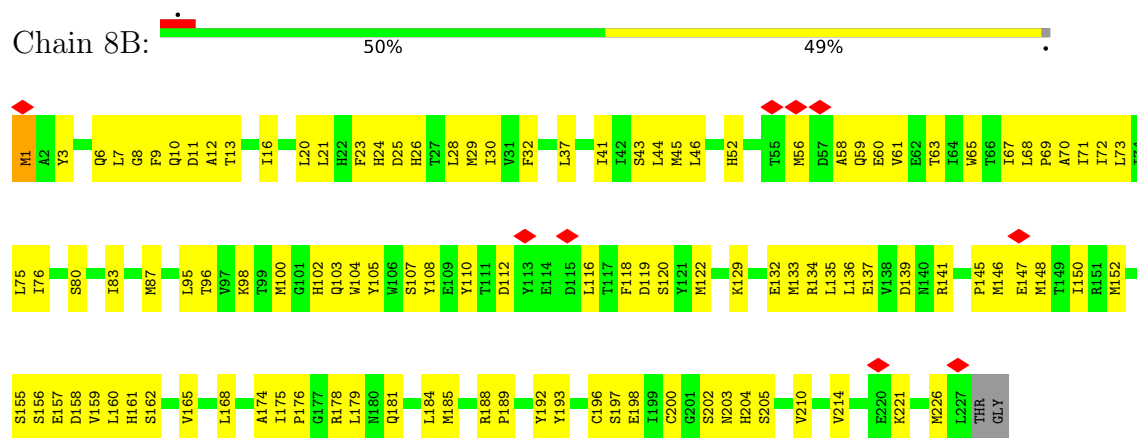
• Molecule 55: Cytochrome c oxidase subunit 1



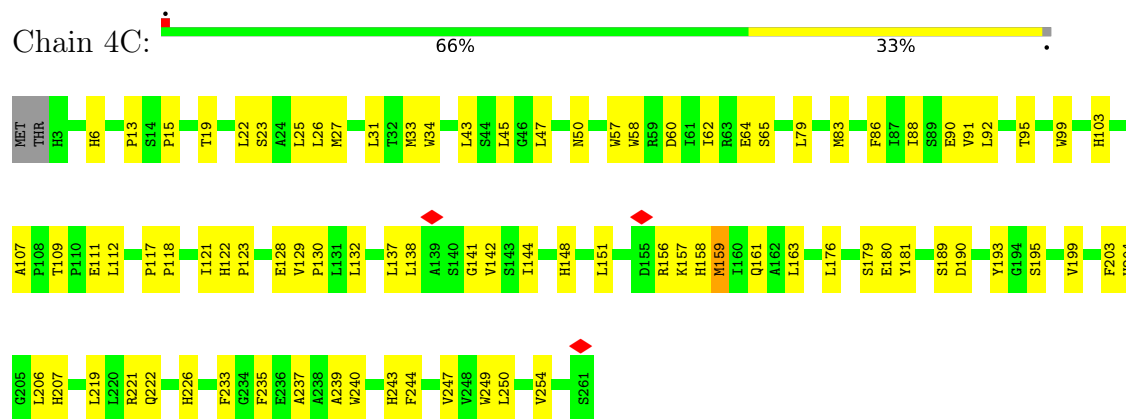
- Molecule 56: Cytochrome c oxidase subunit 2



- Molecule 56: Cytochrome c oxidase subunit 2

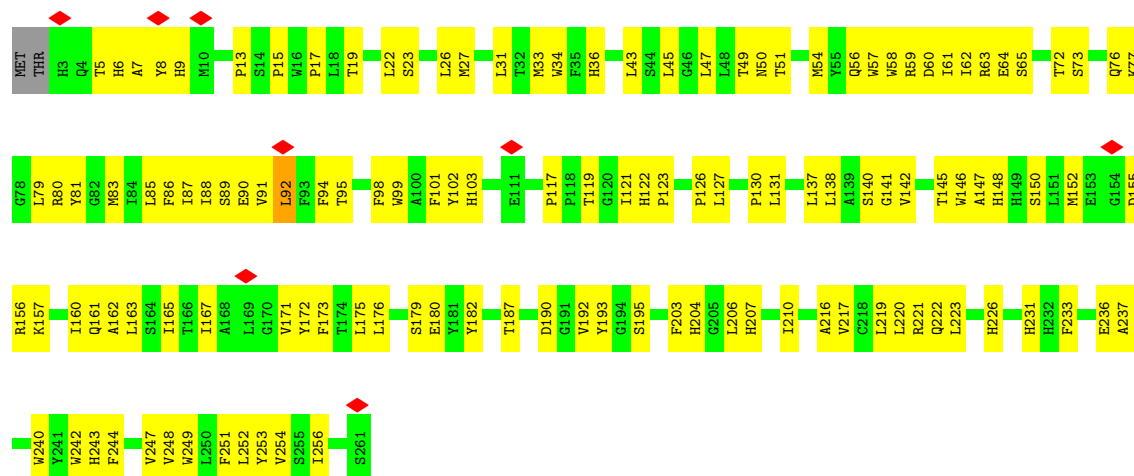


- Molecule 57: Cytochrome c oxidase subunit 3

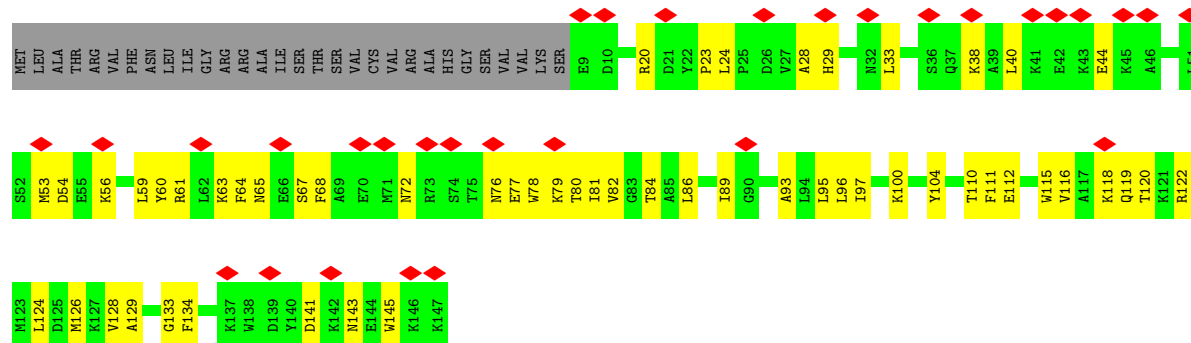


- Molecule 57: Cytochrome c oxidase subunit 3

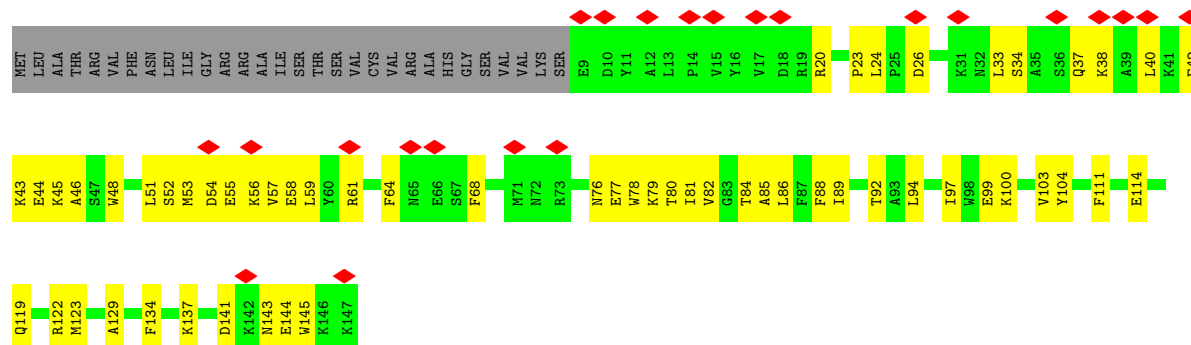




• Molecule 58: Cytochrome c oxidase subunit 4

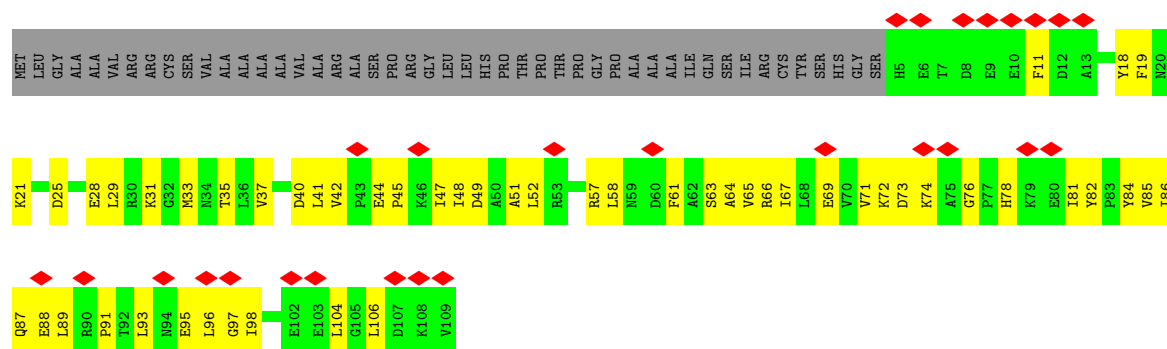


• Molecule 58: Cytochrome c oxidase subunit 4

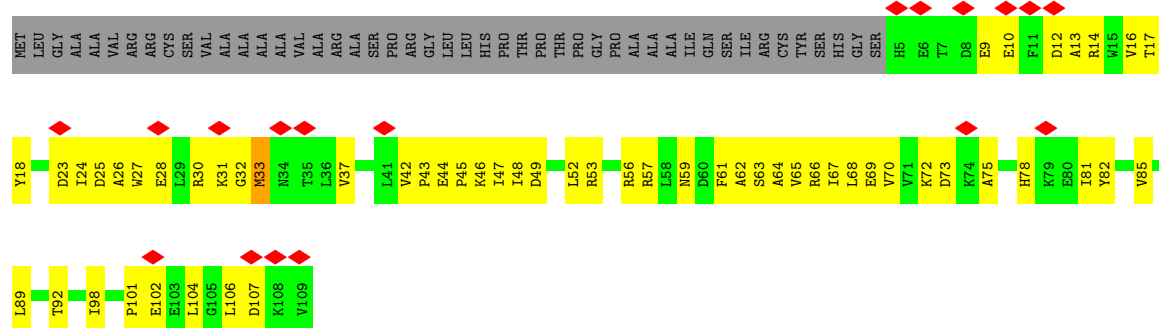


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

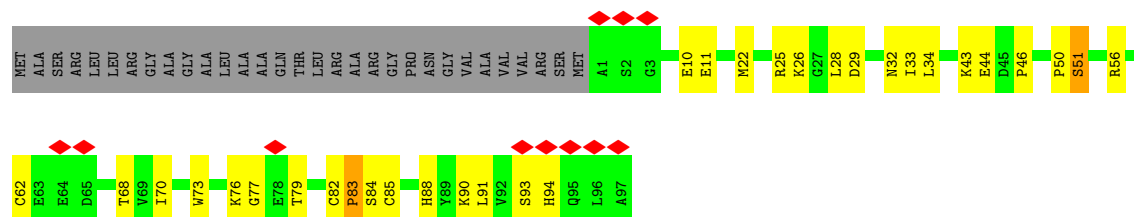




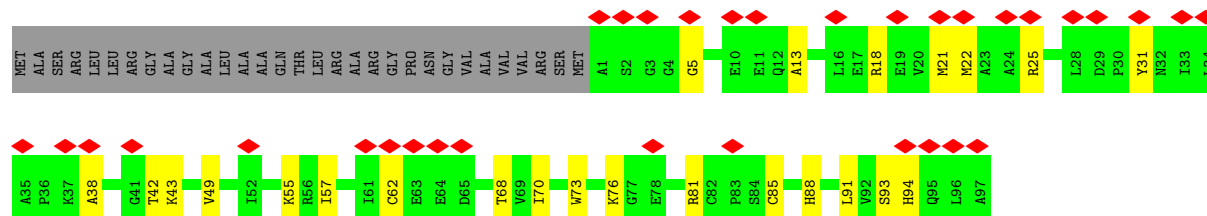
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



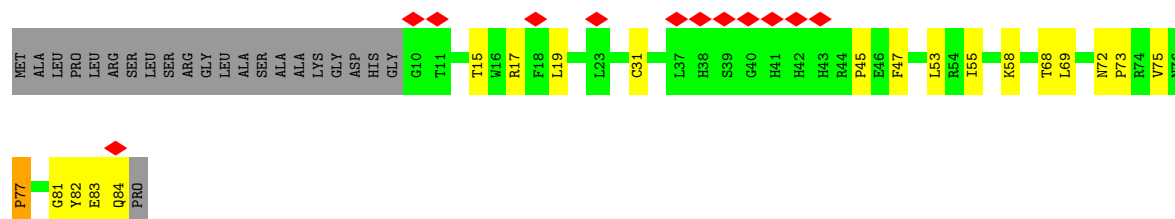
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



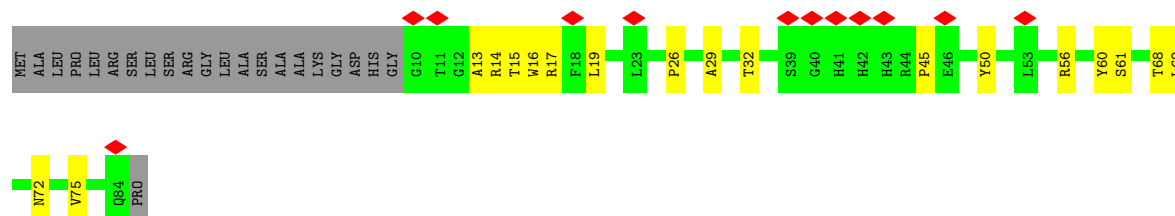
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial



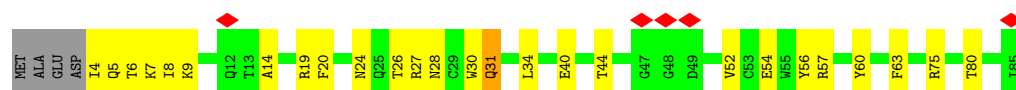
- Molecule 61: Cytochrome c oxidase subunit 6A2



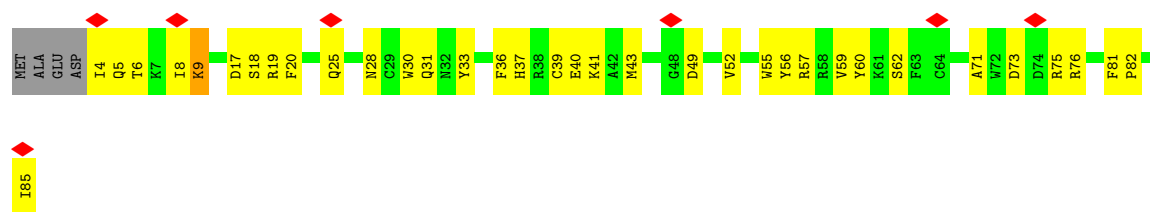
• Molecule 61: Cytochrome c oxidase subunit 6A2



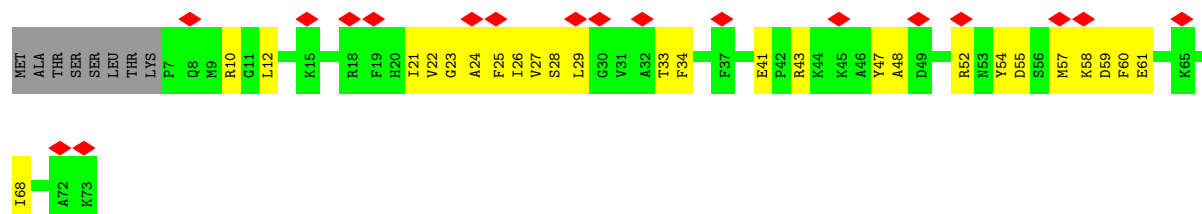
• Molecule 62: Cytochrome c oxidase subunit 6B1



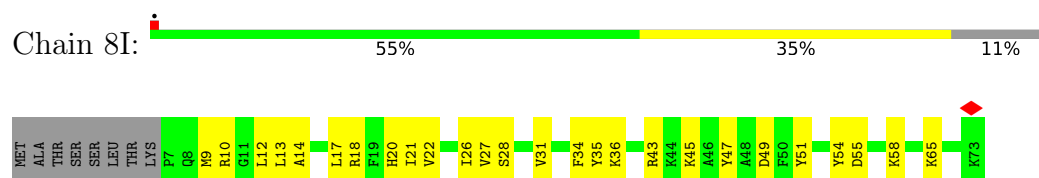
• Molecule 62: Cytochrome c oxidase subunit 6B1



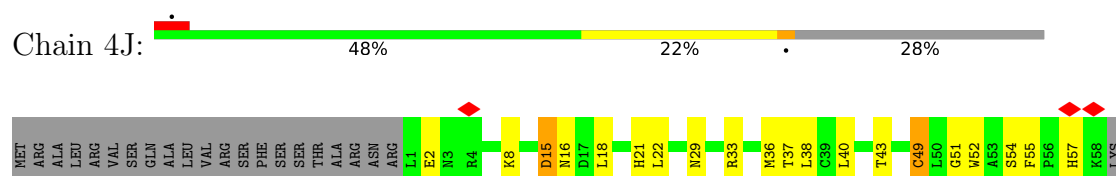
• Molecule 63: Cytochrome c oxidase subunit 6C



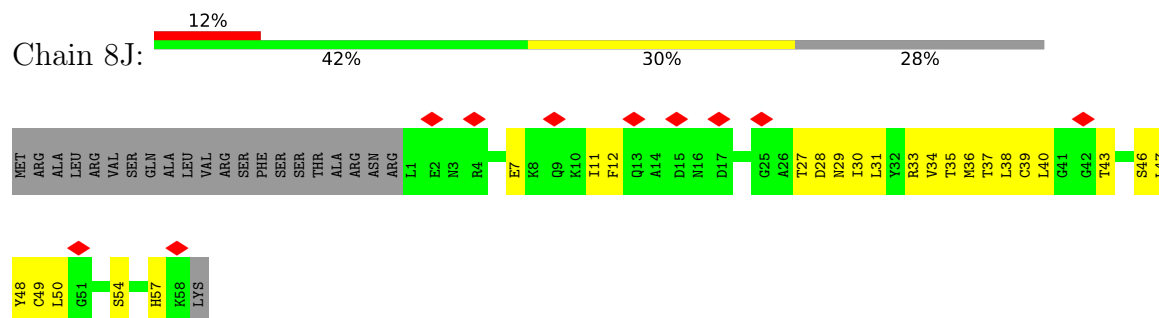
- Molecule 63: Cytochrome c oxidase subunit 6C



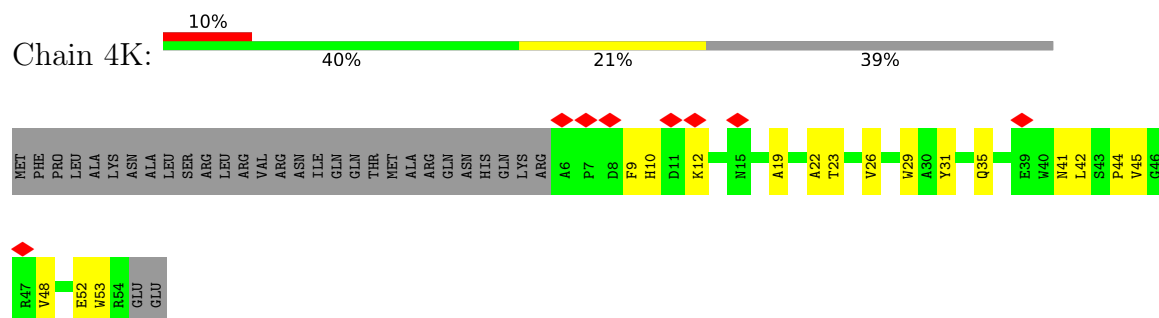
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



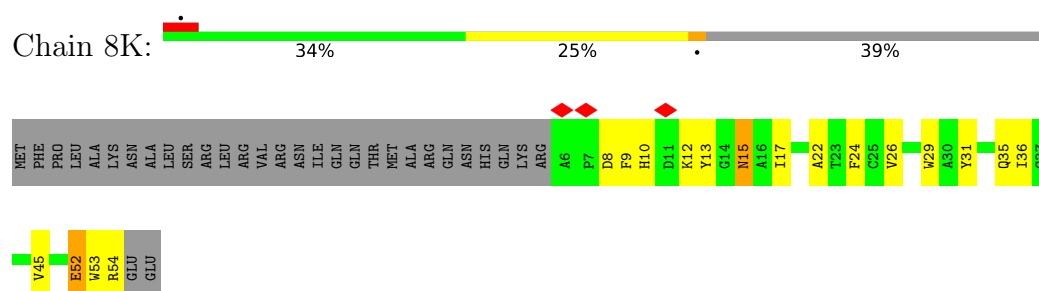
- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



- Molecule 65: Cytochrome c oxidase subunit 7B



- Molecule 65: Cytochrome c oxidase subunit 7B



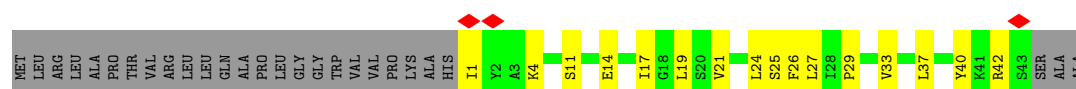
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



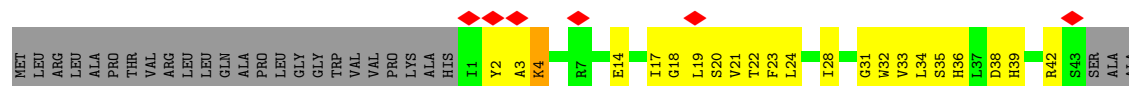
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



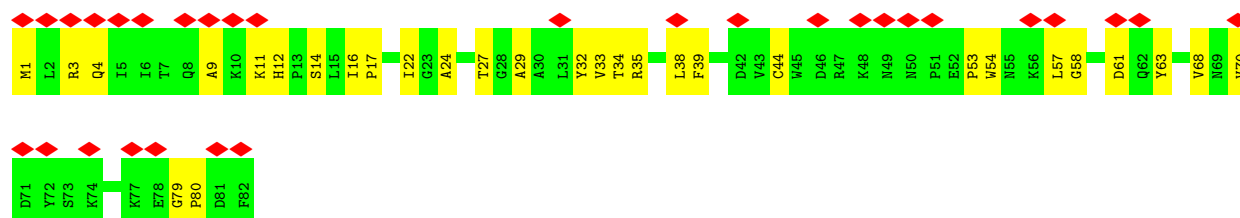
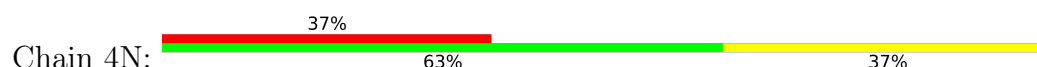
- Molecule 67: Cytochrome c oxidase subunit 8



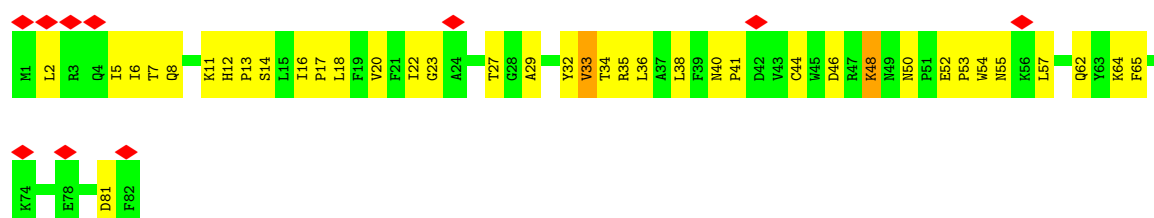
- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



- Molecule 68: Cytochrome c oxidase subunit NDUFA4



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 320000                                  | 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)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOQUANTUM (6k x 4k)           | Depositor |
| Maximum map value                    | 1.149                                   | Depositor |
| Minimum map value                    | 0.000                                   | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.017                                   | Depositor |
| Recommended contour level            | 0.12                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 572.0, 572.0, 572.0                     | wwPDB     |
| Map dimensions                       | 550, 550, 550                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.04, 1.04, 1.04                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, FES, FMN, NDP, 3PE, HEC, ZN, PSC, GTP, CUA, EHZ, MG, AME, PC1, PO4, PEK, SF4, NA, CU, CHD, FME, CDL, PGV, HEA, MYR, HEM, ACE, AYA

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   | 1A    | 0.21         | 0/930         | 0.43        | 0/1271        |
| 2   | 1B    | 0.18         | 0/1273        | 0.39        | 0/1722        |
| 3   | 1C    | 0.12         | 0/1791        | 0.31        | 0/2439        |
| 4   | 1D    | 0.18         | 1/3545 (0.0%) | 0.33        | 0/4806        |
| 5   | 1E    | 0.16         | 0/1698        | 0.37        | 0/2311        |
| 6   | 1F    | 0.16         | 0/3401        | 0.36        | 0/4595        |
| 7   | 1G    | 0.14         | 0/5451        | 0.35        | 0/7387        |
| 8   | 1H    | 0.24         | 0/2566        | 0.42        | 2/3509 (0.1%) |
| 9   | 1I    | 0.12         | 0/1443        | 0.31        | 0/1952        |
| 10  | 1J    | 0.17         | 0/1364        | 0.44        | 0/1850        |
| 11  | 1K    | 0.16         | 0/751         | 0.38        | 0/1018        |
| 12  | 1L    | 0.16         | 0/4939        | 0.36        | 0/6718        |
| 13  | 1M    | 0.15         | 0/3713        | 0.34        | 0/5063        |
| 14  | 1N    | 0.29         | 1/2765 (0.0%) | 0.41        | 1/3758 (0.0%) |
| 15  | 1O    | 0.14         | 0/2650        | 0.34        | 0/3588        |
| 16  | 1P    | 0.15         | 0/2828        | 0.34        | 0/3834        |
| 17  | 1Q    | 0.15         | 0/1070        | 0.36        | 0/1446        |
| 18  | 1R    | 0.14         | 0/755         | 0.32        | 0/1018        |
| 19  | 1S    | 0.17         | 0/711         | 0.44        | 0/956         |
| 20  | 1T    | 0.18         | 0/701         | 0.43        | 0/946         |
| 20  | 1U    | 0.29         | 0/706         | 0.47        | 1/954 (0.1%)  |
| 21  | 1V    | 0.17         | 0/946         | 0.33        | 0/1281        |
| 22  | 1W    | 0.17         | 0/995         | 0.36        | 0/1340        |
| 23  | 1X    | 0.14         | 0/1436        | 0.39        | 0/1938        |
| 24  | 1Y    | 0.11         | 0/1037        | 0.25        | 0/1404        |
| 25  | 1Z    | 0.16         | 0/1199        | 0.31        | 0/1617        |
| 26  | 1a    | 0.14         | 0/577         | 0.38        | 0/777         |
| 27  | 1b    | 0.16         | 0/664         | 0.36        | 0/912         |
| 28  | 1c    | 0.14         | 0/430         | 0.32        | 0/581         |
| 29  | 1d    | 0.11         | 0/1016        | 0.27        | 0/1374        |
| 30  | 1e    | 0.15         | 0/836         | 0.37        | 0/1118        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 31  | 1f    | 0.17         | 0/499         | 0.44        | 0/673         |
| 32  | 1g    | 0.16         | 0/858         | 0.39        | 0/1165        |
| 33  | 1h    | 0.16         | 0/1184        | 0.37        | 0/1603        |
| 34  | 1i    | 0.16         | 0/1138        | 0.38        | 0/1551        |
| 35  | 1j    | 0.17         | 0/627         | 0.36        | 0/858         |
| 36  | 1k    | 0.16         | 0/668         | 0.35        | 0/903         |
| 37  | 1l    | 0.15         | 0/1365        | 0.36        | 0/1867        |
| 38  | 1m    | 0.23         | 0/1092        | 0.35        | 0/1481        |
| 39  | 1n    | 0.39         | 2/1549 (0.1%) | 0.62        | 2/2098 (0.1%) |
| 40  | 1o    | 0.16         | 0/1069        | 0.41        | 0/1430        |
| 41  | 1p    | 0.13         | 0/1481        | 0.35        | 0/1997        |
| 42  | 1q    | 0.13         | 0/1253        | 0.31        | 0/1704        |
| 43  | 1r    | 0.29         | 1/777 (0.1%)  | 0.40        | 0/1051        |
| 44  | 1s    | 0.16         | 0/394         | 0.40        | 0/533         |
| 45  | 3A    | 0.13         | 0/3481        | 0.35        | 0/4722        |
| 45  | 3N    | 0.13         | 0/3496        | 0.32        | 0/4723        |
| 46  | 3B    | 0.13         | 0/3190        | 0.33        | 0/4317        |
| 46  | 3O    | 0.17         | 0/3175        | 0.35        | 0/4292        |
| 47  | 3C    | 0.16         | 0/3123        | 0.36        | 0/4269        |
| 47  | 3P    | 0.15         | 0/3122        | 0.33        | 0/4269        |
| 48  | 3D    | 0.14         | 0/1946        | 0.36        | 0/2641        |
| 48  | 3Q    | 0.13         | 0/1962        | 0.34        | 0/2663        |
| 49  | 3E    | 0.18         | 0/1551        | 0.46        | 0/2098        |
| 49  | 3I    | 1.51         | 4/344 (1.2%)  | 2.00        | 12/468 (2.6%) |
| 49  | 3R    | 0.56         | 2/1551 (0.1%) | 0.76        | 2/2098 (0.1%) |
| 49  | 3V    | 1.68         | 2/225 (0.9%)  | 3.23        | 5/303 (1.7%)  |
| 50  | 3F    | 0.12         | 0/888         | 0.29        | 0/1193        |
| 50  | 3S    | 0.09         | 0/888         | 0.24        | 0/1193        |
| 51  | 3G    | 0.14         | 0/649         | 0.39        | 0/878         |
| 51  | 3T    | 0.15         | 0/649         | 0.35        | 0/878         |
| 52  | 3H    | 0.21         | 0/539         | 0.80        | 2/724 (0.3%)  |
| 52  | 3U    | 0.18         | 0/539         | 0.44        | 0/724         |
| 53  | 3J    | 0.40         | 0/476         | 0.57        | 0/641         |
| 53  | 3W    | 0.37         | 0/476         | 0.50        | 0/641         |
| 54  | 3X    | 0.12         | 0/445         | 0.32        | 0/608         |
| 54  | 3Y    | 0.14         | 0/437         | 0.38        | 0/598         |
| 55  | 4A    | 0.18         | 0/4156        | 0.34        | 0/5679        |
| 55  | 8A    | 0.29         | 1/4156 (0.0%) | 0.46        | 2/5679 (0.0%) |
| 56  | 4B    | 0.25         | 0/1865        | 0.43        | 0/2544        |
| 56  | 8B    | 0.23         | 0/1865        | 0.51        | 0/2544        |
| 57  | 4C    | 0.26         | 1/2179 (0.0%) | 0.35        | 0/2981        |
| 57  | 8C    | 0.22         | 0/2179        | 0.40        | 0/2981        |
| 58  | 4D    | 0.16         | 0/1197        | 0.39        | 0/1617        |

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5          |
| 58  | 8D    | 0.31         | 0/1197           | 0.51        | 0/1617           |
| 59  | 4E    | 0.23         | 0/871            | 0.51        | 0/1182           |
| 59  | 8E    | 0.29         | 0/871            | 0.52        | 0/1182           |
| 60  | 4F    | 0.27         | 0/749            | 0.61        | 1/1016 (0.1%)    |
| 60  | 8F    | 0.14         | 0/749            | 0.38        | 0/1016           |
| 61  | 4G    | 0.19         | 0/644            | 0.47        | 1/881 (0.1%)     |
| 61  | 8G    | 0.13         | 0/644            | 0.37        | 0/881            |
| 62  | 4H    | 0.15         | 0/708            | 0.36        | 0/956            |
| 62  | 8H    | 0.29         | 1/708 (0.1%)     | 0.45        | 0/956            |
| 63  | 4I    | 0.19         | 0/563            | 0.46        | 0/748            |
| 63  | 8I    | 0.25         | 0/563            | 0.46        | 0/748            |
| 64  | 4J    | 0.17         | 0/466            | 0.44        | 0/631            |
| 64  | 8J    | 0.18         | 0/466            | 0.47        | 0/631            |
| 65  | 4K    | 0.15         | 0/396            | 0.40        | 0/543            |
| 65  | 8K    | 0.27         | 0/396            | 0.56        | 0/543            |
| 66  | 4L    | 0.18         | 0/394            | 0.37        | 0/528            |
| 66  | 8L    | 0.27         | 0/394            | 0.51        | 1/528 (0.2%)     |
| 67  | 4M    | 0.23         | 0/349            | 0.49        | 0/477            |
| 67  | 8M    | 0.39         | 0/349            | 0.51        | 0/477            |
| 68  | 4N    | 0.17         | 0/680            | 0.39        | 0/921            |
| 68  | 8N    | 0.33         | 0/680            | 0.62        | 0/921            |
| All | All   | 0.22         | 16/131727 (0.0%) | 0.43        | 32/178746 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | 1F    | 0                   | 1                   |
| 49  | 3V    | 0                   | 1                   |
| 68  | 8N    | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 49  | 3V    | 49  | VAL  | C-N   | 22.83  | 1.70        | 1.33     |
| 49  | 3I    | 73  | PRO  | CG-CD | -19.98 | 0.82        | 1.50     |
| 49  | 3R    | 173 | PRO  | N-CD  | 16.16  | 1.70        | 1.47     |
| 49  | 3I    | 73  | PRO  | N-CD  | 13.25  | 1.66        | 1.47     |
| 14  | 1N    | 255 | PRO  | CA-C  | -11.58 | 1.44        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 39  | 1n    | 144 | PRO  | N-CD  | 10.97 | 1.63        | 1.47     |
| 49  | 3I    | 72  | VAL  | C-O   | 9.89  | 1.36        | 1.24     |
| 49  | 3R    | 173 | PRO  | CG-CD | -9.20 | 1.19        | 1.50     |
| 57  | 4C    | 159 | MET  | CG-SD | -8.28 | 1.60        | 1.80     |
| 49  | 3V    | 48  | SER  | C-N   | -7.96 | 1.19        | 1.33     |
| 43  | 1r    | 37  | PRO  | CA-C  | -6.68 | 1.48        | 1.51     |
| 55  | 8A    | 483 | SER  | CB-OG | -6.61 | 1.28        | 1.42     |
| 4   | 1D    | 359 | PRO  | CA-C  | 6.26  | 1.55        | 1.51     |
| 62  | 8H    | 9   | LYS  | CE-NZ | -5.53 | 1.32        | 1.49     |
| 39  | 1n    | 144 | PRO  | N-CA  | -5.03 | 1.36        | 1.46     |
| 49  | 3I    | 73  | PRO  | CA-CB | -5.02 | 1.46        | 1.53     |

All (32) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 49  | 3V    | 49  | VAL  | O-C-N    | -38.36 | 79.22       | 122.95   |
| 49  | 3R    | 173 | PRO  | CA-N-CD  | -23.12 | 79.64       | 112.00   |
| 49  | 3I    | 73  | PRO  | CB-CG-CD | 23.07  | 179.94      | 106.10   |
| 49  | 3V    | 49  | VAL  | CA-C-N   | 21.55  | 154.96      | 121.98   |
| 49  | 3V    | 49  | VAL  | C-N-CA   | 21.55  | 154.96      | 121.98   |
| 39  | 1n    | 144 | PRO  | CA-N-CD  | -19.71 | 84.41       | 112.00   |
| 49  | 3I    | 73  | PRO  | N-CD-CG  | -18.09 | 76.06       | 103.20   |
| 49  | 3V    | 48  | SER  | CA-C-N   | -16.95 | 100.50      | 122.37   |
| 49  | 3V    | 48  | SER  | C-N-CA   | -16.95 | 100.50      | 122.37   |
| 49  | 3I    | 41  | PRO  | CA-N-CD  | -13.18 | 93.55       | 112.00   |
| 60  | 4F    | 83  | PRO  | CA-N-CD  | -13.07 | 93.69       | 112.00   |
| 49  | 3I    | 73  | PRO  | CA-CB-CG | -13.03 | 79.75       | 104.50   |
| 49  | 3I    | 73  | PRO  | CA-N-CD  | -11.93 | 95.30       | 112.00   |
| 52  | 3H    | 77  | GLU  | CA-C-N   | 11.12  | 141.71      | 121.70   |
| 52  | 3H    | 77  | GLU  | C-N-CA   | 11.12  | 141.71      | 121.70   |
| 14  | 1N    | 255 | PRO  | O-C-N    | -9.00  | 116.92      | 121.15   |
| 8   | 1H    | 60  | PRO  | CA-N-CD  | -7.86  | 101.00      | 112.00   |
| 49  | 3I    | 71  | ASN  | N-CA-C   | -7.68  | 103.21      | 112.58   |
| 49  | 3I    | 41  | PRO  | N-CA-CB  | -7.45  | 98.75       | 102.92   |
| 49  | 3I    | 41  | PRO  | N-CA-C   | 7.33   | 122.90      | 110.74   |
| 49  | 3R    | 172 | LYS  | C-N-CD   | 6.88   | 153.20      | 125.00   |
| 49  | 3I    | 40  | SER  | C-N-CD   | -6.87  | 96.84       | 125.00   |
| 55  | 8A    | 208 | MET  | CB-CG-SD | 6.42   | 131.97      | 112.70   |
| 20  | 1U    | 4   | PRO  | CA-N-CD  | -6.38  | 103.06      | 112.00   |
| 61  | 4G    | 77  | PRO  | CA-N-CD  | -6.15  | 103.39      | 112.00   |
| 55  | 8A    | 208 | MET  | CG-SD-CE | -5.91  | 87.90       | 100.90   |
| 49  | 3I    | 72  | VAL  | CA-C-O   | -5.65  | 112.38      | 119.95   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 49  | 3I    | 72  | VAL  | C-N-CD  | 5.62  | 148.03      | 125.00   |
| 39  | 1n    | 143 | THR  | C-N-CD  | 5.44  | 147.32      | 125.00   |
| 66  | 8L    | 15  | VAL  | N-CA-C  | -5.39 | 107.72      | 112.90   |
| 49  | 3I    | 41  | PRO  | N-CD-CG | -5.26 | 95.31       | 103.20   |
| 8   | 1H    | 124 | ASN  | CB-CA-C | -5.12 | 110.27      | 117.23   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 6   | 1F    | 206 | LYS  | Peptide   |
| 49  | 3V    | 48  | SER  | Mainchain |
| 68  | 8N    | 48  | LYS  | Peptide   |

## 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   | 1A    | 916   | 0        | 950      | 79      | 0            |
| 2   | 1B    | 1242  | 0        | 1249     | 80      | 0            |
| 3   | 1C    | 1740  | 0        | 1691     | 40      | 0            |
| 4   | 1D    | 3452  | 0        | 3389     | 121     | 0            |
| 5   | 1E    | 1658  | 0        | 1662     | 67      | 0            |
| 6   | 1F    | 3325  | 0        | 3288     | 152     | 0            |
| 7   | 1G    | 5362  | 0        | 5388     | 173     | 0            |
| 8   | 1H    | 2504  | 0        | 2602     | 141     | 0            |
| 9   | 1I    | 1412  | 0        | 1366     | 62      | 0            |
| 10  | 1J    | 1329  | 0        | 1326     | 88      | 0            |
| 11  | 1K    | 750   | 0        | 798      | 57      | 0            |
| 12  | 1L    | 4818  | 0        | 4956     | 189     | 0            |
| 13  | 1M    | 3632  | 0        | 3836     | 146     | 0            |
| 14  | 1N    | 2712  | 0        | 2873     | 140     | 0            |
| 15  | 1O    | 2590  | 0        | 2556     | 92      | 0            |
| 16  | 1P    | 2751  | 0        | 2776     | 93      | 0            |
| 17  | 1Q    | 1047  | 0        | 1042     | 39      | 0            |
| 18  | 1R    | 741   | 0        | 704      | 16      | 0            |
| 19  | 1S    | 700   | 0        | 719      | 40      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 20  | 1T    | 689   | 0        | 687      | 42      | 0            |
| 20  | 1U    | 694   | 0        | 691      | 35      | 0            |
| 21  | 1V    | 927   | 0        | 972      | 25      | 0            |
| 22  | 1W    | 971   | 0        | 975      | 42      | 0            |
| 23  | 1X    | 1398  | 0        | 1378     | 45      | 0            |
| 24  | 1Y    | 1016  | 0        | 1020     | 31      | 0            |
| 25  | 1Z    | 1168  | 0        | 1161     | 58      | 0            |
| 26  | 1a    | 562   | 0        | 557      | 21      | 0            |
| 27  | 1b    | 643   | 0        | 645      | 23      | 0            |
| 28  | 1c    | 417   | 0        | 425      | 13      | 0            |
| 29  | 1d    | 985   | 0        | 978      | 29      | 0            |
| 30  | 1e    | 816   | 0        | 823      | 30      | 0            |
| 31  | 1f    | 487   | 0        | 498      | 20      | 0            |
| 32  | 1g    | 835   | 0        | 795      | 46      | 0            |
| 33  | 1h    | 1151  | 0        | 1164     | 32      | 0            |
| 34  | 1i    | 1100  | 0        | 1107     | 45      | 0            |
| 35  | 1j    | 601   | 0        | 546      | 36      | 0            |
| 36  | 1k    | 649   | 0        | 626      | 18      | 0            |
| 37  | 1l    | 1310  | 0        | 1204     | 43      | 0            |
| 38  | 1m    | 1062  | 0        | 1075     | 31      | 0            |
| 39  | 1n    | 1495  | 0        | 1434     | 53      | 0            |
| 40  | 1o    | 1045  | 0        | 1016     | 58      | 0            |
| 41  | 1p    | 1449  | 0        | 1416     | 62      | 0            |
| 42  | 1q    | 1212  | 0        | 1174     | 28      | 0            |
| 43  | 1r    | 759   | 0        | 783      | 29      | 0            |
| 44  | 1s    | 382   | 0        | 351      | 26      | 0            |
| 45  | 3A    | 3411  | 0        | 3308     | 72      | 0            |
| 45  | 3N    | 3424  | 0        | 3350     | 74      | 0            |
| 46  | 3B    | 3138  | 0        | 3116     | 68      | 0            |
| 46  | 3O    | 3124  | 0        | 3108     | 60      | 0            |
| 47  | 3C    | 3025  | 0        | 3090     | 73      | 0            |
| 47  | 3P    | 3024  | 0        | 3090     | 62      | 0            |
| 48  | 3D    | 1888  | 0        | 1834     | 49      | 0            |
| 48  | 3Q    | 1904  | 0        | 1849     | 50      | 0            |
| 49  | 3E    | 1518  | 0        | 1498     | 74      | 0            |
| 49  | 3I    | 340   | 0        | 359      | 18      | 0            |
| 49  | 3R    | 1518  | 0        | 1498     | 108     | 0            |
| 49  | 3V    | 224   | 0        | 241      | 19      | 0            |
| 50  | 3F    | 868   | 0        | 857      | 14      | 0            |
| 50  | 3S    | 868   | 0        | 857      | 9       | 0            |
| 51  | 3G    | 628   | 0        | 634      | 17      | 0            |
| 51  | 3T    | 628   | 0        | 634      | 23      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 52  | 3H    | 533   | 0        | 513      | 21      | 0            |
| 52  | 3U    | 533   | 0        | 513      | 18      | 0            |
| 53  | 3J    | 464   | 0        | 467      | 17      | 0            |
| 53  | 3W    | 464   | 0        | 467      | 15      | 0            |
| 54  | 3X    | 429   | 0        | 430      | 7       | 0            |
| 54  | 3Y    | 421   | 0        | 418      | 13      | 0            |
| 55  | 4A    | 4026  | 0        | 4005     | 196     | 0            |
| 55  | 8A    | 4026  | 0        | 4005     | 322     | 0            |
| 56  | 4B    | 1828  | 0        | 1836     | 123     | 0            |
| 56  | 8B    | 1828  | 0        | 1834     | 132     | 0            |
| 57  | 4C    | 2096  | 0        | 2027     | 100     | 0            |
| 57  | 8C    | 2096  | 0        | 2027     | 168     | 0            |
| 58  | 4D    | 1163  | 0        | 1143     | 79      | 0            |
| 58  | 8D    | 1163  | 0        | 1143     | 112     | 0            |
| 59  | 4E    | 852   | 0        | 845      | 73      | 0            |
| 59  | 8E    | 852   | 0        | 845      | 101     | 0            |
| 60  | 4F    | 734   | 0        | 718      | 34      | 0            |
| 60  | 8F    | 734   | 0        | 718      | 24      | 0            |
| 61  | 4G    | 617   | 0        | 585      | 17      | 0            |
| 61  | 8G    | 617   | 0        | 585      | 24      | 0            |
| 62  | 4H    | 687   | 0        | 645      | 23      | 0            |
| 62  | 8H    | 687   | 0        | 645      | 42      | 0            |
| 63  | 4I    | 550   | 0        | 560      | 32      | 0            |
| 63  | 8I    | 550   | 0        | 560      | 35      | 0            |
| 64  | 4J    | 456   | 0        | 459      | 35      | 0            |
| 64  | 8J    | 456   | 0        | 459      | 33      | 0            |
| 65  | 4K    | 383   | 0        | 366      | 22      | 0            |
| 65  | 8K    | 383   | 0        | 366      | 29      | 0            |
| 66  | 4L    | 381   | 0        | 380      | 27      | 0            |
| 66  | 8L    | 381   | 0        | 380      | 35      | 0            |
| 67  | 4M    | 338   | 0        | 345      | 30      | 0            |
| 67  | 8M    | 338   | 0        | 345      | 35      | 0            |
| 68  | 4N    | 660   | 0        | 664      | 29      | 0            |
| 68  | 8N    | 660   | 0        | 664      | 60      | 0            |
| 69  | 1A    | 47    | 0        | 71       | 3       | 0            |
| 69  | 1K    | 44    | 0        | 62       | 2       | 0            |
| 69  | 1L    | 91    | 0        | 136      | 8       | 0            |
| 69  | 1M    | 194   | 0        | 296      | 30      | 0            |
| 69  | 1N    | 49    | 0        | 75       | 5       | 0            |
| 69  | 1P    | 35    | 0        | 44       | 3       | 0            |
| 69  | 1Y    | 161   | 0        | 195      | 23      | 0            |
| 69  | 1d    | 49    | 0        | 75       | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 69  | 1j    | 44    | 0        | 65       | 0       | 0            |
| 69  | 1m    | 41    | 0        | 59       | 0       | 0            |
| 69  | 3A    | 59    | 0        | 66       | 9       | 0            |
| 69  | 3C    | 69    | 0        | 86       | 9       | 0            |
| 69  | 3D    | 33    | 0        | 40       | 2       | 0            |
| 69  | 3G    | 29    | 0        | 32       | 1       | 0            |
| 69  | 3N    | 58    | 0        | 62       | 8       | 0            |
| 69  | 3P    | 33    | 0        | 40       | 0       | 0            |
| 69  | 3R    | 47    | 0        | 71       | 5       | 0            |
| 69  | 3Y    | 30    | 0        | 34       | 2       | 0            |
| 70  | 1A    | 70    | 0        | 88       | 7       | 0            |
| 70  | 1B    | 94    | 0        | 136      | 15      | 0            |
| 70  | 1H    | 102   | 0        | 161      | 12      | 0            |
| 70  | 1I    | 44    | 0        | 62       | 3       | 0            |
| 70  | 1M    | 79    | 0        | 109      | 10      | 0            |
| 70  | 1P    | 33    | 0        | 40       | 2       | 0            |
| 70  | 1Y    | 46    | 0        | 66       | 7       | 0            |
| 70  | 1d    | 39    | 0        | 52       | 8       | 0            |
| 70  | 1h    | 47    | 0        | 71       | 1       | 0            |
| 70  | 1q    | 49    | 0        | 75       | 4       | 0            |
| 70  | 3J    | 47    | 0        | 68       | 4       | 0            |
| 70  | 3R    | 45    | 0        | 64       | 4       | 0            |
| 70  | 3X    | 29    | 0        | 32       | 2       | 0            |
| 71  | 1B    | 8     | 0        | 0        | 2       | 0            |
| 71  | 1F    | 8     | 0        | 0        | 2       | 0            |
| 71  | 1G    | 16    | 0        | 0        | 3       | 0            |
| 71  | 1I    | 16    | 0        | 0        | 0       | 0            |
| 72  | 1E    | 4     | 0        | 0        | 0       | 0            |
| 72  | 1G    | 4     | 0        | 0        | 2       | 0            |
| 72  | 3E    | 4     | 0        | 0        | 2       | 0            |
| 72  | 3R    | 4     | 0        | 0        | 2       | 0            |
| 73  | 1F    | 31    | 0        | 19       | 4       | 0            |
| 74  | 1G    | 1     | 0        | 0        | 0       | 0            |
| 75  | 1H    | 51    | 0        | 46       | 1       | 0            |
| 75  | 1L    | 76    | 0        | 99       | 6       | 0            |
| 75  | 1N    | 62    | 0        | 68       | 3       | 0            |
| 75  | 1X    | 86    | 0        | 125      | 12      | 0            |
| 75  | 1d    | 65    | 0        | 77       | 6       | 0            |
| 75  | 1h    | 80    | 0        | 104      | 14      | 0            |
| 75  | 1q    | 61    | 0        | 66       | 2       | 0            |
| 75  | 3A    | 58    | 0        | 60       | 3       | 0            |
| 75  | 3G    | 108   | 0        | 104      | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 75  | 3N    | 43    | 0        | 30       | 7       | 0            |
| 75  | 3P    | 56    | 0        | 56       | 9       | 0            |
| 75  | 3T    | 57    | 0        | 58       | 9       | 0            |
| 75  | 4B    | 100   | 0        | 156      | 14      | 0            |
| 75  | 4C    | 100   | 0        | 156      | 15      | 0            |
| 75  | 4D    | 100   | 0        | 156      | 17      | 0            |
| 75  | 8B    | 100   | 0        | 156      | 10      | 0            |
| 75  | 8C    | 100   | 0        | 156      | 16      | 0            |
| 75  | 8D    | 100   | 0        | 156      | 15      | 0            |
| 76  | 1O    | 32    | 0        | 12       | 3       | 0            |
| 77  | 1O    | 1     | 0        | 0        | 0       | 0            |
| 77  | 4A    | 1     | 0        | 0        | 0       | 0            |
| 77  | 8A    | 1     | 0        | 0        | 0       | 0            |
| 78  | 1P    | 48    | 0        | 26       | 2       | 0            |
| 79  | 1R    | 1     | 0        | 0        | 0       | 0            |
| 79  | 4F    | 1     | 0        | 0        | 0       | 0            |
| 79  | 8F    | 1     | 0        | 0        | 0       | 0            |
| 80  | 1T    | 37    | 0        | 0        | 0       | 0            |
| 80  | 1n    | 37    | 0        | 0        | 1       | 0            |
| 81  | 1Y    | 8     | 0        | 8        | 0       | 0            |
| 81  | 1q    | 8     | 0        | 8        | 2       | 0            |
| 82  | 1h    | 11    | 0        | 12       | 1       | 0            |
| 83  | 1i    | 29    | 0        | 39       | 0       | 0            |
| 84  | 1l    | 15    | 0        | 27       | 0       | 0            |
| 85  | 3C    | 86    | 0        | 60       | 2       | 0            |
| 85  | 3P    | 86    | 0        | 60       | 4       | 0            |
| 86  | 3D    | 42    | 0        | 32       | 2       | 0            |
| 86  | 3Q    | 43    | 0        | 32       | 3       | 0            |
| 87  | 4A    | 153   | 0        | 228      | 20      | 0            |
| 87  | 4B    | 102   | 0        | 151      | 8       | 0            |
| 87  | 4C    | 255   | 0        | 380      | 23      | 0            |
| 87  | 4G    | 51    | 0        | 76       | 5       | 0            |
| 87  | 4J    | 51    | 0        | 76       | 10      | 0            |
| 87  | 4K    | 51    | 0        | 76       | 2       | 0            |
| 87  | 4L    | 51    | 0        | 76       | 7       | 0            |
| 87  | 4M    | 51    | 0        | 76       | 3       | 0            |
| 87  | 8A    | 153   | 0        | 228      | 23      | 0            |
| 87  | 8B    | 102   | 0        | 151      | 11      | 0            |
| 87  | 8C    | 306   | 0        | 456      | 42      | 0            |
| 87  | 8G    | 51    | 0        | 76       | 8       | 0            |
| 87  | 8J    | 51    | 0        | 76       | 4       | 0            |
| 87  | 8K    | 51    | 0        | 76       | 3       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 87  | 8L    | 51     | 0        | 76       | 7       | 0            |
| 88  | 4A    | 120    | 0        | 108      | 10      | 0            |
| 88  | 8A    | 120    | 0        | 108      | 12      | 0            |
| 89  | 4A    | 1      | 0        | 0        | 0       | 0            |
| 89  | 8A    | 1      | 0        | 0        | 0       | 0            |
| 90  | 4A    | 1      | 0        | 0        | 0       | 0            |
| 90  | 8A    | 1      | 0        | 0        | 0       | 0            |
| 91  | 4B    | 2      | 0        | 0        | 2       | 0            |
| 91  | 8B    | 2      | 0        | 0        | 2       | 0            |
| 92  | 4B    | 52     | 0        | 80       | 8       | 0            |
| 92  | 8B    | 52     | 0        | 80       | 8       | 0            |
| 93  | 4C    | 52     | 0        | 72       | 5       | 0            |
| 93  | 4G    | 53     | 0        | 77       | 2       | 0            |
| 93  | 8C    | 52     | 0        | 72       | 5       | 0            |
| 93  | 8G    | 53     | 0        | 77       | 5       | 0            |
| 94  | 4H    | 5      | 0        | 0        | 0       | 0            |
| 94  | 8H    | 5      | 0        | 0        | 1       | 0            |
| All | All   | 134346 | 0        | 135606   | 4916    | 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 18.

All (4916) 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) |
|--------------------|-------------------|--------------------------|-------------------|
| 56:8B:52:HIS:CD2   | 56:8B:56:MET:HE1  | 1.45                     | 1.51              |
| 49:3V:49:VAL:C     | 49:3V:50:LEU:N    | 1.69                     | 1.49              |
| 57:4C:151:LEU:HD13 | 57:4C:159:MET:SD  | 1.50                     | 1.48              |
| 59:8E:72:LYS:HB2   | 59:8E:82:TYR:CE2  | 1.47                     | 1.47              |
| 68:8N:7:THR:C      | 68:8N:11:LYS:HZ3  | 1.23                     | 1.43              |
| 69:3A:503:3PE:H362 | 47:3C:11:MET:CE   | 1.58                     | 1.33              |
| 56:4B:61:VAL:HG12  | 56:4B:65:TRP:CZ3  | 1.64                     | 1.30              |
| 55:8A:483:SER:CA   | 67:8M:4:LYS:HZ1   | 1.44                     | 1.30              |
| 55:8A:367:LEU:HD13 | 55:8A:372:TYR:CD2 | 1.68                     | 1.28              |
| 56:8B:52:HIS:HD2   | 56:8B:56:MET:CE   | 1.45                     | 1.28              |
| 69:3A:503:3PE:C36  | 47:3C:11:MET:HE2  | 1.63                     | 1.28              |
| 5:1E:110:LEU:HB3   | 6:1F:261:HIS:NE2  | 1.49                     | 1.27              |
| 66:4L:41:ARG:HG3   | 67:4M:40:TYR:CE2  | 1.71                     | 1.25              |
| 56:8B:200:CYS:SG   | 91:8B:304:CUA:CU2 | 1.27                     | 1.24              |
| 56:8B:196:CYS:SG   | 91:8B:304:CUA:CU1 | 1.26                     | 1.23              |
| 15:1O:265:ASN:OD1  | 15:1O:268:GLU:HG2 | 1.36                     | 1.22              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:86:MET:HA    | 56:4B:89:GLU:OE1   | 1.36                     | 1.22              |
| 49:3R:173:PRO:CD   | 49:3R:173:PRO:N    | 1.70                     | 1.22              |
| 56:8B:52:HIS:CD2   | 56:8B:56:MET:CE    | 2.19                     | 1.22              |
| 55:4A:93:ALA:HA    | 55:4A:171:MET:CE   | 1.70                     | 1.22              |
| 65:8K:38:ILE:HD11  | 65:8K:40:TRP:CZ2   | 1.76                     | 1.21              |
| 49:3R:173:PRO:HD2  | 49:3R:173:PRO:O    | 1.39                     | 1.19              |
| 2:1B:49:THR:HG23   | 2:1B:59:MET:HE1    | 1.23                     | 1.19              |
| 62:8H:6:THR:HB     | 62:8H:9:LYS:NZ     | 1.58                     | 1.17              |
| 8:1H:85:MET:HE3    | 8:1H:233:MET:CE    | 1.74                     | 1.16              |
| 1:1A:18:VAL:HG23   | 8:1H:222:MET:HE2   | 1.21                     | 1.16              |
| 1:1A:18:VAL:CG2    | 8:1H:222:MET:HE2   | 1.75                     | 1.16              |
| 12:1L:140:LEU:HD22 | 12:1L:182:PHE:CZ   | 1.80                     | 1.15              |
| 68:8N:7:THR:C      | 68:8N:11:LYS:NZ    | 2.04                     | 1.15              |
| 57:8C:148:HIS:ND1  | 57:8C:152:MET:HE3  | 1.60                     | 1.15              |
| 55:8A:483:SER:HB3  | 67:8M:4:LYS:NZ     | 1.60                     | 1.14              |
| 55:8A:208:MET:HE1  | 55:8A:219:PHE:CG   | 1.81                     | 1.14              |
| 58:8D:34:SER:N     | 58:8D:37:GLN:OE1   | 1.79                     | 1.14              |
| 57:8C:148:HIS:HD1  | 57:8C:152:MET:HE3  | 1.10                     | 1.14              |
| 58:4D:53:MET:HE1   | 59:4E:104:LEU:HD22 | 1.13                     | 1.13              |
| 49:3R:152:ILE:HD11 | 49:3R:272:ILE:CG2  | 1.77                     | 1.13              |
| 55:8A:483:SER:HA   | 67:8M:4:LYS:HZ1    | 1.08                     | 1.12              |
| 20:1U:22:TYR:CE2   | 20:1U:24:LYS:NZ    | 2.17                     | 1.12              |
| 59:4E:21:LYS:O     | 59:4E:57:ARG:NH1   | 1.83                     | 1.11              |
| 65:8K:13:TYR:O     | 65:8K:17:ILE:HD12  | 1.49                     | 1.11              |
| 55:8A:483:SER:CB   | 67:8M:4:LYS:NZ     | 2.14                     | 1.09              |
| 45:3N:224:VAL:HG13 | 45:3N:225:GLU:H    | 0.97                     | 1.09              |
| 55:8A:172:LYS:NZ   | 55:8A:178:GLN:OE1  | 1.86                     | 1.09              |
| 55:8A:308:ALA:HA   | 55:8A:311:ILE:HD12 | 1.14                     | 1.09              |
| 1:1A:105:GLU:HG3   | 10:1J:169:MET:HE1  | 1.25                     | 1.07              |
| 57:4C:151:LEU:CD1  | 57:4C:159:MET:SD   | 2.43                     | 1.07              |
| 55:8A:409:TRP:HB3  | 55:8A:471:ILE:HD13 | 1.30                     | 1.07              |
| 55:4A:468:MET:HE2  | 55:4A:468:MET:HA   | 1.10                     | 1.06              |
| 56:4B:62:GLU:HB3   | 56:4B:65:TRP:CZ2   | 1.90                     | 1.06              |
| 58:8D:85:ALA:O     | 58:8D:89:ILE:HD12  | 1.56                     | 1.05              |
| 55:4A:93:ALA:HA    | 55:4A:171:MET:HE1  | 1.07                     | 1.05              |
| 12:1L:140:LEU:HD22 | 12:1L:182:PHE:HZ   | 0.98                     | 1.05              |
| 49:3V:49:VAL:O     | 49:3V:50:LEU:N     | 1.90                     | 1.05              |
| 8:1H:85:MET:HE3    | 8:1H:233:MET:HE2   | 1.05                     | 1.04              |
| 57:4C:33:MET:HE3   | 64:4J:49:CYS:HB3   | 1.40                     | 1.04              |
| 38:1m:113:LYS:O    | 38:1m:117:GLU:OE1  | 1.75                     | 1.04              |
| 62:8H:6:THR:HB     | 62:8H:9:LYS:HZ3    | 1.08                     | 1.04              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:61:VAL:CG1   | 56:4B:65:TRP:HZ3   | 1.71                     | 1.03              |
| 6:1F:250:ASN:ND2   | 6:1F:318:ASP:HB2   | 1.73                     | 1.03              |
| 19:1S:88:ARG:NH1   | 19:1S:88:ARG:O     | 1.91                     | 1.03              |
| 55:8A:308:ALA:HA   | 55:8A:311:ILE:CD1  | 1.88                     | 1.03              |
| 49:3R:152:ILE:HD11 | 49:3R:272:ILE:HG23 | 1.07                     | 1.03              |
| 56:4B:61:VAL:HG12  | 56:4B:65:TRP:CE3   | 1.94                     | 1.02              |
| 55:8A:483:SER:HB3  | 67:8M:4:LYS:HZ3    | 1.13                     | 1.02              |
| 59:8E:72:LYS:CB    | 59:8E:82:TYR:HE2   | 1.71                     | 1.02              |
| 55:8A:208:MET:CE   | 55:8A:219:PHE:CD2  | 2.43                     | 1.01              |
| 11:1K:80:MET:HA    | 11:1K:80:MET:HE3   | 1.39                     | 1.01              |
| 45:3A:118:GLN:HG2  | 45:3A:219:LEU:HD21 | 1.40                     | 1.01              |
| 49:3R:173:PRO:HD2  | 49:3R:173:PRO:C    | 1.78                     | 1.01              |
| 59:8E:72:LYS:CB    | 59:8E:82:TYR:CE2   | 2.43                     | 1.00              |
| 59:8E:78:HIS:CE1   | 63:8I:12:LEU:CD1   | 2.44                     | 1.00              |
| 68:8N:8:GLN:N      | 68:8N:11:LYS:HZ3   | 1.58                     | 0.99              |
| 57:8C:60:ASP:HA    | 57:8C:63:ARG:HG3   | 1.44                     | 0.99              |
| 66:4L:41:ARG:CG    | 67:4M:40:TYR:HE2   | 1.75                     | 0.99              |
| 49:3V:64:LEU:HA    | 49:3V:77:ARG:O     | 1.62                     | 0.99              |
| 55:4A:328:HIS:HB2  | 56:4B:45:MET:HE3   | 1.01                     | 0.99              |
| 14:1N:149:ILE:HG21 | 14:1N:154:MET:CE   | 1.93                     | 0.99              |
| 49:3R:173:PRO:CD   | 49:3R:173:PRO:O    | 2.10                     | 0.99              |
| 60:4F:83:PRO:HD2   | 60:4F:84:SER:N     | 1.78                     | 0.99              |
| 7:1G:439:PHE:CD1   | 7:1G:442:ILE:HD11  | 1.96                     | 0.99              |
| 46:3B:396:SER:O    | 46:3B:400:GLN:HG3  | 1.62                     | 0.99              |
| 6:1F:250:ASN:HD21  | 6:1F:318:ASP:CG    | 1.70                     | 0.98              |
| 58:8D:77:GLU:O     | 58:8D:81:ILE:HD12  | 1.63                     | 0.98              |
| 56:8B:52:HIS:CD2   | 56:8B:56:MET:SD    | 2.57                     | 0.98              |
| 45:3N:224:VAL:CG1  | 45:3N:225:GLU:H    | 1.73                     | 0.98              |
| 57:8C:59:ARG:NE    | 57:8C:63:ARG:HH21  | 1.60                     | 0.98              |
| 37:1I:80:ASP:HB3   | 37:1I:83:MET:HE2   | 1.46                     | 0.98              |
| 2:1B:86:MET:HE3    | 2:1B:107:MET:HE2   | 1.46                     | 0.97              |
| 56:4B:62:GLU:HA    | 56:4B:65:TRP:CE2   | 1.99                     | 0.97              |
| 55:8A:208:MET:HE1  | 55:8A:219:PHE:CB   | 1.94                     | 0.97              |
| 13:1M:453:MET:HE2  | 32:1g:77:VAL:HG13  | 1.46                     | 0.97              |
| 55:4A:328:HIS:CB   | 56:4B:45:MET:HE3   | 1.95                     | 0.97              |
| 68:8N:7:THR:O      | 68:8N:11:LYS:NZ    | 1.94                     | 0.96              |
| 1:1A:57:LEU:HD21   | 10:1J:172:THR:HG21 | 1.48                     | 0.96              |
| 55:4A:28:MET:HA    | 55:4A:28:MET:HE3   | 1.47                     | 0.96              |
| 55:8A:483:SER:CA   | 67:8M:4:LYS:NZ     | 2.28                     | 0.95              |
| 58:8D:48:TRP:CZ3   | 59:8E:61:PHE:CD2   | 2.54                     | 0.95              |
| 56:4B:62:GLU:HA    | 56:4B:65:TRP:CD2   | 2.02                     | 0.95              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 39:1n:144:PRO:HD2  | 39:1n:144:PRO:O    | 1.55                     | 0.95              |
| 66:8L:18:LYS:NZ    | 66:8L:19:TRP:CZ2   | 2.34                     | 0.95              |
| 55:8A:367:LEU:HD13 | 55:8A:372:TYR:CE2  | 2.00                     | 0.95              |
| 55:4A:468:MET:HA   | 55:4A:468:MET:CE   | 1.97                     | 0.94              |
| 59:4E:52:LEU:HD12  | 59:4E:98:ILE:HD12  | 1.48                     | 0.94              |
| 65:8K:38:ILE:HD11  | 65:8K:40:TRP:CE2   | 2.02                     | 0.94              |
| 45:3N:224:VAL:HG13 | 45:3N:225:GLU:N    | 1.75                     | 0.94              |
| 66:8L:37:PHE:HB3   | 67:8M:33:VAL:HG11  | 1.49                     | 0.94              |
| 2:1B:49:THR:CG2    | 2:1B:59:MET:HE1    | 1.98                     | 0.94              |
| 66:4L:41:ARG:HG3   | 67:4M:40:TYR:HE2   | 1.04                     | 0.94              |
| 55:8A:208:MET:HE1  | 55:8A:219:PHE:HB3  | 1.48                     | 0.93              |
| 55:4A:468:MET:HE2  | 55:4A:468:MET:CA   | 1.98                     | 0.93              |
| 55:4A:328:HIS:HB2  | 56:4B:45:MET:CE    | 1.95                     | 0.93              |
| 62:8H:6:THR:CB     | 62:8H:9:LYS:NZ     | 2.32                     | 0.93              |
| 57:8C:33:MET:HE2   | 64:8J:49:CYS:HB3   | 1.51                     | 0.93              |
| 12:1L:73:THR:HG22  | 12:1L:194:ASN:HD21 | 1.29                     | 0.93              |
| 16:1P:89:ASN:OD1   | 16:1P:90:VAL:HG12  | 1.69                     | 0.93              |
| 20:1U:17:TYR:O     | 20:1U:21:LEU:HD23  | 1.69                     | 0.93              |
| 55:8A:409:TRP:CB   | 55:8A:471:ILE:HD13 | 1.99                     | 0.93              |
| 7:1G:101:HIS:CE1   | 71:1G:801:SF4:S3   | 2.61                     | 0.92              |
| 56:4B:196:CYS:HG   | 91:4B:304:CUA:CU2  | 0.73                     | 0.92              |
| 5:1E:216:GLY:C     | 5:1E:217:LEU:HD23  | 1.94                     | 0.92              |
| 55:8A:308:ALA:CA   | 55:8A:311:ILE:HD12 | 2.00                     | 0.92              |
| 55:8A:483:SER:CB   | 67:8M:4:LYS:HZ3    | 1.75                     | 0.92              |
| 57:8C:122:HIS:CE1  | 61:8G:45:PRO:HB3   | 2.04                     | 0.92              |
| 7:1G:570:SER:HA    | 7:1G:583:THR:O     | 1.69                     | 0.92              |
| 55:8A:155:VAL:O    | 55:8A:159:LEU:HD12 | 1.69                     | 0.92              |
| 14:1N:1:FME:O1     | 15:1O:258:ARG:NH1  | 2.01                     | 0.92              |
| 17:1Q:39:VAL:HG21  | 17:1Q:108:ARG:HG3  | 1.50                     | 0.92              |
| 55:4A:93:ALA:CA    | 55:4A:171:MET:HE1  | 1.98                     | 0.92              |
| 14:1N:149:ILE:HG21 | 14:1N:154:MET:HE2  | 1.50                     | 0.91              |
| 1:1A:1:FME:H       | 1:1A:4:MET:HE3     | 1.35                     | 0.91              |
| 57:8C:148:HIS:CE1  | 57:8C:152:MET:HE3  | 2.04                     | 0.91              |
| 1:1A:18:VAL:HG23   | 8:1H:222:MET:CE    | 1.99                     | 0.91              |
| 8:1H:85:MET:CE     | 8:1H:233:MET:HE2   | 1.97                     | 0.91              |
| 38:1m:117:GLU:OE1  | 38:1m:117:GLU:N    | 2.03                     | 0.91              |
| 49:3R:173:PRO:CD   | 49:3R:173:PRO:C    | 2.33                     | 0.91              |
| 61:8G:15:THR:O     | 61:8G:19:LEU:HD12  | 1.71                     | 0.90              |
| 43:1r:57:ASP:OD2   | 43:1r:60:ARG:HB2   | 1.70                     | 0.90              |
| 57:4C:129:VAL:CG1  | 57:4C:180:GLU:OE1  | 2.20                     | 0.90              |
| 58:8D:99:GLU:OE2   | 58:8D:104:TYR:CE2  | 2.25                     | 0.90              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:1M:453:MET:HE1  | 32:1g:80:LEU:HD12  | 1.53                     | 0.90              |
| 60:4F:83:PRO:HD2   | 60:4F:84:SER:H     | 1.34                     | 0.90              |
| 62:8H:31:GLN:OE1   | 68:8N:54:TRP:NE1   | 2.05                     | 0.89              |
| 58:8D:48:TRP:HZ3   | 59:8E:61:PHE:CD2   | 1.88                     | 0.89              |
| 58:8D:68:PHE:CE1   | 59:8E:69:GLU:HB2   | 2.07                     | 0.89              |
| 58:4D:96:LEU:HD23  | 58:4D:96:LEU:O     | 1.71                     | 0.89              |
| 8:1H:156:MET:HE2   | 25:1Z:50:MET:HG2   | 1.53                     | 0.88              |
| 40:1o:32:GLU:O     | 40:1o:34:LYS:NZ    | 2.05                     | 0.88              |
| 12:1L:73:THR:CG2   | 12:1L:194:ASN:HD21 | 1.87                     | 0.88              |
| 57:8C:182:TYR:HE2  | 87:8C:305:PGV:H042 | 1.38                     | 0.88              |
| 46:3B:222:ARG:NE   | 46:3B:223:PHE:CE1  | 2.42                     | 0.88              |
| 37:1l:12:PRO:HA    | 38:1m:78:ASN:OD1   | 1.73                     | 0.88              |
| 61:4G:77:PRO:HD3   | 61:4G:82:TYR:CE1   | 2.08                     | 0.88              |
| 39:1n:144:PRO:O    | 39:1n:144:PRO:CD   | 2.22                     | 0.88              |
| 16:1P:108:ASP:HA   | 16:1P:112:LYS:HG2  | 1.56                     | 0.87              |
| 55:8A:208:MET:CE   | 55:8A:219:PHE:CG   | 2.57                     | 0.87              |
| 19:1S:43:LEU:CD1   | 19:1S:47:ASN:HD21  | 1.87                     | 0.87              |
| 20:1U:22:TYR:CZ    | 20:1U:24:LYS:NZ    | 2.41                     | 0.87              |
| 55:4A:91:ASP:OD1   | 55:4A:92:MET:N     | 2.06                     | 0.87              |
| 58:4D:53:MET:CE    | 59:4E:104:LEU:HD22 | 2.04                     | 0.87              |
| 57:8C:83:MET:HE2   | 57:8C:237:ALA:HB1  | 1.55                     | 0.87              |
| 16:1P:115:HIS:NE2  | 16:1P:119:GLN:OE1  | 2.08                     | 0.86              |
| 1:1A:27:LEU:HG     | 8:1H:59:GLU:HG3    | 1.55                     | 0.86              |
| 10:1J:86:ASN:OD1   | 10:1J:88:THR:N     | 2.07                     | 0.86              |
| 16:1P:147:ARG:HH12 | 59:8E:9:GLU:H      | 1.20                     | 0.86              |
| 58:4D:77:GLU:HG3   | 65:4K:10:HIS:NE2   | 1.88                     | 0.86              |
| 12:1L:161:ARG:HG2  | 12:1L:164:ALA:H    | 1.38                     | 0.86              |
| 32:1g:120:LEU:HD22 | 41:1p:163:LEU:HD21 | 1.58                     | 0.86              |
| 56:4B:61:VAL:CG1   | 56:4B:65:TRP:CZ3   | 2.49                     | 0.86              |
| 49:3E:165:MET:HA   | 49:3E:165:MET:HE3  | 1.57                     | 0.86              |
| 56:8B:58:ALA:HB2   | 92:8B:305:PSC:H031 | 1.56                     | 0.86              |
| 3:1C:114:LEU:O     | 22:1W:20:ILE:HD11  | 1.76                     | 0.86              |
| 8:1H:156:MET:SD    | 8:1H:174:MET:CE    | 2.64                     | 0.86              |
| 12:1L:140:LEU:CD2  | 12:1L:182:PHE:CZ   | 2.58                     | 0.86              |
| 55:4A:468:MET:HE1  | 55:4A:471:ILE:HD11 | 1.56                     | 0.86              |
| 12:1L:140:LEU:CD2  | 12:1L:182:PHE:HZ   | 1.88                     | 0.86              |
| 2:1B:49:THR:HG23   | 2:1B:59:MET:CE     | 2.06                     | 0.86              |
| 34:1i:77:PRO:O     | 34:1i:81:ILE:HG12  | 1.76                     | 0.86              |
| 59:4E:33:MET:HE3   | 59:4E:67:ILE:CG2   | 2.06                     | 0.85              |
| 59:8E:78:HIS:CE1   | 63:8I:12:LEU:HD11  | 2.10                     | 0.85              |
| 14:1N:149:ILE:HD13 | 14:1N:154:MET:HE1  | 1.58                     | 0.85              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:1S:88:ARG:NH2   | 19:1S:92:ASN:OD1   | 2.08                     | 0.85              |
| 40:1o:41:THR:O     | 40:1o:45:MET:HB3   | 1.77                     | 0.85              |
| 14:1N:270:MET:HE1  | 14:1N:282:MET:HE2  | 1.57                     | 0.84              |
| 87:4M:101:PGV:H61  | 87:4M:101:PGV:H221 | 1.59                     | 0.84              |
| 57:8C:50:ASN:OD1   | 57:8C:54:MET:HE2   | 1.77                     | 0.84              |
| 58:8D:78:TRP:HA    | 58:8D:81:ILE:HD13  | 1.58                     | 0.84              |
| 1:1A:68:GLU:HG2    | 10:1J:161:LEU:HD13 | 1.58                     | 0.84              |
| 57:8C:148:HIS:CE1  | 57:8C:152:MET:CE   | 2.59                     | 0.84              |
| 68:8N:8:GLN:HA     | 68:8N:11:LYS:NZ    | 1.92                     | 0.84              |
| 68:8N:8:GLN:N      | 68:8N:11:LYS:NZ    | 2.22                     | 0.84              |
| 34:1i:74:VAL:O     | 34:1i:78:VAL:HG12  | 1.77                     | 0.84              |
| 37:1l:127:PRO:HG3  | 40:1o:3:HIS:HD2    | 1.42                     | 0.84              |
| 6:1F:250:ASN:ND2   | 6:1F:318:ASP:CB    | 2.40                     | 0.84              |
| 55:4A:412:ILE:HD13 | 58:4D:84:THR:OG1   | 1.76                     | 0.84              |
| 55:8A:483:SER:CB   | 67:8M:4:LYS:HZ1    | 1.83                     | 0.84              |
| 57:8C:122:HIS:HE1  | 61:8G:45:PRO:HB3   | 1.40                     | 0.84              |
| 57:4C:45:LEU:HD11  | 64:4J:38:LEU:HD22  | 1.60                     | 0.84              |
| 46:3B:222:ARG:HE   | 46:3B:223:PHE:HE1  | 1.26                     | 0.84              |
| 56:8B:63:THR:HG22  | 56:8B:67:ILE:HD11  | 1.59                     | 0.84              |
| 22:1W:23:ARG:O     | 22:1W:23:ARG:HD3   | 1.77                     | 0.83              |
| 37:1l:127:PRO:HG3  | 40:1o:3:HIS:CD2    | 2.13                     | 0.83              |
| 56:4B:61:VAL:HG12  | 56:4B:65:TRP:HZ3   | 1.09                     | 0.83              |
| 55:8A:124:THR:CG2  | 55:8A:128:VAL:HA   | 2.08                     | 0.83              |
| 7:1G:105:CYS:HA    | 7:1G:108:CYS:HB2   | 1.58                     | 0.83              |
| 12:1L:584:ILE:HD11 | 14:1N:58:LYS:HG2   | 1.60                     | 0.83              |
| 58:8D:97:ILE:HG22  | 65:8K:36:ILE:HD11  | 1.60                     | 0.83              |
| 49:3R:239:HIS:CD2  | 49:3R:240:GLY:H    | 1.97                     | 0.83              |
| 13:1M:19:LYS:HD2   | 31:1f:9:ASP:OD1    | 1.79                     | 0.83              |
| 44:1s:42:GLN:N     | 44:1s:42:GLN:OE1   | 2.10                     | 0.83              |
| 55:8A:69:MET:CE    | 88:8A:604:HEA:H272 | 2.08                     | 0.83              |
| 49:3V:62:ARG:O     | 49:3V:77:ARG:NH2   | 2.11                     | 0.83              |
| 22:1W:62:LYS:HD2   | 22:1W:66:MET:HE3   | 1.59                     | 0.82              |
| 57:8C:27:MET:HE1   | 57:8C:50:ASN:HD22  | 1.43                     | 0.82              |
| 55:8A:212:ASP:OD1  | 55:8A:219:PHE:HB2  | 1.79                     | 0.82              |
| 57:4C:129:VAL:HG11 | 57:4C:180:GLU:OE1  | 1.77                     | 0.82              |
| 59:4E:45:PRO:HB2   | 59:4E:88:GLU:HG3   | 1.61                     | 0.82              |
| 59:8E:33:MET:CE    | 59:8E:67:ILE:HG22  | 2.09                     | 0.82              |
| 58:4D:89:ILE:HG22  | 65:4K:29:TRP:HE1   | 1.44                     | 0.82              |
| 59:8E:78:HIS:ND1   | 63:8I:12:LEU:HD11  | 1.95                     | 0.82              |
| 9:1I:44:GLU:HG3    | 26:1a:1:MET:HE3    | 1.61                     | 0.82              |
| 41:1p:158:GLN:HG2  | 41:1p:162:MET:CE   | 2.10                     | 0.81              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:8C:59:ARG:CD    | 57:8C:63:ARG:HH21  | 1.92                     | 0.81              |
| 12:1L:525:MET:HE2  | 39:1n:76:PRO:HB3   | 1.60                     | 0.81              |
| 27:1b:51:ASN:OD1   | 33:1h:139:THR:HG22 | 1.79                     | 0.81              |
| 47:3C:9:PRO:HB3    | 47:3P:202:GLU:OE2  | 1.80                     | 0.81              |
| 55:8A:250:GLY:O    | 55:8A:254:ILE:HG12 | 1.79                     | 0.81              |
| 49:3R:232:GLY:HA3  | 49:3R:244:ASP:HA   | 1.61                     | 0.81              |
| 56:8B:59:GLN:OE1   | 68:8N:14:SER:OG    | 1.97                     | 0.81              |
| 1:1A:18:VAL:CG2    | 8:1H:222:MET:CE    | 2.57                     | 0.81              |
| 55:4A:463:THR:HA   | 55:4A:466:MET:HE3  | 1.63                     | 0.81              |
| 55:4A:462:LEU:HG   | 55:4A:466:MET:HE2  | 1.62                     | 0.81              |
| 6:1F:17:ASP:HA     | 6:1F:20:ARG:HG2    | 1.61                     | 0.80              |
| 49:3R:197:ASP:O    | 49:3R:248:ARG:NH2  | 2.14                     | 0.80              |
| 55:4A:271:MET:HA   | 55:4A:271:MET:HE3  | 1.63                     | 0.80              |
| 55:8A:208:MET:CE   | 55:8A:219:PHE:HB3  | 2.12                     | 0.80              |
| 66:8L:18:LYS:NZ    | 67:8M:14:GLU:OE1   | 2.13                     | 0.80              |
| 10:1J:99:MET:SD    | 10:1J:99:MET:C     | 2.64                     | 0.80              |
| 55:8A:381:LEU:HD13 | 88:8A:604:HEA:HAC  | 1.61                     | 0.80              |
| 59:8E:33:MET:HE1   | 59:8E:67:ILE:HG22  | 1.63                     | 0.80              |
| 56:4B:133:MET:HE1  | 58:4D:119:GLN:HG3  | 1.64                     | 0.80              |
| 61:4G:77:PRO:HD3   | 61:4G:82:TYR:CZ    | 2.16                     | 0.80              |
| 35:1j:65:GLY:HA3   | 40:1o:30:PHE:CE1   | 2.16                     | 0.80              |
| 55:8A:241:PRO:O    | 55:8A:245:ILE:HG13 | 1.82                     | 0.80              |
| 62:8H:57:ARG:HA    | 62:8H:60:TYR:CE1   | 2.17                     | 0.80              |
| 32:1g:112:CYS:HA   | 41:1p:141:ARG:HH21 | 1.46                     | 0.80              |
| 57:8C:86:PHE:CZ    | 57:8C:90:GLU:OE2   | 2.35                     | 0.80              |
| 56:8B:68:LEU:HA    | 56:8B:71:ILE:HD12  | 1.64                     | 0.80              |
| 2:1B:81:ARG:HE     | 8:1H:61:LEU:CD2    | 1.95                     | 0.80              |
| 55:8A:208:MET:SD   | 55:8A:219:PHE:CD2  | 2.75                     | 0.80              |
| 2:1B:42:ARG:HH22   | 70:1B:203:PC1:H12  | 1.47                     | 0.79              |
| 14:1N:270:MET:HE1  | 14:1N:282:MET:CE   | 2.12                     | 0.79              |
| 12:1L:576:MET:HG2  | 69:1Y:202:3PE:H32  | 1.65                     | 0.79              |
| 19:1S:18:ILE:HD11  | 19:1S:52:ILE:HG23  | 1.65                     | 0.79              |
| 55:8A:124:THR:HG23 | 55:8A:128:VAL:HA   | 1.62                     | 0.79              |
| 56:8B:59:GLN:NE2   | 68:8N:14:SER:H     | 1.81                     | 0.79              |
| 16:1P:248:VAL:HG22 | 16:1P:334:VAL:HG21 | 1.65                     | 0.79              |
| 39:1n:97:LYS:HG2   | 39:1n:177:PRO:HG3  | 1.65                     | 0.79              |
| 48:3D:249:MET:HE3  | 48:3D:252:PRO:HG3  | 1.64                     | 0.79              |
| 55:8A:483:SER:HA   | 67:8M:4:LYS:NZ     | 1.92                     | 0.79              |
| 1:1A:105:GLU:CG    | 10:1J:169:MET:HE1  | 2.11                     | 0.79              |
| 32:1g:55:LEU:O     | 32:1g:59:ARG:HG3   | 1.81                     | 0.79              |
| 68:8N:18:LEU:O     | 68:8N:22:ILE:HD12  | 1.81                     | 0.79              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:49:LEU:HD12   | 8:1H:126:LYS:HG3   | 1.65                     | 0.79              |
| 59:4E:33:MET:HE3   | 59:4E:67:ILE:HG21  | 1.64                     | 0.79              |
| 68:8N:8:GLN:CA     | 68:8N:11:LYS:NZ    | 2.46                     | 0.79              |
| 66:4L:24:MET:HG3   | 87:4L:101:PGV:H201 | 1.65                     | 0.78              |
| 15:1O:14:THR:O     | 15:1O:18:LEU:HD13  | 1.83                     | 0.78              |
| 92:4B:305:PSC:H261 | 92:4B:305:PSC:H10  | 1.66                     | 0.78              |
| 58:4D:53:MET:HE1   | 59:4E:104:LEU:CD2  | 2.05                     | 0.78              |
| 56:8B:52:HIS:NE2   | 56:8B:56:MET:SD    | 2.56                     | 0.78              |
| 4:1D:20:TYR:HB2    | 12:1L:575:ILE:HD11 | 1.65                     | 0.78              |
| 87:4C:301:PGV:H162 | 93:4G:102:PEK:H162 | 1.65                     | 0.78              |
| 57:8C:148:HIS:ND1  | 57:8C:152:MET:CE   | 2.45                     | 0.78              |
| 4:1D:52:GLY:H      | 4:1D:53:PRO:HD3    | 1.49                     | 0.78              |
| 7:1G:226:GLU:HG2   | 7:1G:253:ARG:HD3   | 1.64                     | 0.78              |
| 52:3U:21:ARG:O     | 52:3U:25:GLU:HG3   | 1.84                     | 0.78              |
| 55:4A:381:LEU:HD13 | 88:4A:604:HEA:HAC  | 1.66                     | 0.78              |
| 52:3H:77:GLU:HA    | 52:3H:79:ASP:HB2   | 1.66                     | 0.77              |
| 65:4K:52:GLU:N     | 65:4K:52:GLU:OE2   | 2.17                     | 0.77              |
| 58:8D:34:SER:OG    | 58:8D:37:GLN:HG3   | 1.83                     | 0.77              |
| 35:1j:38:TRP:CE3   | 35:1j:42:HIS:HE1   | 2.02                     | 0.77              |
| 65:8K:52:GLU:OE1   | 65:8K:54:ARG:O     | 2.01                     | 0.77              |
| 49:3R:199:GLN:HB2  | 49:3R:248:ARG:HH21 | 1.49                     | 0.77              |
| 57:8C:119:THR:HG22 | 61:8G:50:TYR:CE2   | 2.19                     | 0.77              |
| 58:8D:43:LYS:NZ    | 58:8D:46:ALA:HB3   | 1.99                     | 0.77              |
| 58:8D:77:GLU:O     | 58:8D:81:ILE:CD1   | 2.32                     | 0.77              |
| 26:1a:59:ARG:HE    | 26:1a:61:HIS:CE1   | 2.02                     | 0.77              |
| 45:3A:172:GLU:OE1  | 45:3A:173:ASN:N    | 2.18                     | 0.77              |
| 58:8D:78:TRP:HA    | 58:8D:81:ILE:CD1   | 2.13                     | 0.77              |
| 59:8E:18:TYR:OH    | 59:8E:28:GLU:O     | 2.02                     | 0.77              |
| 36:1k:29:GLU:OE1   | 36:1k:33:GLU:OE2   | 2.02                     | 0.77              |
| 37:1l:80:ASP:HB3   | 37:1l:83:MET:CE    | 2.15                     | 0.77              |
| 41:1p:88:GLU:O     | 41:1p:92:ARG:HG2   | 1.83                     | 0.77              |
| 55:8A:69:MET:HE3   | 88:8A:604:HEA:H272 | 1.65                     | 0.77              |
| 58:8D:68:PHE:CE1   | 59:8E:69:GLU:CB    | 2.67                     | 0.77              |
| 23:1X:87:CYS:SG    | 23:1X:102:GLN:NE2  | 2.58                     | 0.77              |
| 67:4M:29:PRO:O     | 67:4M:33:VAL:HG23  | 1.84                     | 0.77              |
| 12:1L:176:ARG:HA   | 12:1L:179:ASP:OD2  | 1.85                     | 0.77              |
| 55:8A:409:TRP:CB   | 55:8A:471:ILE:CD1  | 2.62                     | 0.77              |
| 15:1O:189:PRO:HA   | 15:1O:192:MET:HG2  | 1.67                     | 0.77              |
| 58:4D:64:PHE:CD2   | 59:4E:66:ARG:HD3   | 2.19                     | 0.77              |
| 55:8A:208:MET:SD   | 55:8A:219:PHE:CE2  | 2.78                     | 0.77              |
| 12:1L:23:ASN:HD22  | 75:1L:702:CDL:H321 | 1.50                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:1J:86:ASN:OD1   | 10:1J:87:LYS:N     | 2.17                     | 0.76              |
| 66:8L:26:THR:HG21  | 67:8M:21:VAL:HG22  | 1.65                     | 0.76              |
| 17:1Q:9:GLN:HB3    | 22:1W:23:ARG:HH21  | 1.51                     | 0.76              |
| 58:4D:82:VAL:O     | 58:4D:86:LEU:HD13  | 1.84                     | 0.76              |
| 57:8C:6:HIS:CD2    | 57:8C:8:TYR:H      | 2.02                     | 0.76              |
| 57:8C:47:LEU:CD2   | 87:8C:303:PGV:H12  | 2.15                     | 0.76              |
| 25:1Z:59:ARG:O     | 25:1Z:62:ILE:HG22  | 1.86                     | 0.76              |
| 30:1e:4:ASP:OD1    | 30:1e:7:LYS:HB3    | 1.86                     | 0.76              |
| 87:8C:302:PGV:H162 | 93:8G:102:PEK:H162 | 1.66                     | 0.76              |
| 55:8A:409:TRP:HB3  | 55:8A:471:ILE:CD1  | 2.15                     | 0.76              |
| 4:1D:50:ASN:HA     | 4:1D:65:VAL:HA     | 1.66                     | 0.76              |
| 8:1H:204:GLU:HG2   | 8:1H:279:ARG:HH22  | 1.49                     | 0.76              |
| 58:4D:20:ARG:HD3   | 58:4D:72:ASN:HD21  | 1.50                     | 0.76              |
| 6:1F:250:ASN:ND2   | 6:1F:318:ASP:CG    | 2.43                     | 0.76              |
| 23:1X:122:GLY:HA3  | 27:1b:77:LEU:HD12  | 1.67                     | 0.76              |
| 59:4E:85:VAL:O     | 59:4E:89:LEU:HD13  | 1.86                     | 0.76              |
| 55:8A:362:SER:HA   | 56:8B:87:MET:HE1   | 1.67                     | 0.76              |
| 6:1F:43:TYR:CE1    | 6:1F:44:LYS:HG3    | 2.21                     | 0.76              |
| 1:1A:18:VAL:HG22   | 8:1H:222:MET:HE2   | 1.68                     | 0.76              |
| 4:1D:328:ALA:HB3   | 7:1G:126:ASP:HB2   | 1.66                     | 0.76              |
| 23:1X:36:ASP:OD2   | 27:1b:68:HIS:ND1   | 2.12                     | 0.76              |
| 1:1A:90:MET:HA     | 1:1A:90:MET:HE3    | 1.67                     | 0.75              |
| 12:1L:378:LEU:HD22 | 12:1L:383:MET:HE3  | 1.68                     | 0.75              |
| 16:1P:249:ALA:HB2  | 16:1P:318:LEU:HD12 | 1.68                     | 0.75              |
| 57:4C:151:LEU:HD22 | 57:4C:159:MET:HE1  | 1.68                     | 0.75              |
| 56:8B:185:MET:HA   | 56:8B:185:MET:HE2  | 1.68                     | 0.75              |
| 10:1J:17:PHE:HB3   | 11:1K:14:ILE:HD11  | 1.68                     | 0.75              |
| 62:8H:6:THR:CA     | 62:8H:9:LYS:NZ     | 2.50                     | 0.75              |
| 5:1E:144:CYS:O     | 6:1F:139:ARG:NH2   | 2.18                     | 0.75              |
| 55:8A:393:PHE:HE2  | 55:8A:472:ILE:HD11 | 1.52                     | 0.75              |
| 19:1S:43:LEU:HD11  | 19:1S:47:ASN:HD21  | 1.50                     | 0.75              |
| 20:1T:49:GLU:OE2   | 22:1W:40:TYR:CZ    | 2.39                     | 0.75              |
| 56:4B:94:ALA:HB3   | 56:4B:148:MET:SD   | 2.26                     | 0.75              |
| 11:1K:36:MET:HE3   | 14:1N:68:MET:HG3   | 1.67                     | 0.75              |
| 49:3R:200:HIS:HB3  | 49:3R:203:GLU:HG2  | 1.66                     | 0.75              |
| 16:1P:4:ALA:HB2    | 18:1R:24:ARG:NH2   | 2.02                     | 0.75              |
| 4:1D:269:LEU:HD11  | 4:1D:373:GLU:HG3   | 1.69                     | 0.74              |
| 13:1M:46:GLY:HA2   | 32:1g:84:ARG:NH2   | 2.02                     | 0.74              |
| 35:1j:69:ASP:HB3   | 40:1o:117:ARG:NH1  | 2.02                     | 0.74              |
| 58:8D:34:SER:OG    | 58:8D:37:GLN:CD    | 2.30                     | 0.74              |
| 55:4A:468:MET:HE1  | 55:4A:471:ILE:CD1  | 2.15                     | 0.74              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:194:GLU:HG2   | 6:1F:28:ARG:HH21   | 1.50                     | 0.74              |
| 66:4L:41:ARG:HG3   | 67:4M:40:TYR:CZ    | 2.19                     | 0.74              |
| 57:8C:27:MET:HE1   | 57:8C:50:ASN:ND2   | 2.01                     | 0.74              |
| 24:1Y:38:TYR:HB3   | 69:1Y:202:3PE:H232 | 1.67                     | 0.74              |
| 26:1a:22:ALA:O     | 26:1a:26:ILE:HG12  | 1.88                     | 0.74              |
| 75:4C:305:CDL:H822 | 75:4C:305:CDL:H612 | 1.69                     | 0.74              |
| 14:1N:70:LEU:HG    | 14:1N:98:MET:HE2   | 1.69                     | 0.74              |
| 19:1S:88:ARG:NH1   | 19:1S:92:ASN:OD1   | 2.19                     | 0.74              |
| 40:1o:45:MET:HE1   | 40:1o:59:ALA:HB3   | 1.68                     | 0.74              |
| 62:8H:73:ASP:OD1   | 62:8H:76:ARG:NH2   | 2.20                     | 0.74              |
| 43:1r:11:ARG:HG3   | 43:1r:19:LEU:HD11  | 1.69                     | 0.74              |
| 57:8C:33:MET:HE2   | 64:8J:49:CYS:CB    | 2.17                     | 0.74              |
| 59:8E:69:GLU:HG2   | 59:8E:101:PRO:HG3  | 1.70                     | 0.74              |
| 5:1E:76:PRO:HB2    | 5:1E:79:ARG:HG2    | 1.70                     | 0.74              |
| 7:1G:648:LEU:HD21  | 19:1S:44:LYS:HG2   | 1.69                     | 0.74              |
| 20:1T:18:VAL:HG21  | 20:1T:54:MET:HG3   | 1.69                     | 0.74              |
| 14:1N:149:ILE:HG21 | 14:1N:154:MET:HE1  | 1.68                     | 0.74              |
| 58:8D:77:GLU:HG2   | 58:8D:81:ILE:HD11  | 1.69                     | 0.74              |
| 13:1M:307:TRP:HA   | 13:1M:310:MET:HE2  | 1.70                     | 0.74              |
| 17:1Q:10:LEU:HD13  | 22:1W:16:SER:HB3   | 1.68                     | 0.74              |
| 41:1p:158:GLN:HG2  | 41:1p:162:MET:HE2  | 1.68                     | 0.74              |
| 61:4G:15:THR:O     | 61:4G:19:LEU:HD12  | 1.87                     | 0.74              |
| 64:4J:21:HIS:CD2   | 64:4J:22:LEU:HD13  | 2.22                     | 0.74              |
| 55:4A:222:PRO:HG2  | 56:4B:176:PRO:HB2  | 1.70                     | 0.74              |
| 57:4C:151:LEU:CD2  | 57:4C:159:MET:HE1  | 2.17                     | 0.74              |
| 48:3D:269:SER:OG   | 52:3H:42:LEU:HB2   | 1.88                     | 0.73              |
| 51:3T:40:ARG:NH1   | 75:3T:101:CDL:OA3  | 2.20                     | 0.73              |
| 55:4A:31:THR:HG21  | 55:4A:465:VAL:HG11 | 1.70                     | 0.73              |
| 55:4A:306:THR:HG23 | 55:4A:310:MET:CE   | 2.18                     | 0.73              |
| 12:1L:217:LEU:HD13 | 12:1L:277:THR:HG22 | 1.69                     | 0.73              |
| 25:1Z:68:ARG:O     | 25:1Z:72:MET:HG3   | 1.87                     | 0.73              |
| 59:8E:78:HIS:CE1   | 63:8I:12:LEU:HD12  | 2.23                     | 0.73              |
| 2:1B:109:GLU:OE2   | 16:1P:54:TYR:OH    | 2.06                     | 0.73              |
| 10:1J:34:ILE:HA    | 10:1J:61:LEU:HD11  | 1.70                     | 0.73              |
| 13:1M:216:LEU:HD23 | 13:1M:291:VAL:HG22 | 1.69                     | 0.73              |
| 48:3Q:139:THR:OG1  | 52:3U:41:ASP:OD1   | 2.07                     | 0.73              |
| 55:4A:271:MET:HE3  | 55:4A:271:MET:CA   | 2.19                     | 0.73              |
| 12:1L:297:ASP:HB3  | 12:1L:300:LYS:HB2  | 1.68                     | 0.73              |
| 55:8A:333:LYS:HZ2  | 55:8A:335:SER:N    | 1.87                     | 0.73              |
| 59:8E:85:VAL:O     | 59:8E:89:LEU:HG    | 1.88                     | 0.73              |
| 2:1B:86:MET:HE3    | 2:1B:107:MET:CE    | 2.18                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:1O:162:GLU:HG3  | 15:1O:262:LEU:HD22 | 1.70                     | 0.73              |
| 35:1j:38:TRP:CD2   | 35:1j:42:HIS:CE1   | 2.77                     | 0.73              |
| 56:4B:86:MET:CA    | 56:4B:89:GLU:OE1   | 2.27                     | 0.73              |
| 57:4C:151:LEU:HD22 | 57:4C:159:MET:CE   | 2.19                     | 0.73              |
| 59:4E:33:MET:HE3   | 59:4E:67:ILE:CB    | 2.18                     | 0.73              |
| 68:8N:32:TYR:O     | 68:8N:34:THR:N     | 2.21                     | 0.73              |
| 49:3R:172:LYS:HD2  | 49:3R:214:ILE:HG21 | 1.69                     | 0.73              |
| 54:3Y:8:PRO:O      | 54:3Y:12:GLU:HG3   | 1.89                     | 0.73              |
| 87:8A:601:PGV:H182 | 87:8A:601:PGV:H332 | 1.69                     | 0.73              |
| 62:8H:6:THR:CB     | 62:8H:9:LYS:HZ1    | 2.02                     | 0.73              |
| 66:8L:34:ALA:HA    | 66:8L:37:PHE:HD2   | 1.52                     | 0.73              |
| 25:1Z:76:GLN:NE2   | 25:1Z:80:ASP:OD1   | 2.22                     | 0.72              |
| 59:4E:48:ILE:CD1   | 59:4E:71:VAL:HG21  | 2.19                     | 0.72              |
| 52:3H:61:ARG:NH2   | 52:3H:86:ASP:OD2   | 2.23                     | 0.72              |
| 57:4C:33:MET:CE    | 64:4J:49:CYS:HB3   | 2.17                     | 0.72              |
| 55:8A:74:MET:HE3   | 55:8A:249:PRO:HB2  | 1.69                     | 0.72              |
| 6:1F:30:ASP:O      | 6:1F:39:ARG:NH2    | 2.23                     | 0.72              |
| 8:1H:196:ALA:HB3   | 8:1H:197:PRO:HD3   | 1.71                     | 0.72              |
| 13:1M:108:MET:HB3  | 13:1M:121:LEU:HD13 | 1.72                     | 0.72              |
| 55:8A:110:LEU:HD11 | 87:8A:601:PGV:H181 | 1.71                     | 0.72              |
| 69:1L:703:3PE:N    | 70:1M:505:PC1:O12  | 2.22                     | 0.72              |
| 47:3C:229:ILE:HG23 | 70:3J:101:PC1:H3A1 | 1.71                     | 0.72              |
| 46:3O:124:LEU:HD22 | 46:3O:224:LEU:HD21 | 1.71                     | 0.72              |
| 62:4H:6:THR:HA     | 62:4H:9:LYS:HE2    | 1.71                     | 0.72              |
| 55:8A:208:MET:HE3  | 55:8A:219:PHE:CD2  | 2.24                     | 0.72              |
| 2:1B:81:ARG:HE     | 8:1H:61:LEU:HD23   | 1.54                     | 0.72              |
| 7:1G:451:VAL:HG22  | 7:1G:489:VAL:HG12  | 1.72                     | 0.72              |
| 49:3R:173:PRO:HG2  | 49:3R:215:GLY:O    | 1.89                     | 0.72              |
| 49:3R:204:ARG:NH1  | 49:3R:246:SER:O    | 2.23                     | 0.72              |
| 68:8N:8:GLN:HA     | 68:8N:11:LYS:CE    | 2.20                     | 0.72              |
| 56:8B:59:GLN:CD    | 68:8N:14:SER:OG    | 2.33                     | 0.72              |
| 2:1B:48:MET:HE2    | 2:1B:80:PRO:HG3    | 1.72                     | 0.72              |
| 75:3P:504:CDL:HA61 | 75:3P:504:CDL:H532 | 1.71                     | 0.72              |
| 10:1J:99:MET:HE3   | 10:1J:100:GLU:N    | 2.05                     | 0.72              |
| 40:1o:45:MET:HE1   | 40:1o:59:ALA:CB    | 2.20                     | 0.72              |
| 55:8A:483:SER:HB3  | 67:8M:4:LYS:CE     | 2.19                     | 0.72              |
| 7:1G:477:ILE:HD11  | 7:1G:489:VAL:HG11  | 1.71                     | 0.72              |
| 12:1L:528:TYR:CG   | 37:1l:101:MET:HG2  | 2.25                     | 0.72              |
| 55:4A:353:LEU:HB3  | 56:4B:31:VAL:HG13  | 1.72                     | 0.72              |
| 59:4E:33:MET:HE3   | 59:4E:67:ILE:HB    | 1.72                     | 0.72              |
| 55:8A:222:PRO:HG2  | 56:8B:176:PRO:HB2  | 1.72                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:8C:247:VAL:HG12 | 57:8C:251:PHE:HE1  | 1.54                     | 0.72              |
| 64:8J:36:MET:HA    | 64:8J:39:CYS:SG    | 2.30                     | 0.72              |
| 49:3R:150:SER:HB3  | 49:3R:170:ARG:H    | 1.53                     | 0.71              |
| 55:4A:28:MET:HE2   | 67:4M:26:PHE:CE2   | 2.24                     | 0.71              |
| 60:4F:83:PRO:CD    | 60:4F:84:SER:N     | 2.52                     | 0.71              |
| 68:4N:32:TYR:O     | 68:4N:34:THR:N     | 2.23                     | 0.71              |
| 20:1T:34:SER:HB3   | 20:1T:40:LEU:HD11  | 1.72                     | 0.71              |
| 57:8C:127:LEU:HA   | 57:8C:131:LEU:HD11 | 1.71                     | 0.71              |
| 20:1T:25:ILE:HD12  | 20:1T:40:LEU:HD22  | 1.71                     | 0.71              |
| 69:1M:504:3PE:H3I1 | 14:1N:256:PRO:HD2  | 1.72                     | 0.71              |
| 32:1g:120:LEU:HD23 | 32:1g:121:PRO:HD2  | 1.72                     | 0.71              |
| 55:8A:367:LEU:CD1  | 55:8A:372:TYR:CE2  | 2.73                     | 0.71              |
| 56:8B:45:MET:CE    | 92:8B:305:PSC:H81  | 2.20                     | 0.71              |
| 56:8B:52:HIS:CG    | 56:8B:56:MET:HE1   | 2.19                     | 0.71              |
| 56:8B:45:MET:HE1   | 92:8B:305:PSC:H81  | 1.73                     | 0.71              |
| 66:8L:36:PRO:O     | 66:8L:40:VAL:HG23  | 1.91                     | 0.71              |
| 55:8A:390:MET:HA   | 55:8A:390:MET:HE3  | 1.73                     | 0.71              |
| 57:8C:27:MET:CE    | 57:8C:50:ASN:HD22  | 2.02                     | 0.71              |
| 7:1G:110:GLN:HE21  | 17:1Q:45:MET:HB3   | 1.55                     | 0.71              |
| 56:4B:58:ALA:HB2   | 92:4B:305:PSC:H031 | 1.71                     | 0.71              |
| 6:1F:365:CYS:HB2   | 71:1F:502:SF4:S3   | 2.30                     | 0.71              |
| 47:3P:111:GLU:OE1  | 47:3P:111:GLU:N    | 2.19                     | 0.71              |
| 58:4D:63:LYS:HG2   | 58:4D:64:PHE:CE1   | 2.24                     | 0.71              |
| 58:8D:44:GLU:OE2   | 59:8E:59:ASN:HB3   | 1.91                     | 0.71              |
| 65:8K:13:TYR:O     | 65:8K:17:ILE:CD1   | 2.36                     | 0.71              |
| 12:1L:503:GLU:HG3  | 64:4J:33:ARG:HE    | 1.55                     | 0.71              |
| 14:1N:270:MET:HE3  | 14:1N:279:PRO:HG3  | 1.72                     | 0.71              |
| 45:3A:269:PRO:HB2  | 45:3A:410:VAL:HG11 | 1.72                     | 0.71              |
| 55:4A:28:MET:HE2   | 67:4M:26:PHE:HE2   | 1.56                     | 0.71              |
| 59:4E:63:SER:O     | 59:4E:67:ILE:HG23  | 1.89                     | 0.71              |
| 2:1B:86:MET:CE     | 2:1B:107:MET:HE2   | 2.20                     | 0.71              |
| 10:1J:88:THR:HG23  | 69:1K:101:3PE:H232 | 1.72                     | 0.71              |
| 15:1O:105:LEU:HA   | 15:1O:128:ILE:HD11 | 1.73                     | 0.71              |
| 53:3W:10:TYR:HA    | 53:3W:14:PHE:HB2   | 1.73                     | 0.71              |
| 55:4A:93:ALA:CA    | 55:4A:171:MET:CE   | 2.61                     | 0.71              |
| 60:4F:76:LYS:HD3   | 60:4F:77:GLY:N     | 2.06                     | 0.71              |
| 11:1K:80:MET:HA    | 11:1K:80:MET:CE    | 2.20                     | 0.70              |
| 15:1O:24:VAL:HG23  | 15:1O:167:HIS:H    | 1.54                     | 0.70              |
| 13:1M:423:ILE:HG12 | 38:1m:58:VAL:HG12  | 1.72                     | 0.70              |
| 25:1Z:108:GLU:H    | 30:1e:74:ARG:NH2   | 1.89                     | 0.70              |
| 68:8N:2:LEU:O      | 68:8N:6:ILE:HG12   | 1.91                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:73:ALA:HB2   | 14:1N:97:MET:HB3   | 1.72                     | 0.70              |
| 55:4A:176:MET:HE3  | 55:4A:181:THR:HG22 | 1.72                     | 0.70              |
| 56:4B:30:ILE:HG21  | 56:4B:76:ILE:HD11  | 1.73                     | 0.70              |
| 68:4N:11:LYS:O     | 68:4N:11:LYS:NZ    | 2.21                     | 0.70              |
| 58:8D:68:PHE:CD1   | 59:8E:69:GLU:HB3   | 2.27                     | 0.70              |
| 62:8H:6:THR:HA     | 62:8H:9:LYS:NZ     | 2.06                     | 0.70              |
| 36:1k:24:GLU:OE1   | 36:1k:24:GLU:N     | 2.19                     | 0.70              |
| 47:3C:103:TYR:HA   | 47:3C:315:MET:HE3  | 1.72                     | 0.70              |
| 66:4L:41:ARG:O     | 66:4L:45:LEU:HD23  | 1.91                     | 0.70              |
| 2:1B:104:TYR:O     | 2:1B:111:ARG:NH1   | 2.24                     | 0.70              |
| 6:1F:164:LYS:N     | 44:1s:63:MET:HE1   | 2.05                     | 0.70              |
| 14:1N:270:MET:HB3  | 14:1N:275:SER:HB3  | 1.72                     | 0.70              |
| 8:1H:169:GLN:HG2   | 8:1H:174:MET:HG3   | 1.74                     | 0.70              |
| 55:4A:383:MET:HE2  | 55:4A:421:VAL:HG13 | 1.74                     | 0.70              |
| 55:8A:195:LEU:HG   | 55:8A:245:ILE:HG21 | 1.72                     | 0.70              |
| 62:8H:36:PHE:O     | 62:8H:40:GLU:HG2   | 1.92                     | 0.70              |
| 63:8I:65:LYS:HD2   | 63:8I:65:LYS:O     | 1.92                     | 0.70              |
| 1:1A:36:PRO:HB2    | 1:1A:43:PRO:HG2    | 1.73                     | 0.70              |
| 69:1M:502:3PE:H372 | 69:1M:502:3PE:H272 | 1.73                     | 0.70              |
| 38:1m:111:LYS:O    | 38:1m:115:ILE:HG13 | 1.91                     | 0.70              |
| 55:4A:96:ARG:NH2   | 57:4C:64:GLU:OE1   | 2.24                     | 0.70              |
| 67:4M:17:ILE:O     | 67:4M:21:VAL:HG23  | 1.91                     | 0.70              |
| 55:8A:333:LYS:NZ   | 55:8A:335:SER:CA   | 2.54                     | 0.70              |
| 6:1F:276:LEU:HD13  | 6:1F:315:VAL:HG23  | 1.71                     | 0.70              |
| 8:1H:32:GLN:OE1    | 8:1H:34:ARG:NH1    | 2.23                     | 0.70              |
| 9:1I:150:ASN:HD21  | 42:1q:127:TYR:H    | 1.40                     | 0.70              |
| 16:1P:89:ASN:OD1   | 16:1P:90:VAL:N     | 2.25                     | 0.70              |
| 37:1I:158:ILE:HG12 | 40:1o:99:LYS:HB3   | 1.74                     | 0.70              |
| 55:8A:367:LEU:CD1  | 55:8A:372:TYR:CD2  | 2.62                     | 0.70              |
| 59:8E:63:SER:O     | 59:8E:67:ILE:HG23  | 1.92                     | 0.70              |
| 6:1F:287:VAL:HG11  | 6:1F:294:LEU:HD12  | 1.73                     | 0.70              |
| 23:1X:36:ASP:OD1   | 23:1X:37:LYS:N     | 2.25                     | 0.70              |
| 87:4B:301:PGV:H22  | 75:4D:201:CDL:H312 | 1.74                     | 0.70              |
| 63:4I:54:TYR:OH    | 63:4I:59:ASP:OD2   | 2.09                     | 0.70              |
| 64:4J:2:GLU:N      | 64:4J:2:GLU:OE2    | 2.25                     | 0.70              |
| 14:1N:6:TYR:CE2    | 14:1N:46:LYS:HD2   | 2.27                     | 0.69              |
| 49:3E:159:ILE:HG12 | 49:3E:165:MET:HG2  | 1.73                     | 0.69              |
| 49:3E:261:PRO:HB2  | 49:3E:273:VAL:HG11 | 1.73                     | 0.69              |
| 87:4A:601:PGV:H332 | 87:4A:601:PGV:H162 | 1.72                     | 0.69              |
| 13:1M:225:ILE:O    | 13:1M:229:MET:HG3  | 1.92                     | 0.69              |
| 5:1E:55:GLN:HE22   | 5:1E:90:TYR:HA     | 1.56                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:1Q:28:GLU:OE1   | 17:1Q:28:GLU:N     | 2.25                     | 0.69              |
| 53:3J:14:TYR:HA    | 53:3J:18:PHE:HB2   | 1.75                     | 0.69              |
| 49:3R:239:HIS:HD2  | 49:3R:240:GLY:H    | 1.41                     | 0.69              |
| 56:4B:62:GLU:CB    | 56:4B:65:TRP:CZ2   | 2.71                     | 0.69              |
| 55:8A:333:LYS:HZ1  | 55:8A:335:SER:HA   | 1.58                     | 0.69              |
| 68:8N:2:LEU:HA     | 68:8N:5:ILE:HG22   | 1.74                     | 0.69              |
| 68:8N:50:ASN:HD21  | 68:8N:53:PRO:HB3   | 1.56                     | 0.69              |
| 7:1G:101:HIS:HE1   | 71:1G:801:SF4:S3   | 1.94                     | 0.69              |
| 10:1J:20:PHE:HE1   | 11:1K:32:CYS:HA    | 1.56                     | 0.69              |
| 14:1N:332:LEU:HD21 | 75:1d:203:CDL:H431 | 1.74                     | 0.69              |
| 6:1F:43:TYR:CD1    | 6:1F:44:LYS:HG3    | 2.28                     | 0.69              |
| 6:1F:250:ASN:OD1   | 6:1F:250:ASN:O     | 2.11                     | 0.69              |
| 7:1G:129:ARG:HB3   | 43:1r:48:LEU:HD22  | 1.74                     | 0.69              |
| 34:1i:105:PRO:HG2  | 34:1i:119:MET:HE2  | 1.74                     | 0.69              |
| 40:1o:74:PRO:HG3   | 41:1p:28:PRO:HD3   | 1.75                     | 0.69              |
| 60:4F:83:PRO:CD    | 60:4F:84:SER:H     | 2.06                     | 0.69              |
| 55:8A:176:MET:HE2  | 55:8A:181:THR:HG22 | 1.73                     | 0.69              |
| 57:8C:23:SER:OG    | 57:8C:50:ASN:HB2   | 1.91                     | 0.69              |
| 58:8D:48:TRP:NE1   | 59:8E:56:ARG:HD3   | 2.08                     | 0.69              |
| 4:1D:249:ASP:OD2   | 4:1D:404:LYS:NZ    | 2.25                     | 0.69              |
| 16:1P:138:ASP:HB3  | 16:1P:141:SER:HB2  | 1.74                     | 0.69              |
| 20:1U:21:LEU:HD13  | 36:1k:18:TYR:OH    | 1.92                     | 0.69              |
| 26:1a:1:MET:HE2    | 26:1a:1:MET:N      | 2.07                     | 0.69              |
| 34:1i:100:LYS:O    | 40:1o:49:GLN:NE2   | 2.26                     | 0.69              |
| 46:3B:166:ALA:HB2  | 46:3B:244:ILE:HG13 | 1.73                     | 0.69              |
| 55:8A:242:GLU:HA   | 55:8A:245:ILE:HD12 | 1.75                     | 0.69              |
| 87:8B:302:PGV:H91  | 87:8B:302:PGV:H251 | 1.74                     | 0.69              |
| 68:8N:7:THR:O      | 68:8N:11:LYS:CE    | 2.40                     | 0.69              |
| 15:1O:101:TYR:HE1  | 15:1O:128:ILE:HG23 | 1.58                     | 0.69              |
| 29:1d:107:LYS:HB2  | 29:1d:112:ILE:HD11 | 1.73                     | 0.69              |
| 64:4J:8:LYS:HA     | 64:4J:8:LYS:HE3    | 1.75                     | 0.69              |
| 55:8A:393:PHE:CE2  | 55:8A:472:ILE:HD11 | 2.28                     | 0.69              |
| 56:8B:16:ILE:O     | 56:8B:20:LEU:HD23  | 1.92                     | 0.69              |
| 68:8N:8:GLN:CA     | 68:8N:11:LYS:HZ3   | 2.04                     | 0.69              |
| 2:1B:62:MET:HE3    | 2:1B:69:MET:SD     | 2.33                     | 0.69              |
| 12:1L:102:GLU:OE1  | 12:1L:456:ARG:NH2  | 2.25                     | 0.69              |
| 12:1L:290:LEU:O    | 12:1L:523:SER:OG   | 2.10                     | 0.69              |
| 22:1W:62:LYS:HD2   | 22:1W:66:MET:CE    | 2.22                     | 0.69              |
| 23:1X:17:VAL:HG11  | 25:1Z:74:LEU:HD11  | 1.75                     | 0.69              |
| 23:1X:29:HIS:HB3   | 23:1X:119:PRO:HD2  | 1.74                     | 0.69              |
| 31:1f:47:GLU:OE1   | 31:1f:47:GLU:N     | 2.25                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:1o:55:ARG:HH22  | 41:1p:119:SER:HB3  | 1.56                     | 0.69              |
| 43:1r:29:GLU:OE2   | 43:1r:29:GLU:N     | 2.23                     | 0.69              |
| 45:3A:118:GLN:CG   | 45:3A:219:LEU:HD21 | 2.20                     | 0.69              |
| 47:3C:129:MET:HE1  | 47:3C:181:PHE:HB3  | 1.74                     | 0.69              |
| 49:3R:162:GLY:H    | 49:3R:178:HIS:HB3  | 1.57                     | 0.69              |
| 57:4C:90:GLU:OE2   | 57:4C:207:HIS:NE2  | 2.26                     | 0.69              |
| 57:4C:176:LEU:HD12 | 57:4C:179:SER:OG   | 1.93                     | 0.69              |
| 55:8A:495:LEU:HD11 | 60:8F:73:TRP:CD1   | 2.28                     | 0.69              |
| 56:8B:25:ASP:O     | 56:8B:29:MET:HG3   | 1.92                     | 0.69              |
| 20:1U:8:LEU:N      | 20:1U:88:GLU:OE2   | 2.26                     | 0.69              |
| 29:1d:99:GLU:OE1   | 29:1d:99:GLU:N     | 2.26                     | 0.69              |
| 52:3U:47:ARG:HG2   | 52:3U:50:THR:HB    | 1.75                     | 0.69              |
| 59:4E:52:LEU:HD12  | 59:4E:98:ILE:CD1   | 2.22                     | 0.69              |
| 59:4E:82:TYR:HA    | 59:4E:85:VAL:HG12  | 1.74                     | 0.69              |
| 55:8A:379:TYR:CE1  | 55:8A:383:MET:HE1  | 2.27                     | 0.69              |
| 59:8E:25:ASP:HB3   | 59:8E:28:GLU:OE2   | 1.93                     | 0.69              |
| 1:1A:69:ILE:HD11   | 8:1H:144:VAL:HG13  | 1.75                     | 0.69              |
| 7:1G:537:LEU:HD12  | 7:1G:543:ILE:HD11  | 1.74                     | 0.69              |
| 56:8B:100:MET:SD   | 56:8B:155:SER:OG   | 2.50                     | 0.69              |
| 87:8A:602:PGV:H221 | 87:8A:602:PGV:H61  | 1.74                     | 0.68              |
| 58:8D:100:LYS:HA   | 58:8D:104:TYR:HD2  | 1.58                     | 0.68              |
| 20:1T:12:LYS:HZ1   | 20:1T:32:VAL:HG13  | 1.58                     | 0.68              |
| 25:1Z:59:ARG:O     | 25:1Z:62:ILE:CG2   | 2.42                     | 0.68              |
| 55:4A:28:MET:HA    | 55:4A:28:MET:CE    | 2.22                     | 0.68              |
| 55:8A:208:MET:CE   | 55:8A:219:PHE:CB   | 2.70                     | 0.68              |
| 66:8L:20:ARG:NH1   | 66:8L:24:MET:HE2   | 2.08                     | 0.68              |
| 13:1M:46:GLY:HA2   | 32:1g:84:ARG:CZ    | 2.24                     | 0.68              |
| 16:1P:52:GLU:HG3   | 16:1P:54:TYR:H     | 1.58                     | 0.68              |
| 57:4C:60:ASP:O     | 57:4C:64:GLU:HG3   | 1.94                     | 0.68              |
| 59:4E:48:ILE:HD11  | 59:4E:71:VAL:CG2   | 2.24                     | 0.68              |
| 55:8A:362:SER:HA   | 56:8B:87:MET:CE    | 2.23                     | 0.68              |
| 62:8H:6:THR:HB     | 62:8H:9:LYS:HZ1    | 1.53                     | 0.68              |
| 1:1A:27:LEU:HD22   | 70:1A:202:PC1:H122 | 1.76                     | 0.68              |
| 1:1A:73:LEU:HD23   | 8:1H:151:LEU:HD12  | 1.74                     | 0.68              |
| 12:1L:82:MET:HA    | 12:1L:82:MET:HE3   | 1.74                     | 0.68              |
| 57:8C:77:LYS:HD2   | 57:8C:80:ARG:HD3   | 1.76                     | 0.68              |
| 70:1H:403:PC1:H331 | 70:1H:403:PC1:H2A2 | 1.76                     | 0.68              |
| 10:1J:74:MET:CE    | 10:1J:75:ALA:HB2   | 2.24                     | 0.68              |
| 59:4E:48:ILE:HG21  | 59:4E:89:LEU:HD21  | 1.76                     | 0.68              |
| 56:8B:141:ARG:HD3  | 56:8B:210:VAL:HG11 | 1.74                     | 0.68              |
| 2:1B:101:ARG:NH1   | 2:1B:105:ASP:OD1   | 2.26                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:190:MET:CG    | 7:1G:192:MET:HE3   | 2.24                     | 0.68              |
| 13:1M:341:THR:HG21 | 38:1m:64:LEU:HD21  | 1.75                     | 0.68              |
| 16:1P:264:ARG:HH12 | 16:1P:285:GLU:HB2  | 1.57                     | 0.68              |
| 23:1X:46:ARG:NH2   | 33:1h:142:ASP:OD1  | 2.27                     | 0.68              |
| 56:8B:133:MET:HE1  | 58:8D:123:MET:HG3  | 1.76                     | 0.68              |
| 75:8C:306:CDL:H141 | 75:8C:306:CDL:H541 | 1.76                     | 0.68              |
| 7:1G:672:TYR:HB3   | 7:1G:684:MET:HE3   | 1.74                     | 0.68              |
| 12:1L:145:GLU:HA   | 12:1L:145:GLU:OE2  | 1.94                     | 0.68              |
| 15:1O:45:LYS:HE3   | 15:1O:232:GLU:HG3  | 1.75                     | 0.68              |
| 49:3I:32:ALA:N     | 49:3I:71:ASN:O     | 2.26                     | 0.68              |
| 49:3V:65:VAL:H     | 49:3V:77:ARG:C     | 2.00                     | 0.68              |
| 57:8C:65:SER:HB2   | 87:8C:307:PGV:H041 | 1.75                     | 0.68              |
| 64:8J:39:CYS:O     | 64:8J:43:THR:HG23  | 1.94                     | 0.68              |
| 15:1O:73:LEU:HD21  | 15:1O:295:LYS:HB3  | 1.76                     | 0.68              |
| 59:8E:78:HIS:HE1   | 63:8I:12:LEU:CD1   | 2.03                     | 0.68              |
| 12:1L:556:ILE:HD11 | 38:1m:75:ILE:HG22  | 1.76                     | 0.68              |
| 25:1Z:108:GLU:H    | 30:1e:74:ARG:HH22  | 1.38                     | 0.68              |
| 58:8D:48:TRP:HE1   | 59:8E:56:ARG:HH11  | 1.42                     | 0.68              |
| 34:1i:68:ILE:O     | 34:1i:72:THR:HG22  | 1.95                     | 0.67              |
| 13:1M:453:MET:HE2  | 32:1g:77:VAL:CG1   | 2.22                     | 0.67              |
| 56:4B:132:GLU:HB3  | 56:4B:137:GLU:HG3  | 1.75                     | 0.67              |
| 56:4B:161:HIS:CE1  | 56:4B:207:MET:HE1  | 2.30                     | 0.67              |
| 57:8C:157:LYS:HA   | 57:8C:157:LYS:HE3  | 1.76                     | 0.67              |
| 67:8M:18:GLY:O     | 67:8M:22:THR:HG23  | 1.93                     | 0.67              |
| 39:1n:178:MET:HE2  | 39:1n:178:MET:HA   | 1.76                     | 0.67              |
| 47:3C:125:ALA:O    | 47:3C:129:MET:HG3  | 1.94                     | 0.67              |
| 23:1X:122:GLY:CA   | 27:1b:77:LEU:HD12  | 2.23                     | 0.67              |
| 55:4A:22:PHE:CE2   | 55:4A:105:LEU:HB3  | 2.29                     | 0.67              |
| 55:8A:15:ILE:HD11  | 55:8A:99:ASN:HA    | 1.76                     | 0.67              |
| 56:8B:41:ILE:HG23  | 56:8B:45:MET:HE2   | 1.76                     | 0.67              |
| 59:8E:75:ALA:HB1   | 59:8E:81:ILE:HD13  | 1.76                     | 0.67              |
| 7:1G:324:ASP:HB3   | 7:1G:571:ALA:HB1   | 1.77                     | 0.67              |
| 52:3U:49:GLN:OE1   | 52:3U:49:GLN:O     | 2.13                     | 0.67              |
| 55:8A:124:THR:CG2  | 55:8A:128:VAL:HG22 | 2.25                     | 0.67              |
| 55:8A:343:GLY:O    | 55:8A:347:LEU:HD22 | 1.94                     | 0.67              |
| 55:8A:434:SER:O    | 56:8B:10:GLN:NE2   | 2.28                     | 0.67              |
| 6:1F:364:PRO:HB2   | 6:1F:403:THR:HG22  | 1.75                     | 0.67              |
| 7:1G:190:MET:SD    | 7:1G:192:MET:HE3   | 2.35                     | 0.67              |
| 48:3D:284:GLU:OE2  | 48:3D:290:ARG:NH1  | 2.26                     | 0.67              |
| 49:3R:176:VAL:HG22 | 49:3R:212:ILE:HG23 | 1.77                     | 0.67              |
| 49:3V:53:GLU:HA    | 49:3V:56:ARG:HD2   | 1.75                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:418:PHE:HE2  | 75:4D:201:CDL:HB21 | 1.58                     | 0.67              |
| 57:4C:204:HIS:CE1  | 57:4C:249:TRP:HB2  | 2.30                     | 0.67              |
| 87:8C:307:PGV:H152 | 87:8C:307:PGV:H291 | 1.77                     | 0.67              |
| 66:8L:20:ARG:CZ    | 66:8L:24:MET:HE2   | 2.24                     | 0.67              |
| 20:1U:28:GLU:OE2   | 20:1U:29:LYS:HG2   | 1.94                     | 0.67              |
| 41:1p:5:ASP:HB3    | 41:1p:8:VAL:HG12   | 1.76                     | 0.67              |
| 47:3C:8:HIS:HB3    | 47:3C:11:MET:HB2   | 1.77                     | 0.67              |
| 49:3R:180:THR:O    | 49:3R:182:LYS:N    | 2.28                     | 0.67              |
| 63:4I:55:ASP:OD1   | 63:4I:58:LYS:HB2   | 1.94                     | 0.67              |
| 66:4L:41:ARG:CG    | 67:4M:40:TYR:CE2   | 2.57                     | 0.67              |
| 58:8D:34:SER:OG    | 58:8D:37:GLN:CG    | 2.42                     | 0.67              |
| 58:8D:81:ILE:HD12  | 58:8D:81:ILE:H     | 1.59                     | 0.67              |
| 69:1M:502:3PE:H371 | 29:1d:43:LEU:HB3   | 1.77                     | 0.67              |
| 36:1k:74:PHE:O     | 36:1k:78:VAL:HG22  | 1.95                     | 0.67              |
| 56:8B:28:LEU:HG    | 63:8I:35:TYR:HE2   | 1.59                     | 0.67              |
| 62:8H:57:ARG:HA    | 62:8H:60:TYR:HE1   | 1.58                     | 0.67              |
| 66:8L:35:ALA:O     | 66:8L:39:ILE:HD12  | 1.95                     | 0.67              |
| 12:1L:599:MET:HE1  | 14:1N:97:MET:SD    | 2.35                     | 0.67              |
| 58:4D:20:ARG:CD    | 58:4D:72:ASN:HD21  | 2.08                     | 0.67              |
| 55:8A:496:HIS:CE1  | 60:8F:57:ILE:HD11  | 2.30                     | 0.67              |
| 49:3E:151:LYS:HG3  | 49:3E:152:ILE:HG23 | 1.75                     | 0.67              |
| 55:8A:426:PHE:HZ   | 75:8B:303:CDL:H142 | 1.60                     | 0.67              |
| 60:8F:18:ARG:HD3   | 60:8F:22:MET:HE3   | 1.77                     | 0.67              |
| 22:1W:42:GLU:O     | 22:1W:42:GLU:OE2   | 2.14                     | 0.66              |
| 55:8A:124:THR:HG21 | 55:8A:128:VAL:HG22 | 1.76                     | 0.66              |
| 56:8B:13:THR:HA    | 56:8B:188:ARG:HH12 | 1.60                     | 0.66              |
| 62:8H:71:ALA:O     | 62:8H:75:ARG:HG2   | 1.95                     | 0.66              |
| 12:1L:499:MET:HE1  | 64:4J:37:THR:HG21  | 1.77                     | 0.66              |
| 23:1X:121:LEU:HD11 | 25:1Z:62:ILE:HG23  | 1.76                     | 0.66              |
| 33:1h:44:ASN:ND2   | 75:1h:202:CDL:OB9  | 2.28                     | 0.66              |
| 55:8A:147:ILE:HG23 | 55:8A:206:ILE:HB   | 1.77                     | 0.66              |
| 6:1F:224:ASN:ND2   | 73:1F:501:FMN:O2   | 2.29                     | 0.66              |
| 12:1L:151:SER:HB2  | 12:1L:248:HIS:HE1  | 1.60                     | 0.66              |
| 26:1a:44:GLN:HA    | 26:1a:47:LEU:HD12  | 1.76                     | 0.66              |
| 45:3A:250:LEU:HD12 | 49:3I:44:ASP:HB2   | 1.76                     | 0.66              |
| 45:3N:224:VAL:HG13 | 45:3N:225:GLU:OE1  | 1.94                     | 0.66              |
| 3:1C:40:VAL:HG12   | 3:1C:50:ILE:HG23   | 1.78                     | 0.66              |
| 41:1p:119:SER:O    | 41:1p:123:ASN:ND2  | 2.28                     | 0.66              |
| 63:4I:23:GLY:O     | 63:4I:27:VAL:HG12  | 1.95                     | 0.66              |
| 55:8A:407:GLN:OE1  | 55:8A:407:GLN:N    | 2.22                     | 0.66              |
| 1:1A:73:LEU:O      | 8:1H:160:TYR:OH    | 2.13                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:200:THR:HG21  | 6:1F:283:HIS:HA    | 1.77                     | 0.66              |
| 8:1H:24:GLU:OE2    | 8:1H:274:ARG:NH1   | 2.29                     | 0.66              |
| 45:3A:146:ARG:NH2  | 45:3A:308:GLN:OE1  | 2.29                     | 0.66              |
| 48:3D:161:GLY:HA2  | 48:3D:168:MET:HE1  | 1.77                     | 0.66              |
| 56:4B:216:LEU:HD22 | 56:4B:220:GLU:OE1  | 1.94                     | 0.66              |
| 58:8D:40:LEU:CD2   | 58:8D:59:LEU:HD21  | 2.25                     | 0.66              |
| 58:8D:43:LYS:HZ1   | 58:8D:46:ALA:HB3   | 1.61                     | 0.66              |
| 2:1B:34:ASP:HB2    | 2:1B:173:LEU:HB2   | 1.76                     | 0.66              |
| 9:1I:156:ASN:ND2   | 18:1R:34:GLU:OE1   | 2.27                     | 0.66              |
| 20:1T:58:PHE:HD2   | 20:1T:80:ILE:HG21  | 1.58                     | 0.66              |
| 26:1a:1:MET:HE2    | 26:1a:1:MET:H1     | 1.60                     | 0.66              |
| 42:1q:60:ARG:HH22  | 42:1q:95:ASP:HA    | 1.60                     | 0.66              |
| 48:3D:162:PRO:HB2  | 48:3Q:99:GLU:HG3   | 1.77                     | 0.66              |
| 57:8C:86:PHE:CE1   | 57:8C:90:GLU:OE2   | 2.48                     | 0.66              |
| 31:1f:5:GLN:O      | 31:1f:9:ASP:HB3    | 1.96                     | 0.66              |
| 69:3A:503:3PE:H362 | 47:3C:11:MET:HE2   | 0.74                     | 0.66              |
| 49:3R:209:GLU:HG2  | 49:3R:210:TRP:CD2  | 2.30                     | 0.66              |
| 1:1A:60:ILE:HG21   | 10:1J:168:ILE:HG21 | 1.78                     | 0.66              |
| 11:1K:55:LEU:HD13  | 30:1e:16:TRP:HE3   | 1.61                     | 0.66              |
| 20:1T:70:LEU:HD23  | 20:1T:76:ILE:HG23  | 1.76                     | 0.66              |
| 25:1Z:93:GLU:O     | 25:1Z:97:ILE:HG13  | 1.96                     | 0.66              |
| 49:3R:266:THR:OG1  | 49:3R:270:LEU:O    | 2.14                     | 0.66              |
| 55:8A:230:LEU:O    | 55:8A:234:LEU:HD22 | 1.95                     | 0.66              |
| 58:8D:78:TRP:O     | 58:8D:82:VAL:HG23  | 1.95                     | 0.66              |
| 6:1F:426:LEU:O     | 6:1F:430:MET:HG2   | 1.96                     | 0.66              |
| 7:1G:226:GLU:OE1   | 17:1Q:36:ARG:NH2   | 2.28                     | 0.66              |
| 11:1K:1:FME:O1     | 30:1e:72:MET:SD    | 2.54                     | 0.66              |
| 13:1M:312:ALA:O    | 13:1M:316:MET:HG3  | 1.95                     | 0.66              |
| 15:1O:63:THR:OG1   | 15:1O:302:ARG:NH2  | 2.29                     | 0.66              |
| 55:4A:412:ILE:HG12 | 58:4D:81:ILE:HG23  | 1.76                     | 0.66              |
| 87:8C:304:PGV:H221 | 87:8C:304:PGV:H31  | 1.78                     | 0.66              |
| 62:8H:20:PHE:HB2   | 62:8H:28:ASN:HD21  | 1.61                     | 0.66              |
| 4:1D:34:ASN:HB3    | 4:1D:36:VAL:HG22   | 1.77                     | 0.66              |
| 6:1F:105:CYS:H     | 6:1F:257:ASN:ND2   | 1.93                     | 0.66              |
| 13:1M:385:SER:CB   | 13:1M:396:MET:HE1  | 2.25                     | 0.66              |
| 55:8A:93:ALA:HA    | 55:8A:171:MET:CE   | 2.26                     | 0.66              |
| 7:1G:579:ARG:HG2   | 7:1G:636:VAL:HB    | 1.77                     | 0.65              |
| 55:8A:232:GLN:HB3  | 55:8A:292:MET:HE2  | 1.78                     | 0.65              |
| 3:1C:149:ARG:NH2   | 4:1D:77:ASP:OD2    | 2.29                     | 0.65              |
| 62:4H:56:TYR:CZ    | 68:4N:80:PRO:HD2   | 2.31                     | 0.65              |
| 57:8C:9:HIS:NE2    | 57:8C:64:GLU:OE2   | 2.24                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:127:HIS:O     | 2:1B:134:ARG:NH1   | 2.30                     | 0.65              |
| 6:1F:25:LEU:HD11   | 6:1F:267:THR:HG22  | 1.78                     | 0.65              |
| 11:1K:73:LEU:HD21  | 14:1N:41:ILE:HG13  | 1.78                     | 0.65              |
| 45:3N:240:GLU:HG3  | 45:3N:422:VAL:HB   | 1.79                     | 0.65              |
| 60:4F:70:ILE:HG21  | 60:4F:83:PRO:CD    | 2.26                     | 0.65              |
| 3:1C:195:ARG:NH2   | 9:1I:92:ILE:O      | 2.29                     | 0.65              |
| 55:8A:138:HIS:O    | 55:8A:213:ARG:NH2  | 2.29                     | 0.65              |
| 70:1M:503:PC1:H272 | 70:1M:503:PC1:H371 | 1.78                     | 0.65              |
| 55:8A:321:PHE:HA   | 55:8A:324:LEU:HD12 | 1.78                     | 0.65              |
| 20:1T:35:HIS:CE1   | 20:1T:38:LYS:HE3   | 2.32                     | 0.65              |
| 41:1p:158:GLN:O    | 41:1p:162:MET:HE3  | 1.97                     | 0.65              |
| 70:1B:203:PC1:H341 | 70:1q:201:PC1:H352 | 1.77                     | 0.65              |
| 7:1G:350:PRO:HB3   | 7:1G:464:THR:HG22  | 1.78                     | 0.65              |
| 20:1T:12:LYS:NZ    | 20:1T:32:VAL:HG13  | 2.11                     | 0.65              |
| 23:1X:72:GLN:HG2   | 23:1X:114:LEU:HD21 | 1.78                     | 0.65              |
| 46:3O:28:ARG:HH22  | 46:3O:390:GLY:HA3  | 1.62                     | 0.65              |
| 49:3V:77:ARG:O     | 49:3V:77:ARG:NE    | 2.30                     | 0.65              |
| 54:3X:38:TRP:HA    | 70:3X:101:PC1:H32  | 1.78                     | 0.65              |
| 87:4A:601:PGV:H62  | 64:4J:40:LEU:HD11  | 1.78                     | 0.65              |
| 55:8A:33:LEU:HB3   | 55:8A:61:HIS:HB2   | 1.78                     | 0.65              |
| 55:8A:232:GLN:HB3  | 55:8A:292:MET:CE   | 2.27                     | 0.65              |
| 6:1F:185:ILE:HG12  | 6:1F:359:CYS:HB2   | 1.79                     | 0.65              |
| 39:1n:12:GLN:HE22  | 39:1n:13:GLN:HG3   | 1.62                     | 0.65              |
| 55:4A:406:ASN:HD22 | 55:4A:409:TRP:HD1  | 1.43                     | 0.65              |
| 56:4B:89:GLU:HG2   | 68:4N:70:VAL:CG2   | 2.27                     | 0.65              |
| 59:4E:48:ILE:HD13  | 59:4E:71:VAL:HG21  | 1.79                     | 0.65              |
| 55:8A:151:HIS:NE2  | 55:8A:206:ILE:HG13 | 2.12                     | 0.65              |
| 55:8A:333:LYS:HZ1  | 55:8A:335:SER:CA   | 2.10                     | 0.65              |
| 57:8C:247:VAL:HG12 | 57:8C:251:PHE:CE1  | 2.32                     | 0.65              |
| 59:8E:33:MET:HE1   | 59:8E:67:ILE:CG2   | 2.27                     | 0.65              |
| 8:1H:31:MET:HE3    | 9:1I:41:LEU:HD22   | 1.79                     | 0.65              |
| 26:1a:67:GLU:OE1   | 26:1a:67:GLU:N     | 2.25                     | 0.65              |
| 75:1d:203:CDL:HA4  | 75:1d:203:CDL:H512 | 1.79                     | 0.65              |
| 49:3R:209:GLU:OE2  | 49:3R:209:GLU:N    | 2.21                     | 0.65              |
| 56:4B:61:VAL:O     | 56:4B:65:TRP:CE3   | 2.50                     | 0.65              |
| 55:8A:298:ASP:OD2  | 55:8A:300:ASP:HB2  | 1.97                     | 0.65              |
| 24:1Y:11:ILE:HG13  | 24:1Y:20:LYS:HE3   | 1.79                     | 0.65              |
| 48:3D:160:ASP:HB2  | 48:3D:171:ARG:HG2  | 1.79                     | 0.65              |
| 55:8A:190:ILE:HG23 | 87:8A:603:PGV:H252 | 1.79                     | 0.65              |
| 55:8A:271:MET:HG3  | 68:8N:12:HIS:HE1   | 1.60                     | 0.65              |
| 4:1D:34:ASN:HB2    | 15:1O:158:VAL:HG13 | 1.78                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:36:LYS:O      | 44:1s:65:GLN:NE2   | 2.30                     | 0.64              |
| 12:1L:2:ASN:HB3    | 12:1L:3:PRO:HD2    | 1.79                     | 0.64              |
| 12:1L:562:LEU:HD22 | 69:1N:901:3PE:H3B2 | 1.79                     | 0.64              |
| 17:1Q:9:GLN:CB     | 22:1W:23:ARG:HH21  | 2.10                     | 0.64              |
| 49:3E:231:PHE:HE1  | 49:3E:242:HIS:HB3  | 1.61                     | 0.64              |
| 56:4B:28:LEU:HD21  | 75:4B:303:CDL:H561 | 1.77                     | 0.64              |
| 55:8A:314:ILE:H    | 55:8A:314:ILE:HD12 | 1.62                     | 0.64              |
| 75:8B:303:CDL:HB21 | 75:8B:303:CDL:HB61 | 1.78                     | 0.64              |
| 66:8L:34:ALA:HA    | 66:8L:37:PHE:CD2   | 2.32                     | 0.64              |
| 1:1A:27:LEU:HD13   | 70:1A:202:PC1:H132 | 1.78                     | 0.64              |
| 14:1N:69:MET:HE3   | 14:1N:97:MET:CE    | 2.27                     | 0.64              |
| 22:1W:25:MET:O     | 22:1W:29:LYS:HG3   | 1.97                     | 0.64              |
| 52:3H:83:GLU:OE1   | 52:3H:83:GLU:N     | 2.26                     | 0.64              |
| 49:3R:151:LYS:HD3  | 49:3R:152:ILE:HB   | 1.78                     | 0.64              |
| 56:4B:89:GLU:OE2   | 68:4N:68:VAL:HB    | 1.97                     | 0.64              |
| 59:4E:52:LEU:HD22  | 59:4E:67:ILE:HD11  | 1.79                     | 0.64              |
| 65:4K:19:ALA:O     | 65:4K:23:THR:HG23  | 1.96                     | 0.64              |
| 59:8E:81:ILE:H     | 59:8E:81:ILE:HD12  | 1.62                     | 0.64              |
| 61:8G:29:ALA:O     | 61:8G:32:THR:HG22  | 1.98                     | 0.64              |
| 1:1A:41:PHE:HB2    | 4:1D:51:PHE:CE2    | 2.31                     | 0.64              |
| 5:1E:100:ILE:HD13  | 5:1E:156:ILE:HD12  | 1.78                     | 0.64              |
| 13:1M:365:THR:HG21 | 13:1M:444:LEU:HD21 | 1.80                     | 0.64              |
| 16:1P:92:ILE:HD11  | 16:1P:218:ILE:HD11 | 1.79                     | 0.64              |
| 69:1d:201:3PE:H221 | 70:1d:202:PC1:H221 | 1.78                     | 0.64              |
| 40:1o:56:ASP:OD1   | 40:1o:57:TYR:N     | 2.28                     | 0.64              |
| 47:3P:32:ASN:ND2   | 47:3P:228:ASP:OD1  | 2.29                     | 0.64              |
| 2:1B:33:LEU:HD13   | 70:1B:202:PC1:H381 | 1.80                     | 0.64              |
| 20:1T:73:PRO:O     | 20:1T:77:VAL:HG23  | 1.97                     | 0.64              |
| 47:3C:181:PHE:CE1  | 47:3P:53:MET:HE2   | 2.33                     | 0.64              |
| 52:3H:45:VAL:HG12  | 52:3H:95:VAL:HG22  | 1.79                     | 0.64              |
| 45:3N:141:ASN:HA   | 49:3V:47:ARG:HH21  | 1.61                     | 0.64              |
| 59:4E:48:ILE:CG2   | 59:4E:89:LEU:HD21  | 2.27                     | 0.64              |
| 59:8E:42:VAL:HG21  | 59:8E:81:ILE:HG21  | 1.78                     | 0.64              |
| 12:1L:528:TYR:CD1  | 37:1l:101:MET:HG2  | 2.33                     | 0.64              |
| 53:3J:36:GLU:OE1   | 54:3Y:34:TRP:NE1   | 2.30                     | 0.64              |
| 75:4B:303:CDL:HB21 | 75:4B:303:CDL:HB61 | 1.79                     | 0.64              |
| 7:1G:190:MET:HG2   | 7:1G:192:MET:HG2   | 1.80                     | 0.64              |
| 12:1L:401:MET:SD   | 12:1L:482:MET:HG3  | 2.37                     | 0.64              |
| 13:1M:54:LEU:HD21  | 33:1h:96:ILE:HD11  | 1.79                     | 0.64              |
| 13:1M:118:PHE:O    | 13:1M:122:PHE:HB3  | 1.97                     | 0.64              |
| 20:1U:25:ILE:HG12  | 20:1U:40:LEU:HD13  | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:3E:199:GLN:HB3  | 49:3E:204:ARG:HD3  | 1.78                     | 0.64              |
| 46:3O:196:GLN:HA   | 46:3O:227:ARG:HD3  | 1.79                     | 0.64              |
| 57:8C:59:ARG:CZ    | 57:8C:63:ARG:HH21  | 2.11                     | 0.64              |
| 12:1L:194:ASN:ND2  | 41:1p:106:GLN:OE1  | 2.31                     | 0.64              |
| 55:8A:409:TRP:HB2  | 55:8A:471:ILE:CD1  | 2.27                     | 0.64              |
| 58:8D:77:GLU:HB2   | 65:8K:10:HIS:CD2   | 2.33                     | 0.64              |
| 7:1G:620:ARG:NH1   | 7:1G:633:TYR:OH    | 2.31                     | 0.64              |
| 43:1r:45:SER:O     | 43:1r:51:ASN:ND2   | 2.26                     | 0.64              |
| 46:3O:28:ARG:NH2   | 46:3O:390:GLY:HA3  | 2.12                     | 0.64              |
| 56:4B:115:ASP:OD1  | 56:4B:115:ASP:O    | 2.16                     | 0.64              |
| 61:4G:83:GLU:OE1   | 61:4G:83:GLU:N     | 2.22                     | 0.64              |
| 33:1h:63:HIS:NE2   | 33:1h:76:ALA:O     | 2.30                     | 0.64              |
| 55:4A:35:LEU:HD21  | 55:4A:462:LEU:HB2  | 1.79                     | 0.64              |
| 87:4B:302:PGV:H91  | 87:4B:302:PGV:H251 | 1.80                     | 0.64              |
| 87:8A:601:PGV:H131 | 57:8C:22:LEU:HD21  | 1.80                     | 0.64              |
| 87:8B:301:PGV:H22  | 75:8D:201:CDL:H312 | 1.80                     | 0.64              |
| 34:1i:108:THR:HG22 | 34:1i:115:VAL:HB   | 1.79                     | 0.64              |
| 56:4B:200:CYS:SG   | 91:4B:304:CUA:CU2  | 1.88                     | 0.64              |
| 57:4C:180:GLU:HA   | 57:4C:180:GLU:OE2  | 1.97                     | 0.64              |
| 55:8A:407:GLN:NE2  | 87:8A:602:PGV:O05  | 2.31                     | 0.64              |
| 68:8N:23:GLY:O     | 68:8N:27:THR:OG1   | 2.11                     | 0.64              |
| 8:1H:156:MET:SD    | 8:1H:174:MET:HE3   | 2.36                     | 0.63              |
| 46:3B:34:VAL:HG11  | 46:3B:386:ALA:HB1  | 1.81                     | 0.63              |
| 51:3T:36:ASN:ND2   | 75:3T:101:CDL:OA4  | 2.31                     | 0.63              |
| 58:4D:126:MET:HG2  | 63:4I:68:ILE:HG21  | 1.80                     | 0.63              |
| 66:4L:28:TYR:CE2   | 87:4L:101:PGV:H302 | 2.33                     | 0.63              |
| 15:1O:320:LYS:O    | 29:1d:60:ARG:NH2   | 2.30                     | 0.63              |
| 46:3B:227:ARG:HG3  | 46:3B:229:GLY:H    | 1.64                     | 0.63              |
| 45:3N:444:LEU:HB2  | 75:3N:502:CDL:HB31 | 1.80                     | 0.63              |
| 68:8N:13:PRO:HA    | 68:8N:16:ILE:HG13  | 1.78                     | 0.63              |
| 1:1A:37:TYR:CE2    | 2:1B:80:PRO:HD2    | 2.33                     | 0.63              |
| 8:1H:223:PHE:O     | 8:1H:227:GLU:HG2   | 1.98                     | 0.63              |
| 10:1J:130:THR:HG22 | 25:1Z:121:MET:HE2  | 1.79                     | 0.63              |
| 14:1N:107:GLY:O    | 14:1N:187:MET:HE1  | 1.98                     | 0.63              |
| 22:1W:29:LYS:HZ2   | 22:1W:29:LYS:HB3   | 1.63                     | 0.63              |
| 24:1Y:35:VAL:HG23  | 69:1Y:202:3PE:H252 | 1.80                     | 0.63              |
| 53:3J:20:ARG:HB2   | 53:3J:23:THR:HG22  | 1.81                     | 0.63              |
| 55:8A:144:ASP:OD1  | 55:8A:213:ARG:NH1  | 2.30                     | 0.63              |
| 15:1O:265:ASN:CG   | 15:1O:268:GLU:HG2  | 2.22                     | 0.63              |
| 39:1n:13:GLN:O     | 39:1n:17:ARG:HG2   | 1.98                     | 0.63              |
| 41:1p:29:VAL:O     | 41:1p:33:THR:HG23  | 1.97                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:4K:44:PRO:HB3   | 65:4K:48:VAL:HG21  | 1.81                     | 0.63              |
| 55:8A:173:PRO:HB3  | 55:8A:511:ILE:HD13 | 1.81                     | 0.63              |
| 59:8E:24:ILE:HD12  | 59:8E:25:ASP:H     | 1.63                     | 0.63              |
| 60:8F:81:ARG:HG2   | 60:8F:88:HIS:CD2   | 2.34                     | 0.63              |
| 7:1G:672:TYR:HD1   | 7:1G:684:MET:HE1   | 1.64                     | 0.63              |
| 12:1L:6:SER:O      | 12:1L:10:THR:OG1   | 2.14                     | 0.63              |
| 58:4D:77:GLU:HG2   | 58:4D:81:ILE:HD11  | 1.79                     | 0.63              |
| 59:4E:41:LEU:O     | 59:4E:41:LEU:HD12  | 1.99                     | 0.63              |
| 55:8A:271:MET:HG3  | 68:8N:12:HIS:CE1   | 2.32                     | 0.63              |
| 55:8A:336:PRO:HB2  | 55:8A:394:VAL:HG11 | 1.80                     | 0.63              |
| 66:8L:18:LYS:NZ    | 66:8L:19:TRP:CH2   | 2.66                     | 0.63              |
| 8:1H:114:TYR:OH    | 10:1J:65:LEU:O     | 2.17                     | 0.63              |
| 12:1L:159:HIS:HB2  | 13:1M:416:ARG:HB3  | 1.81                     | 0.63              |
| 35:1j:65:GLY:CA    | 40:1o:30:PHE:CE1   | 2.82                     | 0.63              |
| 52:3H:49:CYS:O     | 52:3H:52:ILE:HG12  | 1.99                     | 0.63              |
| 75:3P:504:CDL:H151 | 75:3T:101:CDL:H521 | 1.80                     | 0.63              |
| 57:4C:107:ALA:HB1  | 62:4H:27:ARG:HH21  | 1.64                     | 0.63              |
| 58:4D:96:LEU:HD23  | 58:4D:96:LEU:C     | 2.22                     | 0.63              |
| 59:4E:31:LYS:HE2   | 60:4F:83:PRO:O     | 1.99                     | 0.63              |
| 55:8A:343:GLY:O    | 55:8A:347:LEU:CD2  | 2.46                     | 0.63              |
| 70:1B:203:PC1:H3C1 | 8:1H:53:LEU:HD11   | 1.81                     | 0.63              |
| 14:1N:280:THR:O    | 14:1N:284:MET:HG2  | 1.99                     | 0.63              |
| 55:4A:273:MET:HE3  | 55:4A:319:LYS:HE3  | 1.80                     | 0.63              |
| 59:4E:44:GLU:H     | 59:4E:47:ILE:HD11  | 1.64                     | 0.63              |
| 56:8B:100:MET:HE2  | 56:8B:157:GLU:HG3  | 1.81                     | 0.63              |
| 57:8C:87:ILE:O     | 57:8C:91:VAL:HG23  | 1.99                     | 0.63              |
| 58:8D:48:TRP:NE1   | 59:8E:56:ARG:HH11  | 1.95                     | 0.63              |
| 63:8I:22:VAL:O     | 63:8I:26:ILE:HG13  | 1.98                     | 0.63              |
| 8:1H:156:MET:HE1   | 8:1H:177:THR:HG21  | 1.81                     | 0.63              |
| 9:1I:146:GLU:OE2   | 42:1q:123:GLN:NE2  | 2.31                     | 0.63              |
| 27:1b:56:LEU:O     | 27:1b:56:LEU:HD12  | 1.99                     | 0.63              |
| 49:3I:71:ASN:O     | 49:3I:71:ASN:OD1   | 2.15                     | 0.63              |
| 47:3P:8:HIS:HB3    | 47:3P:11:MET:HB2   | 1.80                     | 0.63              |
| 53:3W:32:GLU:OE1   | 54:3X:34:TRP:NE1   | 2.32                     | 0.63              |
| 58:4D:40:LEU:HD21  | 58:4D:59:LEU:HG    | 1.80                     | 0.63              |
| 58:4D:56:LYS:NZ    | 59:4E:97:GLY:O     | 2.30                     | 0.63              |
| 62:4H:6:THR:HA     | 62:4H:9:LYS:CE     | 2.29                     | 0.63              |
| 75:8C:306:CDL:H212 | 75:8C:306:CDL:H311 | 1.80                     | 0.63              |
| 68:8N:7:THR:O      | 68:8N:11:LYS:HD3   | 1.98                     | 0.63              |
| 6:1F:250:ASN:ND2   | 6:1F:318:ASP:OD2   | 2.20                     | 0.63              |
| 7:1G:36:GLN:NE2    | 17:1Q:47:SER:O     | 2.32                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:207:ILE:HG22 | 14:1N:211:MET:HE2  | 1.80                     | 0.63              |
| 31:1f:23:GLY:O     | 31:1f:27:ASP:OD1   | 2.17                     | 0.63              |
| 38:1m:105:LYS:O    | 38:1m:109:ASP:OD1  | 2.17                     | 0.63              |
| 87:4A:603:PGV:H131 | 68:4N:22:ILE:HG21  | 1.79                     | 0.63              |
| 56:8B:141:ARG:HD3  | 56:8B:210:VAL:CG1  | 2.28                     | 0.63              |
| 12:1L:86:SER:O     | 12:1L:90:ILE:HG12  | 1.98                     | 0.62              |
| 51:3T:63:THR:O     | 51:3T:67:GLU:OE2   | 2.17                     | 0.62              |
| 59:4E:41:LEU:HD23  | 63:4I:10:ARG:HE    | 1.64                     | 0.62              |
| 61:4G:68:THR:HG22  | 61:4G:69:LEU:H     | 1.63                     | 0.62              |
| 87:4G:101:PGV:H261 | 87:4G:101:PGV:H92  | 1.81                     | 0.62              |
| 69:1M:504:3PE:H281 | 14:1N:246:VAL:HG11 | 1.81                     | 0.62              |
| 70:1M:505:PC1:H2D2 | 70:1M:505:PC1:H292 | 1.81                     | 0.62              |
| 14:1N:6:TYR:HE2    | 14:1N:46:LYS:HD2   | 1.64                     | 0.62              |
| 23:1X:19:VAL:O     | 26:1a:50:ARG:NH2   | 2.31                     | 0.62              |
| 56:8B:52:HIS:HD2   | 56:8B:56:MET:HE1   | 0.88                     | 0.62              |
| 57:8C:47:LEU:HD23  | 87:8C:303:PGV:H12  | 1.80                     | 0.62              |
| 58:8D:24:LEU:HD11  | 59:8E:33:MET:HE2   | 1.80                     | 0.62              |
| 1:1A:38:GLU:HB2    | 1:1A:43:PRO:HG3    | 1.79                     | 0.62              |
| 13:1M:16:TRP:NE1   | 13:1M:97:THR:OG1   | 2.32                     | 0.62              |
| 49:3E:123:VAL:HG13 | 53:3J:32:ALA:HA    | 1.81                     | 0.62              |
| 75:8C:306:CDL:H822 | 75:8C:306:CDL:H612 | 1.81                     | 0.62              |
| 4:1D:246:THR:HG23  | 21:1V:12:GLY:HA3   | 1.79                     | 0.62              |
| 13:1M:325:MET:HE1  | 13:1M:441:ILE:HB   | 1.82                     | 0.62              |
| 20:1T:54:MET:SD    | 20:1T:76:ILE:HG21  | 2.39                     | 0.62              |
| 56:4B:41:ILE:O     | 56:4B:45:MET:HG2   | 2.00                     | 0.62              |
| 55:8A:93:ALA:HA    | 55:8A:171:MET:HE1  | 1.80                     | 0.62              |
| 57:8C:59:ARG:NE    | 57:8C:63:ARG:NH2   | 2.41                     | 0.62              |
| 58:8D:53:MET:H     | 58:8D:53:MET:HE2   | 1.64                     | 0.62              |
| 3:1C:116:PRO:HD2   | 22:1W:18:LYS:HE2   | 1.81                     | 0.62              |
| 13:1M:147:LEU:HB3  | 69:1N:901:3PE:H332 | 1.81                     | 0.62              |
| 29:1d:89:ASP:HB2   | 33:1h:121:PRO:HG2  | 1.82                     | 0.62              |
| 65:8K:22:ALA:O     | 65:8K:26:VAL:HG12  | 2.00                     | 0.62              |
| 19:1S:88:ARG:CZ    | 19:1S:92:ASN:OD1   | 2.48                     | 0.62              |
| 38:1m:7:PRO:HB3    | 38:1m:13:LEU:HB2   | 1.82                     | 0.62              |
| 57:4C:129:VAL:CB   | 57:4C:180:GLU:OE1  | 2.47                     | 0.62              |
| 8:1H:156:MET:SD    | 8:1H:174:MET:HE1   | 2.40                     | 0.62              |
| 31:1f:56:TRP:HE1   | 33:1h:88:GLU:HG3   | 1.64                     | 0.62              |
| 63:4I:48:ALA:O     | 63:4I:52:ARG:HG3   | 1.99                     | 0.62              |
| 57:8C:6:HIS:NE2    | 57:8C:8:TYR:HB2    | 2.14                     | 0.62              |
| 57:8C:126:PRO:HA   | 57:8C:130:PRO:HG2  | 1.80                     | 0.62              |
| 65:8K:38:ILE:O     | 65:8K:38:ILE:HG13  | 1.97                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:1N:902:CDL:H221 | 75:1N:902:CDL:H371 | 1.80                     | 0.62              |
| 47:3C:149:LEU:HG   | 47:3C:291:VAL:HG22 | 1.79                     | 0.62              |
| 55:4A:241:PRO:O    | 55:4A:245:ILE:HG13 | 2.00                     | 0.62              |
| 55:8A:254:ILE:HG13 | 55:8A:344:PHE:CD2  | 2.34                     | 0.62              |
| 87:8A:603:PGV:H151 | 68:8N:22:ILE:HB    | 1.81                     | 0.62              |
| 92:8B:305:PSC:H261 | 92:8B:305:PSC:H10  | 1.82                     | 0.62              |
| 3:1C:22:LEU:HD12   | 3:1C:48:LEU:HB2    | 1.80                     | 0.62              |
| 6:1F:197:GLU:OE1   | 6:1F:204:ARG:NH2   | 2.33                     | 0.62              |
| 13:1M:108:MET:HE1  | 75:1X:201:CDL:H232 | 1.82                     | 0.62              |
| 54:3X:14:ALA:O     | 54:3X:18:ILE:HG12  | 1.99                     | 0.62              |
| 75:4C:305:CDL:H141 | 75:4C:305:CDL:H541 | 1.82                     | 0.62              |
| 55:8A:510:TYR:CG   | 60:8F:49:VAL:HG23  | 2.34                     | 0.62              |
| 57:8C:81:TYR:O     | 57:8C:85:LEU:HG    | 1.99                     | 0.62              |
| 3:1C:40:VAL:HG23   | 43:1r:68:VAL:HG23  | 1.80                     | 0.62              |
| 9:1I:7:MET:HG3     | 9:1I:7:MET:O       | 2.00                     | 0.62              |
| 12:1L:316:THR:HA   | 12:1L:319:ILE:HG12 | 1.82                     | 0.62              |
| 38:1m:105:LYS:O    | 38:1m:109:ASP:CG   | 2.43                     | 0.62              |
| 55:4A:195:LEU:HG   | 55:4A:245:ILE:HD13 | 1.80                     | 0.62              |
| 58:4D:54:ASP:C     | 58:4D:54:ASP:OD1   | 2.43                     | 0.62              |
| 75:4D:201:CDL:H402 | 75:4D:201:CDL:H592 | 1.81                     | 0.62              |
| 58:8D:84:THR:O     | 58:8D:88:PHE:HD1   | 1.82                     | 0.62              |
| 7:1G:273:GLY:O     | 7:1G:549:HIS:NE2   | 2.29                     | 0.61              |
| 16:1P:27:THR:HG21  | 16:1P:56:THR:HG22  | 1.82                     | 0.61              |
| 47:3C:112:THR:O    | 47:3C:196:HIS:NE2  | 2.33                     | 0.61              |
| 58:4D:120:THR:HG23 | 58:4D:134:PHE:HZ   | 1.65                     | 0.61              |
| 55:8A:333:LYS:NZ   | 55:8A:335:SER:HA   | 2.14                     | 0.61              |
| 55:8A:484:ALA:HB3  | 67:8M:2:TYR:HB2    | 1.81                     | 0.61              |
| 35:1j:38:TRP:CE3   | 35:1j:42:HIS:CE1   | 2.85                     | 0.61              |
| 49:3E:209:GLU:OE1  | 49:3E:209:GLU:N    | 2.24                     | 0.61              |
| 45:3N:444:LEU:HD11 | 69:3N:503:3PE:H12  | 1.81                     | 0.61              |
| 57:8C:22:LEU:O     | 57:8C:26:LEU:HG    | 2.00                     | 0.61              |
| 7:1G:229:ASP:OD2   | 7:1G:231:MET:HG2   | 2.00                     | 0.61              |
| 69:1Y:202:3PE:H341 | 69:1Y:203:3PE:H331 | 1.83                     | 0.61              |
| 33:1h:41:THR:O     | 33:1h:45:VAL:HG23  | 2.00                     | 0.61              |
| 57:8C:182:TYR:CE2  | 87:8C:305:PGV:H042 | 2.29                     | 0.61              |
| 64:8J:27:THR:O     | 64:8J:31:LEU:HD12  | 1.99                     | 0.61              |
| 1:1A:7:LEU:HD11    | 70:1H:403:PC1:H342 | 1.83                     | 0.61              |
| 6:1F:21:ILE:HG23   | 6:1F:117:LYS:HZ1   | 1.66                     | 0.61              |
| 75:1q:203:CDL:H181 | 75:1q:203:CDL:H331 | 1.82                     | 0.61              |
| 53:3J:33:LEU:HD11  | 54:3Y:48:ILE:HG21  | 1.81                     | 0.61              |
| 49:3R:214:ILE:N    | 49:3R:259:GLU:O    | 2.25                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:8A:333:LYS:NZ   | 55:8A:335:SER:HB3  | 2.14                     | 0.61              |
| 87:8B:301:PGV:H05  | 75:8D:201:CDL:HA32 | 1.81                     | 0.61              |
| 62:8H:25:GLN:NE2   | 62:8H:28:ASN:OD1   | 2.34                     | 0.61              |
| 13:1M:6:ILE:HG12   | 75:1X:201:CDL:H652 | 1.82                     | 0.61              |
| 19:1S:43:LEU:HD12  | 19:1S:47:ASN:HD21  | 1.66                     | 0.61              |
| 20:1T:32:VAL:HG12  | 20:1T:74:GLN:HE21  | 1.65                     | 0.61              |
| 46:3O:116:ILE:HG13 | 46:3O:120:MET:HE2  | 1.82                     | 0.61              |
| 47:3P:377:LEU:HG   | 50:3S:20:TYR:HE2   | 1.66                     | 0.61              |
| 64:4J:16:ASN:CG    | 64:4J:18:LEU:HD13  | 2.25                     | 0.61              |
| 56:8B:133:MET:SD   | 58:8D:119:GLN:NE2  | 2.73                     | 0.61              |
| 6:1F:21:ILE:HG21   | 6:1F:230:VAL:HG12  | 1.81                     | 0.61              |
| 7:1G:11:VAL:HG11   | 7:1G:73:VAL:HB     | 1.82                     | 0.61              |
| 19:1S:43:LEU:HD12  | 19:1S:43:LEU:O     | 2.00                     | 0.61              |
| 49:3R:239:HIS:CE1  | 49:3R:253:PRO:HD2  | 2.36                     | 0.61              |
| 55:4A:469:ILE:CD1  | 67:4M:26:PHE:CZ    | 2.83                     | 0.61              |
| 55:8A:86:MET:HB3   | 55:8A:182:PRO:HG2  | 1.82                     | 0.61              |
| 87:8A:601:PGV:H62  | 64:8J:40:LEU:HD11  | 1.82                     | 0.61              |
| 57:8C:182:TYR:HE2  | 87:8C:305:PGV:C04  | 2.12                     | 0.61              |
| 15:1O:294:GLN:O    | 15:1O:298:GLU:HG3  | 2.01                     | 0.61              |
| 20:1T:5:PRO:HB2    | 20:1T:86:VAL:HG13  | 1.83                     | 0.61              |
| 34:1i:86:LYS:HG2   | 34:1i:87:TYR:CE1   | 2.36                     | 0.61              |
| 40:1o:21:MET:HE1   | 40:1o:101:PHE:HA   | 1.81                     | 0.61              |
| 7:1G:347:GLU:HB2   | 7:1G:496:ILE:HD12  | 1.82                     | 0.61              |
| 70:1I:203:PC1:H31  | 25:1Z:28:ARG:HG3   | 1.83                     | 0.61              |
| 13:1M:71:TRP:CG    | 70:1M:505:PC1:H2C2 | 2.36                     | 0.61              |
| 49:3E:261:PRO:HG2  | 49:3E:273:VAL:HG21 | 1.82                     | 0.61              |
| 47:3P:216:ASP:OD1  | 47:3P:216:ASP:O    | 2.18                     | 0.61              |
| 57:4C:86:PHE:HZ    | 87:4C:306:PGV:H301 | 1.65                     | 0.61              |
| 3:1C:137:MET:HE1   | 3:1C:153:THR:HG23  | 1.82                     | 0.61              |
| 7:1G:594:ARG:NH1   | 22:1W:122:PHE:O    | 2.34                     | 0.61              |
| 75:3A:501:CDL:H151 | 75:3A:501:CDL:H321 | 1.82                     | 0.61              |
| 52:3H:60:GLU:O     | 52:3H:64:LEU:HG    | 2.00                     | 0.61              |
| 47:3P:132:VAL:HA   | 47:3P:139:SER:HB3  | 1.83                     | 0.61              |
| 47:3P:215:MET:HB2  | 51:3T:10:MET:HE2   | 1.83                     | 0.61              |
| 48:3Q:132:THR:HA   | 48:3Q:179:MET:HE3  | 1.83                     | 0.61              |
| 57:8C:45:LEU:HD11  | 64:8J:38:LEU:HG    | 1.82                     | 0.61              |
| 70:1A:202:PC1:H331 | 70:1A:202:PC1:H262 | 1.82                     | 0.61              |
| 4:1D:52:GLY:N      | 4:1D:53:PRO:HD3    | 2.14                     | 0.61              |
| 8:1H:253:GLU:O     | 8:1H:257:ILE:HD12  | 2.01                     | 0.61              |
| 12:1L:90:ILE:HD12  | 12:1L:129:MET:SD   | 2.40                     | 0.61              |
| 19:1S:24:GLN:HE22  | 19:1S:56:GLU:HG3   | 1.66                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:91:LYS:HB2    | 6:1F:131:ALA:HA    | 1.81                     | 0.60              |
| 7:1G:104:ASP:O     | 7:1G:108:CYS:N     | 2.33                     | 0.60              |
| 7:1G:284:ILE:HG23  | 7:1G:294:THR:HG21  | 1.83                     | 0.60              |
| 15:1O:303:LYS:H    | 15:1O:309:ASN:HD21 | 1.47                     | 0.60              |
| 35:1j:69:ASP:HB3   | 40:1o:117:ARG:HH12 | 1.67                     | 0.60              |
| 36:1k:77:PHE:O     | 36:1k:81:VAL:HG13  | 2.01                     | 0.60              |
| 37:1l:157:GLU:O    | 40:1o:33:ARG:NH2   | 2.32                     | 0.60              |
| 58:8D:52:SER:OG    | 58:8D:54:ASP:OD1   | 2.19                     | 0.60              |
| 62:8H:57:ARG:HA    | 62:8H:60:TYR:CD1   | 2.35                     | 0.60              |
| 7:1G:46:LEU:O      | 17:1Q:116:LYS:NZ   | 2.34                     | 0.60              |
| 13:1M:12:LEU:HD22  | 13:1M:97:THR:HG23  | 1.83                     | 0.60              |
| 37:1l:138:LEU:O    | 37:1l:142:ARG:HB2  | 2.01                     | 0.60              |
| 49:3E:161:GLU:HA   | 49:3E:178:HIS:HB3  | 1.82                     | 0.60              |
| 64:4J:33:ARG:NH1   | 87:4J:101:PGV:H181 | 2.16                     | 0.60              |
| 57:8C:233:PHE:HA   | 57:8C:236:GLU:OE1  | 2.01                     | 0.60              |
| 58:8D:68:PHE:HE1   | 59:8E:69:GLU:HB2   | 1.61                     | 0.60              |
| 4:1D:166:PRO:HG3   | 4:1D:228:MET:HG3   | 1.83                     | 0.60              |
| 12:1L:596:MET:O    | 12:1L:600:THR:OG1  | 2.10                     | 0.60              |
| 45:3A:354:VAL:HG21 | 45:3A:404:ALA:HA   | 1.83                     | 0.60              |
| 55:4A:336:PRO:HB2  | 55:4A:394:VAL:HG11 | 1.83                     | 0.60              |
| 55:8A:6:TRP:HE3    | 55:8A:18:LEU:HD21  | 1.66                     | 0.60              |
| 8:1H:149:ILE:HG21  | 8:1H:185:TRP:HB2   | 1.84                     | 0.60              |
| 13:1M:332:THR:HG22 | 13:1M:433:GLU:HG2  | 1.83                     | 0.60              |
| 45:3N:173:ASN:HA   | 45:3N:176:LYS:HG2  | 1.84                     | 0.60              |
| 46:3O:107:TYR:HB3  | 46:3O:123:LEU:HD11 | 1.84                     | 0.60              |
| 58:4D:80:THR:HG21  | 65:4K:10:HIS:ND1   | 2.15                     | 0.60              |
| 58:8D:48:TRP:HZ3   | 59:8E:61:PHE:CG    | 2.17                     | 0.60              |
| 64:8J:30:ILE:O     | 64:8J:34:VAL:HG12  | 2.01                     | 0.60              |
| 68:8N:5:ILE:HG23   | 68:8N:6:ILE:HD13   | 1.82                     | 0.60              |
| 5:1E:52:ASP:OD2    | 6:1F:179:ARG:NH1   | 2.35                     | 0.60              |
| 6:1F:105:CYS:H     | 6:1F:257:ASN:HD22  | 1.50                     | 0.60              |
| 12:1L:288:THR:HG21 | 12:1L:307:SER:HB3  | 1.84                     | 0.60              |
| 13:1M:243:MET:HE3  | 13:1M:301:ILE:HG21 | 1.82                     | 0.60              |
| 16:1P:4:ALA:HB2    | 18:1R:24:ARG:HH21  | 1.65                     | 0.60              |
| 25:1Z:86:MET:HE1   | 25:1Z:125:TYR:CE2  | 2.36                     | 0.60              |
| 33:1h:74:TRP:O     | 33:1h:78:THR:HG22  | 2.02                     | 0.60              |
| 49:3E:164:ASN:HB3  | 49:3E:177:ARG:HD3  | 1.84                     | 0.60              |
| 49:3R:212:ILE:HD13 | 49:3R:271:VAL:HG21 | 1.83                     | 0.60              |
| 55:4A:426:PHE:HZ   | 75:4B:303:CDL:H142 | 1.66                     | 0.60              |
| 59:4E:33:MET:HE1   | 59:4E:67:ILE:HD12  | 1.83                     | 0.60              |
| 68:8N:8:GLN:HA     | 68:8N:11:LYS:HE2   | 1.83                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:150:PRO:HG3   | 4:1D:189:MET:HE3   | 1.83                     | 0.60              |
| 4:1D:165:THR:OG1   | 8:1H:275:ALA:O     | 2.19                     | 0.60              |
| 7:1G:194:GLU:HG2   | 7:1G:195:LEU:HG    | 1.83                     | 0.60              |
| 14:1N:95:MET:HE2   | 14:1N:149:ILE:HG23 | 1.84                     | 0.60              |
| 48:3D:289:HIS:O    | 48:3D:293:MET:HG3  | 2.01                     | 0.60              |
| 46:3O:212:SER:OG   | 46:3O:215:VAL:HG12 | 2.02                     | 0.60              |
| 49:3R:239:HIS:CD2  | 49:3R:240:GLY:N    | 2.67                     | 0.60              |
| 55:4A:33:LEU:HB3   | 55:4A:61:HIS:HB2   | 1.84                     | 0.60              |
| 56:4B:112:ASP:OD1  | 56:4B:113:TYR:N    | 2.35                     | 0.60              |
| 57:8C:59:ARG:CZ    | 57:8C:63:ARG:NH2   | 2.65                     | 0.60              |
| 1:1A:92:LEU:O      | 1:1A:96:ILE:HG12   | 2.02                     | 0.60              |
| 5:1E:37:ASN:ND2    | 44:1s:55:ASN:HD21  | 2.00                     | 0.60              |
| 5:1E:110:LEU:HB3   | 6:1F:261:HIS:CD2   | 2.31                     | 0.60              |
| 6:1F:31:TRP:HE1    | 44:1s:42:GLN:NE2   | 2.00                     | 0.60              |
| 10:1J:7:PHE:CE1    | 11:1K:3:LEU:HD13   | 2.37                     | 0.60              |
| 48:3D:228:GLY:HA3  | 52:3H:79:ASP:H     | 1.65                     | 0.60              |
| 46:3O:49:LEU:HD21  | 46:3O:204:MET:HE3  | 1.83                     | 0.60              |
| 58:4D:82:VAL:O     | 58:4D:86:LEU:CD1   | 2.50                     | 0.60              |
| 55:8A:106:PRO:O    | 55:8A:110:LEU:HD13 | 2.01                     | 0.60              |
| 57:8C:47:LEU:HD21  | 87:8C:303:PGV:H12  | 1.84                     | 0.60              |
| 2:1B:81:ARG:NE     | 8:1H:61:LEU:HD21   | 2.17                     | 0.60              |
| 4:1D:143:GLU:OE2   | 4:1D:278:TYR:OH    | 2.17                     | 0.60              |
| 6:1F:125:GLY:O     | 6:1F:129:MET:HG3   | 2.01                     | 0.60              |
| 7:1G:117:GLN:O     | 7:1G:121:MET:HG2   | 2.02                     | 0.60              |
| 7:1G:316:ALA:HB3   | 7:1G:519:PRO:HG3   | 1.83                     | 0.60              |
| 14:1N:339:MET:HE2  | 29:1d:34:MET:SD    | 2.41                     | 0.60              |
| 37:1l:112:MET:HA   | 37:1l:112:MET:HE3  | 1.83                     | 0.60              |
| 55:4A:80:ASN:OD1   | 55:4A:98:ASN:ND2   | 2.32                     | 0.60              |
| 56:4B:102:HIS:NE2  | 56:4B:107:SER:OG   | 2.30                     | 0.60              |
| 56:8B:95:LEU:HD12  | 56:8B:96:THR:N     | 2.16                     | 0.60              |
| 57:8C:56:GLN:O     | 57:8C:60:ASP:OD1   | 2.19                     | 0.60              |
| 57:8C:59:ARG:HD2   | 57:8C:63:ARG:HH21  | 1.66                     | 0.60              |
| 61:8G:68:THR:HG22  | 61:8G:69:LEU:H     | 1.66                     | 0.60              |
| 64:8J:48:TYR:CE1   | 87:8J:101:PGV:H032 | 2.36                     | 0.60              |
| 1:1A:53:MET:CE     | 10:1J:172:THR:HG23 | 2.32                     | 0.60              |
| 8:1H:156:MET:CG    | 8:1H:174:MET:HE1   | 2.32                     | 0.60              |
| 10:1J:99:MET:CE    | 10:1J:100:GLU:N    | 2.65                     | 0.60              |
| 69:1M:504:3PE:H2   | 14:1N:239:VAL:HG22 | 1.83                     | 0.60              |
| 14:1N:142:LEU:HB3  | 14:1N:194:LEU:HD21 | 1.84                     | 0.60              |
| 55:8A:124:THR:HG21 | 55:8A:128:VAL:HA   | 1.83                     | 0.60              |
| 62:8H:17:ASP:OD1   | 62:8H:19:ARG:N     | 2.27                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:91:THR:HG21   | 4:1D:85:ARG:HG2    | 1.84                     | 0.60              |
| 69:1K:101:3PE:H3C1 | 69:1K:101:3PE:H2C1 | 1.84                     | 0.60              |
| 49:3E:219:HIS:HB3  | 72:3E:301:FES:S1   | 2.42                     | 0.60              |
| 49:3R:123:VAL:HG13 | 53:3W:28:ALA:HA    | 1.84                     | 0.60              |
| 55:4A:253:MET:HG2  | 55:4A:396:TRP:HZ3  | 1.65                     | 0.60              |
| 57:4C:88:ILE:HG12  | 75:4C:305:CDL:H621 | 1.84                     | 0.60              |
| 62:4H:19:ARG:C     | 62:4H:20:PHE:HD1   | 2.09                     | 0.60              |
| 75:8C:306:CDL:H191 | 75:8C:306:CDL:H322 | 1.84                     | 0.60              |
| 8:1H:175:ILE:O     | 8:1H:179:TRP:HB3   | 2.02                     | 0.59              |
| 14:1N:266:ILE:HG22 | 14:1N:270:MET:HE2  | 1.83                     | 0.59              |
| 15:1O:318:TRP:HB2  | 29:1d:58:LEU:HD12  | 1.82                     | 0.59              |
| 51:3G:73:ARG:NH2   | 52:3H:82:GLU:HG2   | 2.16                     | 0.59              |
| 49:3R:219:HIS:HB3  | 72:3R:301:FES:S1   | 2.42                     | 0.59              |
| 55:4A:302:ARG:NH2  | 56:4B:88:ASP:OD1   | 2.35                     | 0.59              |
| 64:8J:40:LEU:HD12  | 87:8J:101:PGV:H142 | 1.83                     | 0.59              |
| 4:1D:130:PRO:HG2   | 4:1D:135:GLN:HE21  | 1.66                     | 0.59              |
| 12:1L:378:LEU:HD12 | 35:1j:32:MET:HE1   | 1.85                     | 0.59              |
| 20:1T:58:PHE:CD2   | 20:1T:80:ILE:HG21  | 2.36                     | 0.59              |
| 32:1g:120:LEU:CD2  | 32:1g:121:PRO:HD2  | 2.32                     | 0.59              |
| 55:4A:321:PHE:HA   | 55:4A:324:LEU:HD12 | 1.84                     | 0.59              |
| 56:4B:33:LEU:HD12  | 63:4I:28:SER:HB2   | 1.84                     | 0.59              |
| 68:4N:9:ALA:HB1    | 68:4N:16:ILE:CD1   | 2.32                     | 0.59              |
| 55:8A:371:TYR:HD2  | 55:8A:428:GLN:HG2  | 1.65                     | 0.59              |
| 55:8A:452:THR:HG22 | 55:8A:456:MET:HE2  | 1.84                     | 0.59              |
| 56:8B:9:PHE:CE1    | 56:8B:24:HIS:CD2   | 2.90                     | 0.59              |
| 65:8K:13:TYR:HB2   | 65:8K:17:ILE:HD11  | 1.83                     | 0.59              |
| 1:1A:105:GLU:HG3   | 10:1J:169:MET:CE   | 2.17                     | 0.59              |
| 6:1F:31:TRP:HE1    | 44:1s:42:GLN:HE22  | 1.50                     | 0.59              |
| 6:1F:305:PRO:HD3   | 6:1F:413:TRP:HB3   | 1.84                     | 0.59              |
| 12:1L:561:ILE:HG23 | 70:1Y:207:PC1:H2B2 | 1.84                     | 0.59              |
| 13:1M:207:MET:HG3  | 13:1M:294:MET:HB3  | 1.82                     | 0.59              |
| 14:1N:316:GLN:HA   | 15:1O:302:ARG:HH12 | 1.66                     | 0.59              |
| 47:3C:149:LEU:HD11 | 47:3C:281:LEU:HD11 | 1.83                     | 0.59              |
| 64:4J:36:MET:HB3   | 87:4J:101:PGV:H182 | 1.84                     | 0.59              |
| 55:8A:100:MET:HE2  | 55:8A:104:LEU:HD21 | 1.84                     | 0.59              |
| 55:8A:265:LYS:HB3  | 55:8A:490:THR:HG21 | 1.84                     | 0.59              |
| 67:8M:24:LEU:HB3   | 67:8M:28:ILE:HD11  | 1.84                     | 0.59              |
| 70:1B:202:PC1:H3G1 | 70:1B:203:PC1:H3E1 | 1.83                     | 0.59              |
| 7:1G:383:ASN:ND2   | 7:1G:665:GLN:O     | 2.35                     | 0.59              |
| 13:1M:453:MET:CE   | 32:1g:80:LEU:HD12  | 2.30                     | 0.59              |
| 32:1g:118:ILE:HD11 | 41:1p:159:LYS:HG3  | 1.85                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:1o:27:ASP:N     | 40:1o:27:ASP:OD1   | 2.35                     | 0.59              |
| 47:3C:53:MET:HE2   | 47:3P:181:PHE:CZ   | 2.38                     | 0.59              |
| 47:3C:270:PRO:HB2  | 47:3C:274:PHE:HB2  | 1.83                     | 0.59              |
| 49:3R:235:TYR:HA   | 49:3R:242:HIS:HA   | 1.83                     | 0.59              |
| 58:4D:95:LEU:HD21  | 67:4M:27:LEU:HD13  | 1.85                     | 0.59              |
| 59:4E:45:PRO:HB2   | 59:4E:88:GLU:CG    | 2.31                     | 0.59              |
| 57:8C:204:HIS:NE2  | 57:8C:249:TRP:HB2  | 2.16                     | 0.59              |
| 58:8D:85:ALA:O     | 58:8D:89:ILE:CD1   | 2.41                     | 0.59              |
| 2:1B:63:ALA:HB2    | 2:1B:69:MET:HE2    | 1.85                     | 0.59              |
| 4:1D:259:MET:HE3   | 4:1D:421:GLN:HA    | 1.84                     | 0.59              |
| 7:1G:243:ARG:HG2   | 7:1G:244:THR:HG23  | 1.84                     | 0.59              |
| 10:1J:130:THR:HG22 | 25:1Z:121:MET:CE   | 2.33                     | 0.59              |
| 12:1L:63:ILE:HD11  | 34:1i:85:LEU:HD22  | 1.84                     | 0.59              |
| 12:1L:566:THR:O    | 12:1L:570:GLN:HG2  | 2.03                     | 0.59              |
| 13:1M:116:ILE:O    | 13:1M:120:ILE:HG12 | 2.03                     | 0.59              |
| 15:1O:3:TYR:HH     | 15:1O:257:HIS:HD1  | 1.49                     | 0.59              |
| 47:3C:129:MET:HE1  | 47:3C:181:PHE:CB   | 2.32                     | 0.59              |
| 5:1E:159:ASN:HB2   | 5:1E:184:PRO:HB3   | 1.82                     | 0.59              |
| 7:1G:693:GLU:HB3   | 7:1G:697:ALA:HB2   | 1.84                     | 0.59              |
| 12:1L:184:LEU:HD13 | 13:1M:393:ILE:HG21 | 1.83                     | 0.59              |
| 35:1j:57:SER:OG    | 35:1j:58:GLN:OE1   | 2.19                     | 0.59              |
| 40:1o:65:LEU:O     | 40:1o:69:LYS:HG3   | 2.02                     | 0.59              |
| 45:3A:140:GLU:O    | 45:3A:143:SER:OG   | 2.20                     | 0.59              |
| 46:3B:124:LEU:HD12 | 46:3B:223:PHE:HB2  | 1.85                     | 0.59              |
| 55:4A:306:THR:HG23 | 55:4A:310:MET:HE1  | 1.83                     | 0.59              |
| 56:4B:146:MET:HE2  | 56:4B:214:VAL:C    | 2.28                     | 0.59              |
| 55:8A:5:ARG:HB2    | 66:8L:3:TYR:CE2    | 2.38                     | 0.59              |
| 57:8C:206:LEU:O    | 57:8C:210:ILE:HG12 | 2.03                     | 0.59              |
| 64:8J:33:ARG:O     | 64:8J:37:THR:HG22  | 2.03                     | 0.59              |
| 68:8N:17:PRO:HD2   | 68:8N:18:LEU:H     | 1.66                     | 0.59              |
| 20:1U:4:PRO:HD2    | 20:1U:4:PRO:O      | 2.02                     | 0.59              |
| 56:4B:27:THR:O     | 56:4B:31:VAL:HG23  | 2.03                     | 0.59              |
| 55:8A:51:ASP:OD2   | 56:8B:204:HIS:HB3  | 2.02                     | 0.59              |
| 59:8E:44:GLU:HG2   | 59:8E:45:PRO:HD2   | 1.84                     | 0.59              |
| 2:1B:86:MET:HE2    | 2:1B:103:VAL:HG23  | 1.84                     | 0.59              |
| 14:1N:272:LYS:HD3  | 33:1h:108:LEU:HD21 | 1.84                     | 0.59              |
| 24:1Y:85:ASP:OD2   | 24:1Y:87:LEU:HB3   | 2.03                     | 0.59              |
| 40:1o:3:HIS:ND1    | 40:1o:4:LEU:HD23   | 2.16                     | 0.59              |
| 42:1q:34:ARG:NH1   | 42:1q:54:GLN:OE1   | 2.35                     | 0.59              |
| 46:3O:35:ILE:HD13  | 46:3O:206:LEU:HB3  | 1.85                     | 0.59              |
| 87:8B:302:PGV:H62  | 68:8N:29:ALA:HB1   | 1.84                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:8C:7:ALA:HB2    | 60:8F:31:TYR:HB3   | 1.85                     | 0.59              |
| 68:8N:16:ILE:O     | 68:8N:20:VAL:HG23  | 2.03                     | 0.59              |
| 2:1B:144:ILE:HG13  | 2:1B:163:LEU:HB2   | 1.83                     | 0.59              |
| 5:1E:151:ALA:HB1   | 5:1E:152:PRO:HD2   | 1.84                     | 0.59              |
| 6:1F:129:MET:HE1   | 6:1F:221:THR:HB    | 1.83                     | 0.59              |
| 12:1L:188:TRP:CD2  | 12:1L:212:PRO:HG3  | 2.38                     | 0.59              |
| 16:1P:325:ARG:HG3  | 16:1P:326:TRP:CE2  | 2.38                     | 0.59              |
| 53:3W:40:ASP:O     | 53:3W:44:GLU:HG3   | 2.02                     | 0.59              |
| 56:4B:61:VAL:C     | 56:4B:65:TRP:CE3   | 2.81                     | 0.59              |
| 87:4B:301:PGV:H312 | 75:4D:201:CDL:H462 | 1.85                     | 0.59              |
| 59:4E:48:ILE:HD11  | 59:4E:71:VAL:HG21  | 1.84                     | 0.59              |
| 61:4G:73:PRO:HA    | 61:4G:83:GLU:OE2   | 2.02                     | 0.59              |
| 55:8A:157:SER:HB2  | 55:8A:199:LEU:HD11 | 1.85                     | 0.59              |
| 75:8B:303:CDL:H811 | 75:8B:303:CDL:H262 | 1.84                     | 0.59              |
| 87:8C:303:PGV:H332 | 93:8C:308:PEK:H322 | 1.85                     | 0.59              |
| 2:1B:50:PHE:CE1    | 2:1B:103:VAL:HG21  | 2.38                     | 0.59              |
| 14:1N:84:TRP:HB2   | 30:1e:18:THR:HA    | 1.83                     | 0.59              |
| 34:1i:39:VAL:HG12  | 34:1i:44:GLN:HG3   | 1.85                     | 0.59              |
| 45:3A:131:ARG:HD3  | 45:3A:175:ARG:HA   | 1.83                     | 0.59              |
| 47:3P:237:LEU:HD13 | 48:3Q:212:MET:HG3  | 1.85                     | 0.59              |
| 55:4A:343:GLY:HA2  | 87:4B:301:PGV:H062 | 1.84                     | 0.59              |
| 59:4E:96:LEU:HD13  | 59:4E:98:ILE:HD11  | 1.84                     | 0.59              |
| 56:8B:116:LEU:HD21 | 56:8B:226:MET:HE2  | 1.83                     | 0.59              |
| 57:8C:6:HIS:HD2    | 57:8C:8:TYR:CD2    | 2.20                     | 0.59              |
| 57:8C:60:ASP:O     | 57:8C:64:GLU:HG3   | 2.02                     | 0.59              |
| 65:8K:38:ILE:HD11  | 65:8K:40:TRP:CH2   | 2.32                     | 0.59              |
| 7:1G:157:THR:HB    | 7:1G:161:ARG:HE    | 1.67                     | 0.58              |
| 11:1K:33:LEU:HA    | 11:1K:36:MET:HE2   | 1.84                     | 0.58              |
| 24:1Y:104:THR:HG22 | 69:1Y:203:3PE:H11  | 1.85                     | 0.58              |
| 34:1i:85:LEU:HD23  | 34:1i:89:VAL:HG21  | 1.85                     | 0.58              |
| 46:3B:314:ALA:HA   | 49:3I:63:PRO:HD3   | 1.83                     | 0.58              |
| 49:3E:125:VAL:HG21 | 70:3J:101:PC1:H362 | 1.85                     | 0.58              |
| 49:3E:242:HIS:O    | 49:3E:250:ARG:N    | 2.35                     | 0.58              |
| 55:4A:138:HIS:O    | 55:4A:213:ARG:NH2  | 2.36                     | 0.58              |
| 57:8C:182:TYR:OH   | 87:8C:305:PGV:H05  | 2.03                     | 0.58              |
| 58:8D:26:ASP:OD1   | 58:8D:26:ASP:N     | 2.36                     | 0.58              |
| 58:8D:99:GLU:OE2   | 58:8D:104:TYR:CD2  | 2.55                     | 0.58              |
| 61:8G:16:TRP:HA    | 61:8G:19:LEU:HD12  | 1.84                     | 0.58              |
| 9:1I:43:ARG:HA     | 43:1r:11:ARG:HH21  | 1.68                     | 0.58              |
| 13:1M:166:TYR:O    | 13:1M:170:THR:HG23 | 2.02                     | 0.58              |
| 13:1M:329:LEU:O    | 13:1M:332:THR:OG1  | 2.21                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:95:MET:HE2   | 14:1N:149:ILE:HA   | 1.85                     | 0.58              |
| 17:1Q:77:ASP:C     | 17:1Q:77:ASP:OD1   | 2.46                     | 0.58              |
| 33:1h:50:ALA:HB2   | 41:1p:60:TYR:CE1   | 2.38                     | 0.58              |
| 48:3Q:212:MET:HA   | 48:3Q:212:MET:HE3  | 1.86                     | 0.58              |
| 55:4A:72:PRO:O     | 55:4A:77:GLY:N     | 2.33                     | 0.58              |
| 56:4B:85:TYR:O     | 56:4B:89:GLU:OE1   | 2.21                     | 0.58              |
| 60:4F:46:PRO:HG2   | 60:4F:90:LYS:HZ1   | 1.67                     | 0.58              |
| 59:8E:64:ALA:O     | 59:8E:67:ILE:HG12  | 2.02                     | 0.58              |
| 59:8E:66:ARG:O     | 59:8E:70:VAL:HG12  | 2.03                     | 0.58              |
| 66:8L:19:TRP:CZ2   | 67:8M:14:GLU:OE1   | 2.55                     | 0.58              |
| 10:1J:60:TYR:HE1   | 11:1K:37:MET:HE1   | 1.68                     | 0.58              |
| 16:1P:143:SER:O    | 16:1P:147:ARG:HG3  | 2.02                     | 0.58              |
| 47:3P:46:LEU:HD21  | 69:3R:302:3PE:H2C1 | 1.84                     | 0.58              |
| 60:8F:22:MET:HE2   | 60:8F:22:MET:N     | 2.18                     | 0.58              |
| 6:1F:326:GLN:O     | 6:1F:420:ARG:NH2   | 2.36                     | 0.58              |
| 22:1W:49:LEU:O     | 22:1W:49:LEU:HD23  | 2.04                     | 0.58              |
| 49:3I:62:ARG:HB2   | 49:3I:77:ARG:HH12  | 1.69                     | 0.58              |
| 49:3V:77:ARG:C     | 49:3V:77:ARG:HE    | 2.11                     | 0.58              |
| 58:4D:78:TRP:HA    | 58:4D:81:ILE:HD12  | 1.86                     | 0.58              |
| 75:4D:201:CDL:H562 | 75:4D:201:CDL:H191 | 1.85                     | 0.58              |
| 67:8M:32:TRP:O     | 67:8M:36:HIS:ND1   | 2.36                     | 0.58              |
| 3:1C:83:VAL:HG12   | 3:1C:85:THR:HG22   | 1.84                     | 0.58              |
| 9:1I:27:TRP:HB3    | 9:1I:30:LEU:HD12   | 1.86                     | 0.58              |
| 23:1X:157:LEU:HD12 | 29:1d:17:GLU:HG2   | 1.84                     | 0.58              |
| 38:1m:82:THR:HG22  | 38:1m:85:THR:HG23  | 1.85                     | 0.58              |
| 46:3O:166:ALA:HB2  | 46:3O:244:ILE:HG13 | 1.85                     | 0.58              |
| 47:3P:207:ASN:ND2  | 47:3P:211:ILE:O    | 2.36                     | 0.58              |
| 54:3Y:38:TRP:HA    | 69:3Y:101:3PE:H11  | 1.84                     | 0.58              |
| 55:4A:92:MET:HE2   | 55:4A:163:ASN:HD22 | 1.68                     | 0.58              |
| 55:8A:420:GLY:O    | 55:8A:424:THR:OG1  | 2.19                     | 0.58              |
| 58:8D:51:LEU:O     | 58:8D:56:LYS:NZ    | 2.33                     | 0.58              |
| 8:1H:24:GLU:HA     | 8:1H:271:LEU:HD13  | 1.84                     | 0.58              |
| 14:1N:242:SER:O    | 14:1N:246:VAL:HG23 | 2.03                     | 0.58              |
| 14:1N:289:ASN:HA   | 14:1N:292:PHE:CE2  | 2.38                     | 0.58              |
| 17:1Q:22:LEU:HD23  | 22:1W:78:VAL:HG13  | 1.84                     | 0.58              |
| 29:1d:8:ARG:NH2    | 70:1d:202:PC1:O14  | 2.36                     | 0.58              |
| 35:1j:61:ASP:HA    | 35:1j:64:LEU:HB2   | 1.86                     | 0.58              |
| 44:1s:43:HIS:CE1   | 44:1s:44:HIS:CE1   | 2.92                     | 0.58              |
| 49:3E:187:GLU:OE1  | 49:3E:248:ARG:NH2  | 2.23                     | 0.58              |
| 52:3H:47:GLU:O     | 52:3H:51:GLN:HG2   | 2.04                     | 0.58              |
| 56:4B:97:VAL:HB    | 56:4B:152:MET:SD   | 2.43                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:4C:65:SER:HB2   | 87:4C:306:PGV:H041 | 1.85                     | 0.58              |
| 87:4C:302:PGV:H332 | 93:4C:307:PEK:H322 | 1.86                     | 0.58              |
| 58:4D:67:SER:HB3   | 59:4E:106:LEU:HB3  | 1.85                     | 0.58              |
| 67:4M:42:ARG:O     | 67:4M:42:ARG:NE    | 2.27                     | 0.58              |
| 68:8N:50:ASN:O     | 68:8N:50:ASN:OD1   | 2.21                     | 0.58              |
| 19:1S:26:SER:O     | 19:1S:33:ARG:NH2   | 2.37                     | 0.58              |
| 20:1U:14:ARG:HB3   | 20:1U:57:GLU:OE2   | 2.04                     | 0.58              |
| 25:1Z:59:ARG:C     | 25:1Z:62:ILE:HG22  | 2.28                     | 0.58              |
| 87:4A:601:PGV:H341 | 87:4L:101:PGV:H152 | 1.85                     | 0.58              |
| 60:8F:43:LYS:HA    | 60:8F:88:HIS:HD1   | 1.68                     | 0.58              |
| 2:1B:69:MET:HB2    | 2:1B:74:VAL:HB     | 1.85                     | 0.58              |
| 10:1J:74:MET:C     | 10:1J:74:MET:SD    | 2.87                     | 0.58              |
| 10:1J:74:MET:HE3   | 10:1J:75:ALA:HB2   | 1.86                     | 0.58              |
| 12:1L:3:PRO:HG2    | 12:1L:53:MET:HE1   | 1.84                     | 0.58              |
| 19:1S:23:CYS:SG    | 19:1S:59:ASP:N     | 2.77                     | 0.58              |
| 48:3Q:147:LEU:HD12 | 48:3Q:157:ALA:HB1  | 1.85                     | 0.58              |
| 48:3Q:203:ARG:NH2  | 53:3W:53:LYS:NZ    | 2.51                     | 0.58              |
| 55:4A:28:MET:HE3   | 55:4A:28:MET:CA    | 2.23                     | 0.58              |
| 55:4A:310:MET:HG2  | 56:4B:73:LEU:HD12  | 1.84                     | 0.58              |
| 55:4A:443:TYR:O    | 56:4B:134:ARG:NH2  | 2.37                     | 0.58              |
| 64:4J:15:ASP:OD1   | 64:4J:15:ASP:N     | 2.37                     | 0.58              |
| 55:8A:6:TRP:CE3    | 55:8A:18:LEU:HD21  | 2.38                     | 0.58              |
| 56:8B:25:ASP:OD2   | 63:8I:43:ARG:NE    | 2.35                     | 0.58              |
| 58:8D:48:TRP:HE1   | 59:8E:56:ARG:CD    | 2.17                     | 0.58              |
| 60:8F:21:MET:O     | 60:8F:25:ARG:HG2   | 2.04                     | 0.58              |
| 87:8L:101:PGV:H131 | 87:8L:101:PGV:H311 | 1.85                     | 0.58              |
| 6:1F:46:LYS:NZ     | 6:1F:167:CYS:O     | 2.32                     | 0.58              |
| 7:1G:118:ASP:OD2   | 17:1Q:46:GLN:NE2   | 2.37                     | 0.58              |
| 13:1M:403:THR:HA   | 13:1M:406:TYR:CE2  | 2.39                     | 0.58              |
| 34:1i:99:ARG:NH1   | 40:1o:49:GLN:OE1   | 2.37                     | 0.58              |
| 48:3D:307:LEU:O    | 48:3D:311:MET:HG3  | 2.03                     | 0.58              |
| 55:4A:113:LEU:O    | 55:4A:117:MET:HG2  | 2.04                     | 0.58              |
| 55:4A:215:LEU:HD11 | 93:4C:307:PEK:H271 | 1.85                     | 0.58              |
| 7:1G:198:ASN:OD1   | 7:1G:268:ARG:NH2   | 2.36                     | 0.58              |
| 14:1N:20:VAL:HG13  | 14:1N:29:ILE:HG23  | 1.86                     | 0.58              |
| 14:1N:149:ILE:CG2  | 14:1N:154:MET:HE2  | 2.32                     | 0.58              |
| 18:1R:38:ASN:HB3   | 18:1R:43:LEU:HD11  | 1.86                     | 0.58              |
| 75:1X:201:CDL:H452 | 75:1X:201:CDL:H251 | 1.85                     | 0.58              |
| 50:3F:82:MET:HE3   | 50:3F:83:ARG:HG3   | 1.86                     | 0.58              |
| 46:3O:46:ARG:HG2   | 46:3O:379:LEU:HD22 | 1.85                     | 0.58              |
| 51:3T:65:GLU:C     | 51:3T:65:GLU:OE1   | 2.47                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:4N:9:ALA:HB1    | 68:4N:16:ILE:HD11  | 1.86                     | 0.58              |
| 75:8C:306:CDL:HB61 | 75:8C:306:CDL:H542 | 1.86                     | 0.58              |
| 59:8E:28:GLU:CD    | 59:8E:28:GLU:H     | 2.12                     | 0.58              |
| 59:8E:107:ASP:N    | 59:8E:107:ASP:OD1  | 2.37                     | 0.58              |
| 87:8G:101:PGV:H282 | 87:8G:101:PGV:H102 | 1.86                     | 0.58              |
| 67:8M:17:ILE:O     | 67:8M:21:VAL:HG12  | 2.03                     | 0.58              |
| 5:1E:101:GLN:OE1   | 5:1E:155:GLN:NE2   | 2.37                     | 0.57              |
| 7:1G:126:ASP:OD1   | 43:1r:56:ARG:NH1   | 2.36                     | 0.57              |
| 14:1N:95:MET:HE2   | 14:1N:149:ILE:HG12 | 1.85                     | 0.57              |
| 35:1j:17:LEU:HD23  | 35:1j:22:LEU:HD21  | 1.85                     | 0.57              |
| 45:3N:42:ASP:HB2   | 45:3N:194:ARG:HB3  | 1.86                     | 0.57              |
| 47:3P:233:LEU:HG   | 48:3Q:212:MET:HE1  | 1.86                     | 0.57              |
| 49:3R:199:GLN:HB2  | 49:3R:248:ARG:NH2  | 2.17                     | 0.57              |
| 55:4A:456:MET:HG2  | 58:4D:96:LEU:CD1   | 2.34                     | 0.57              |
| 66:4L:18:LYS:NZ    | 67:4M:14:GLU:OE1   | 2.34                     | 0.57              |
| 55:8A:491:ASN:HB3  | 55:8A:494:TRP:HD1  | 1.68                     | 0.57              |
| 57:8C:117:PRO:HG2  | 57:8C:123:PRO:HG3  | 1.87                     | 0.57              |
| 1:1A:37:TYR:OH     | 4:1D:54:GLN:OE1    | 2.21                     | 0.57              |
| 8:1H:273:ILE:HG23  | 8:1H:277:TYR:CD2   | 2.40                     | 0.57              |
| 12:1L:481:THR:OG1  | 40:1o:91:HIS:ND1   | 2.29                     | 0.57              |
| 20:1U:36:PHE:HA    | 20:1U:40:LEU:HB2   | 1.86                     | 0.57              |
| 32:1g:118:ILE:HD12 | 41:1p:155:LEU:HD11 | 1.86                     | 0.57              |
| 44:1s:63:MET:HG3   | 44:1s:64:PRO:HD2   | 1.85                     | 0.57              |
| 2:1B:81:ARG:HE     | 8:1H:61:LEU:HD21   | 1.69                     | 0.57              |
| 14:1N:207:ILE:O    | 14:1N:211:MET:HG3  | 2.04                     | 0.57              |
| 19:1S:52:ILE:H     | 19:1S:52:ILE:HD12  | 1.69                     | 0.57              |
| 35:1j:38:TRP:CE2   | 35:1j:42:HIS:CE1   | 2.91                     | 0.57              |
| 57:4C:92:LEU:O     | 57:4C:95:THR:OG1   | 2.23                     | 0.57              |
| 58:4D:78:TRP:CD1   | 75:4D:201:CDL:H202 | 2.39                     | 0.57              |
| 56:8B:59:GLN:HE21  | 68:8N:13:PRO:HD2   | 1.67                     | 0.57              |
| 57:8C:43:LEU:HD21  | 87:8C:303:PGV:H262 | 1.85                     | 0.57              |
| 12:1L:142:ILE:HG21 | 75:1L:702:CDL:H641 | 1.85                     | 0.57              |
| 13:1M:453:MET:CE   | 32:1g:77:VAL:HG13  | 2.28                     | 0.57              |
| 39:1n:170:VAL:HG13 | 39:1n:171:THR:HG23 | 1.86                     | 0.57              |
| 45:3A:142:ASP:OD1  | 49:3E:79:SER:N     | 2.38                     | 0.57              |
| 55:4A:190:ILE:HG23 | 87:4A:603:PGV:H252 | 1.85                     | 0.57              |
| 55:8A:37:ILE:HD11  | 55:8A:58:VAL:HA    | 1.87                     | 0.57              |
| 58:8D:40:LEU:HD21  | 58:8D:59:LEU:HD21  | 1.84                     | 0.57              |
| 62:8H:81:PHE:HD1   | 62:8H:82:PRO:HD2   | 1.69                     | 0.57              |
| 11:1K:1:FME:SD     | 14:1N:79:LEU:HD21  | 2.45                     | 0.57              |
| 14:1N:49:ASN:OD1   | 14:1N:52:ALA:N     | 2.33                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:258:SER:HB2  | 14:1N:336:VAL:HG12 | 1.87                     | 0.57              |
| 46:3B:22:GLN:OE1   | 46:3B:41:TYR:HE2   | 1.86                     | 0.57              |
| 75:3G:103:CDL:H121 | 75:3G:103:CDL:H512 | 1.86                     | 0.57              |
| 46:3O:97:SER:HA    | 49:3V:69:GLY:HA2   | 1.85                     | 0.57              |
| 56:4B:151:ARG:NH2  | 62:4H:14:ALA:O     | 2.37                     | 0.57              |
| 55:8A:5:ARG:HB2    | 66:8L:3:TYR:HE2    | 1.70                     | 0.57              |
| 55:8A:101:SER:OG   | 55:8A:156:SER:O    | 2.20                     | 0.57              |
| 55:8A:510:TYR:CD1  | 60:8F:49:VAL:HG23  | 2.38                     | 0.57              |
| 87:8C:301:PGV:H281 | 87:8C:307:PGV:H312 | 1.86                     | 0.57              |
| 5:1E:37:ASN:C      | 44:1s:65:GLN:HE22  | 2.12                     | 0.57              |
| 8:1H:91:MET:O      | 8:1H:93:TYR:N      | 2.37                     | 0.57              |
| 16:1P:200:THR:HB   | 16:1P:238:LEU:HB2  | 1.87                     | 0.57              |
| 16:1P:216:ASN:ND2  | 16:1P:303:LEU:O    | 2.37                     | 0.57              |
| 45:3A:305:GLN:OE1  | 49:3I:42:VAL:HG12  | 2.04                     | 0.57              |
| 46:3B:365:LYS:HG2  | 46:3B:399:LEU:HD22 | 1.87                     | 0.57              |
| 75:3G:102:CDL:OA7  | 75:3G:102:CDL:O1   | 2.23                     | 0.57              |
| 55:4A:51:ASP:OD2   | 56:4B:205:SER:OG   | 2.21                     | 0.57              |
| 59:4E:41:LEU:HD12  | 59:4E:41:LEU:C     | 2.29                     | 0.57              |
| 60:4F:51:SER:HB3   | 60:4F:91:LEU:CD2   | 2.34                     | 0.57              |
| 57:8C:157:LYS:HZ1  | 87:8C:302:PGV:H02  | 1.69                     | 0.57              |
| 12:1L:142:ILE:HG12 | 13:1M:370:PRO:HB2  | 1.87                     | 0.57              |
| 35:1j:69:ASP:HB3   | 40:1o:117:ARG:CZ   | 2.34                     | 0.57              |
| 40:1o:69:LYS:HG2   | 40:1o:79:CYS:SG    | 2.44                     | 0.57              |
| 70:1q:201:PC1:H2G2 | 70:1q:201:PC1:H3B2 | 1.87                     | 0.57              |
| 55:4A:456:MET:HE2  | 58:4D:96:LEU:HD13  | 1.86                     | 0.57              |
| 55:8A:127:THR:HA   | 55:8A:235:PHE:HE2  | 1.69                     | 0.57              |
| 55:8A:343:GLY:HA2  | 87:8B:301:PGV:H062 | 1.86                     | 0.57              |
| 1:1A:27:LEU:HD11   | 8:1H:60:PRO:HD3    | 1.86                     | 0.57              |
| 4:1D:151:ILE:HD12  | 4:1D:177:MET:HE1   | 1.87                     | 0.57              |
| 7:1G:215:PHE:HB3   | 9:1I:104:ARG:HG3   | 1.86                     | 0.57              |
| 43:1r:57:ASP:OD1   | 43:1r:58:GLY:N     | 2.38                     | 0.57              |
| 45:3N:269:PRO:HB2  | 45:3N:410:VAL:HG11 | 1.87                     | 0.57              |
| 56:4B:62:GLU:CA    | 56:4B:65:TRP:CE2   | 2.81                     | 0.57              |
| 59:4E:82:TYR:CE1   | 59:4E:86:ILE:HG13  | 2.40                     | 0.57              |
| 55:8A:13:LYS:HE2   | 55:8A:500:PRO:HB2  | 1.86                     | 0.57              |
| 55:8A:179:TYR:OH   | 87:8A:603:PGV:O02  | 2.21                     | 0.57              |
| 57:8C:156:ARG:HH22 | 57:8C:223:LEU:HA   | 1.70                     | 0.57              |
| 4:1D:299:CYS:O     | 4:1D:303:GLU:HG2   | 2.04                     | 0.57              |
| 5:1E:159:ASN:ND2   | 5:1E:161:TYR:OH    | 2.37                     | 0.57              |
| 6:1F:28:ARG:NH1    | 44:1s:35:ASN:O     | 2.38                     | 0.57              |
| 6:1F:262:VAL:HA    | 6:1F:287:VAL:HA    | 1.85                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:55:CYS:HB3    | 72:1G:803:FES:S2   | 2.45                     | 0.57              |
| 7:1G:439:PHE:CE1   | 7:1G:442:ILE:HD11  | 2.38                     | 0.57              |
| 12:1L:539:TYR:HB2  | 37:1L:89:VAL:HG21  | 1.87                     | 0.57              |
| 13:1M:319:HIS:HA   | 13:1M:322:THR:HG22 | 1.86                     | 0.57              |
| 46:3B:47:ILE:HD11  | 46:3B:211:VAL:HG11 | 1.86                     | 0.57              |
| 55:4A:124:THR:HG22 | 55:4A:132:LEU:HG   | 1.87                     | 0.57              |
| 57:8C:161:GLN:O    | 57:8C:165:ILE:HG12 | 2.05                     | 0.57              |
| 6:1F:106:LYS:O     | 6:1F:110:ILE:HG22  | 2.04                     | 0.57              |
| 13:1M:153:THR:HG22 | 13:1M:206:LYS:HG2  | 1.87                     | 0.57              |
| 14:1N:314:LYS:NZ   | 15:1O:274:THR:OG1  | 2.28                     | 0.57              |
| 19:1S:82:SER:OG    | 19:1S:84:ASP:OD1   | 2.23                     | 0.57              |
| 33:1h:69:HIS:NE2   | 75:1h:202:CDL:OA4  | 2.33                     | 0.57              |
| 35:1j:9:PRO:HB2    | 36:1k:13:MET:HE1   | 1.85                     | 0.57              |
| 46:3B:23:ASP:OD1   | 46:3B:24:LEU:N     | 2.37                     | 0.57              |
| 53:3J:13:LEU:HD23  | 53:3J:17:LEU:HD12  | 1.87                     | 0.57              |
| 55:4A:179:TYR:OH   | 87:4A:603:PGV:O02  | 2.20                     | 0.57              |
| 55:4A:377:PHE:HA   | 55:4A:380:VAL:HG22 | 1.87                     | 0.57              |
| 57:4C:23:SER:HB3   | 57:4C:50:ASN:HB2   | 1.87                     | 0.57              |
| 57:4C:121:ILE:HG21 | 57:4C:193:TYR:HD2  | 1.69                     | 0.57              |
| 75:4C:305:CDL:H542 | 75:4C:305:CDL:HB61 | 1.87                     | 0.57              |
| 55:8A:460:ILE:CG1  | 58:8D:92:THR:HG21  | 2.35                     | 0.57              |
| 55:8A:481:GLU:OE1  | 66:8L:7:PRO:HG2    | 2.05                     | 0.57              |
| 57:8C:85:LEU:HA    | 57:8C:88:ILE:HD12  | 1.86                     | 0.57              |
| 62:8H:6:THR:HA     | 62:8H:9:LYS:HZ1    | 1.69                     | 0.57              |
| 68:8N:34:THR:O     | 68:8N:38:LEU:HG    | 2.05                     | 0.57              |
| 8:1H:90:PRO:HD2    | 8:1H:240:ILE:HD13  | 1.86                     | 0.56              |
| 24:1Y:123:LEU:HB3  | 69:1Y:204:3PE:H261 | 1.85                     | 0.56              |
| 34:1i:41:PRO:HA    | 34:1i:44:GLN:HB2   | 1.86                     | 0.56              |
| 39:1n:100:GLU:OE1  | 39:1n:121:ARG:NH1  | 2.38                     | 0.56              |
| 43:1r:51:ASN:O     | 43:1r:56:ARG:NH2   | 2.37                     | 0.56              |
| 47:3P:309:THR:OG1  | 47:3P:370:SER:OG   | 2.21                     | 0.56              |
| 56:4B:9:PHE:HE1    | 56:4B:24:HIS:CD2   | 2.23                     | 0.56              |
| 55:8A:495:LEU:O    | 55:8A:495:LEU:HD12 | 2.05                     | 0.56              |
| 57:8C:90:GLU:HB2   | 57:8C:244:PHE:CE2  | 2.40                     | 0.56              |
| 64:8J:7:GLU:OE1    | 64:8J:7:GLU:N      | 2.27                     | 0.56              |
| 5:1E:168:ASP:O     | 5:1E:171:GLU:HG3   | 2.05                     | 0.56              |
| 9:1I:101:ASP:OD1   | 9:1I:101:ASP:N     | 2.35                     | 0.56              |
| 12:1L:9:LEU:O      | 12:1L:13:ILE:HG12  | 2.03                     | 0.56              |
| 47:3C:176:THR:OG1  | 47:3P:53:MET:O     | 2.21                     | 0.56              |
| 55:4A:374:VAL:HA   | 55:4A:377:PHE:CE2  | 2.40                     | 0.56              |
| 56:4B:110:TYR:HB2  | 56:4B:116:LEU:HB3  | 1.86                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:4C:129:VAL:HB   | 57:4C:180:GLU:OE1  | 2.05                     | 0.56              |
| 55:8A:208:MET:O    | 55:8A:211:THR:OG1  | 2.23                     | 0.56              |
| 57:8C:58:TRP:CZ3   | 87:8C:307:PGV:H71  | 2.39                     | 0.56              |
| 3:1C:40:VAL:HG22   | 43:1r:69:MET:HB3   | 1.86                     | 0.56              |
| 4:1D:237:ASN:HB3   | 8:1H:284:GLN:CD    | 2.30                     | 0.56              |
| 6:1F:297:VAL:HG22  | 6:1F:336:VAL:HG12  | 1.86                     | 0.56              |
| 10:1J:130:THR:HA   | 25:1Z:121:MET:HE2  | 1.87                     | 0.56              |
| 10:1J:167:VAL:HG22 | 14:1N:42:PRO:HG2   | 1.85                     | 0.56              |
| 13:1M:207:MET:HG2  | 13:1M:298:ILE:HG13 | 1.87                     | 0.56              |
| 16:1P:171:ILE:HG12 | 16:1P:210:VAL:HG21 | 1.86                     | 0.56              |
| 16:1P:335:LYS:H    | 16:1P:335:LYS:HD3  | 1.70                     | 0.56              |
| 30:1e:88:GLU:HB2   | 30:1e:90:LYS:HZ2   | 1.70                     | 0.56              |
| 32:1g:100:ARG:HD2  | 32:1g:107:LEU:HA   | 1.86                     | 0.56              |
| 45:3N:354:VAL:HG21 | 45:3N:404:ALA:HA   | 1.87                     | 0.56              |
| 46:3O:34:VAL:HG11  | 46:3O:386:ALA:HB1  | 1.87                     | 0.56              |
| 49:3R:236:CYS:HB2  | 49:3R:241:SER:O    | 2.05                     | 0.56              |
| 55:4A:362:SER:HA   | 56:4B:87:MET:CE    | 2.35                     | 0.56              |
| 59:4E:31:LYS:HD2   | 59:4E:35:THR:HG23  | 1.85                     | 0.56              |
| 61:4G:84:GLN:OE1   | 61:4G:84:GLN:N     | 2.38                     | 0.56              |
| 55:8A:162:ILE:HG23 | 57:8C:85:LEU:HD12  | 1.87                     | 0.56              |
| 56:8B:69:PRO:O     | 56:8B:73:LEU:HD22  | 2.05                     | 0.56              |
| 59:8E:12:ASP:O     | 59:8E:16:VAL:HG23  | 2.04                     | 0.56              |
| 59:8E:81:ILE:O     | 59:8E:85:VAL:HG12  | 2.06                     | 0.56              |
| 68:8N:33:VAL:HA    | 68:8N:36:LEU:HD12  | 1.86                     | 0.56              |
| 1:1A:113:TRP:HZ2   | 8:1H:286:MET:HG3   | 1.68                     | 0.56              |
| 6:1F:245:PHE:O     | 6:1F:251:SER:OG    | 2.22                     | 0.56              |
| 10:1J:86:ASN:HD22  | 11:1K:23:ARG:HH22  | 1.52                     | 0.56              |
| 11:1K:47:ILE:CD1   | 14:1N:79:LEU:HB2   | 2.36                     | 0.56              |
| 13:1M:190:TRP:CE3  | 24:1Y:126:MET:HE2  | 2.41                     | 0.56              |
| 23:1X:106:PHE:O    | 23:1X:110:VAL:HG22 | 2.04                     | 0.56              |
| 48:3Q:116:ILE:HG12 | 86:3Q:501:HEC:HMA3 | 1.87                     | 0.56              |
| 55:4A:271:MET:HA   | 55:4A:271:MET:CE   | 2.30                     | 0.56              |
| 56:8B:133:MET:HE1  | 58:8D:123:MET:CG   | 2.35                     | 0.56              |
| 2:1B:81:ARG:NE     | 8:1H:61:LEU:CD2    | 2.67                     | 0.56              |
| 12:1L:136:ASN:HA   | 12:1L:197:ASP:HA   | 1.86                     | 0.56              |
| 13:1M:167:ILE:HG12 | 13:1M:195:MET:CE   | 2.35                     | 0.56              |
| 15:1O:168:VAL:HG11 | 15:1O:238:ILE:HD12 | 1.87                     | 0.56              |
| 55:4A:225:GLY:HA3  | 57:4C:112:LEU:HD13 | 1.88                     | 0.56              |
| 57:4C:190:ASP:HB3  | 61:4G:53:LEU:HD22  | 1.88                     | 0.56              |
| 58:4D:29:HIS:CE1   | 58:4D:65:ASN:CG    | 2.84                     | 0.56              |
| 68:8N:7:THR:O      | 68:8N:11:LYS:CD    | 2.53                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:1A:37:TYR:HE2    | 2:1B:80:PRO:HD2    | 1.70                     | 0.56              |
| 13:1M:1:FME:HE3    | 13:1M:111:THR:HG21 | 1.87                     | 0.56              |
| 15:1O:279:LEU:HD13 | 15:1O:282:ILE:HD11 | 1.87                     | 0.56              |
| 39:1n:134:ARG:HD2  | 39:1n:161:ASP:HB3  | 1.88                     | 0.56              |
| 41:1p:116:GLU:HG3  | 41:1p:123:ASN:HB2  | 1.87                     | 0.56              |
| 43:1r:8:GLN:HA     | 43:1r:11:ARG:HD2   | 1.88                     | 0.56              |
| 47:3C:132:VAL:HA   | 47:3C:139:SER:HB3  | 1.87                     | 0.56              |
| 46:3O:157:ALA:O    | 46:3O:161:GLU:HG2  | 2.05                     | 0.56              |
| 49:3R:210:TRP:CZ3  | 49:3R:267:SER:HA   | 2.41                     | 0.56              |
| 57:8C:216:ALA:O    | 57:8C:220:LEU:HD13 | 2.06                     | 0.56              |
| 57:8C:221:ARG:NH1  | 87:8C:307:PGV:O13  | 2.38                     | 0.56              |
| 75:8C:306:CDL:H342 | 75:8C:306:CDL:H401 | 1.88                     | 0.56              |
| 63:8I:10:ARG:NH1   | 63:8I:10:ARG:HB2   | 2.20                     | 0.56              |
| 3:1C:151:ILE:HG23  | 3:1C:152:LEU:HG    | 1.86                     | 0.56              |
| 7:1G:318:ILE:HD11  | 7:1G:522:LEU:HD21  | 1.87                     | 0.56              |
| 69:1M:501:3PE:H281 | 14:1N:280:THR:HG21 | 1.87                     | 0.56              |
| 14:1N:218:LEU:HB3  | 14:1N:244:MET:HE2  | 1.88                     | 0.56              |
| 17:1Q:27:GLU:OE2   | 17:1Q:27:GLU:N     | 2.26                     | 0.56              |
| 23:1X:7:PRO:HG2    | 25:1Z:84:LEU:HD13  | 1.86                     | 0.56              |
| 24:1Y:128:GLN:HE21 | 69:1Y:204:3PE:P    | 2.28                     | 0.56              |
| 47:3C:207:ASN:ND2  | 47:3C:211:ILE:O    | 2.28                     | 0.56              |
| 48:3Q:158:ILE:HG12 | 48:3Q:160:MET:H    | 1.71                     | 0.56              |
| 55:4A:450:TRP:HH2  | 75:4B:303:CDL:H771 | 1.71                     | 0.56              |
| 57:4C:34:TRP:HZ3   | 93:4C:307:PEK:H272 | 1.70                     | 0.56              |
| 55:8A:297:MET:O    | 55:8A:302:ARG:NH1  | 2.39                     | 0.56              |
| 7:1G:364:LEU:HD12  | 7:1G:491:ASN:HB3   | 1.86                     | 0.56              |
| 10:1J:31:LEU:O     | 10:1J:34:ILE:HG13  | 2.05                     | 0.56              |
| 13:1M:26:ASN:OD1   | 31:1f:13:HIS:NE2   | 2.38                     | 0.56              |
| 13:1M:78:MET:HE1   | 13:1M:439:LEU:HD12 | 1.88                     | 0.56              |
| 19:1S:88:ARG:HH22  | 19:1S:92:ASN:CG    | 2.12                     | 0.56              |
| 48:3Q:172:ASP:OD1  | 48:3Q:172:ASP:N    | 2.36                     | 0.56              |
| 49:3R:152:ILE:CD1  | 49:3R:272:ILE:CG2  | 2.69                     | 0.56              |
| 55:4A:70:VAL:O     | 55:4A:74:MET:HB2   | 2.06                     | 0.56              |
| 55:4A:306:THR:HG23 | 55:4A:310:MET:HE3  | 1.88                     | 0.56              |
| 87:4C:306:PGV:H291 | 87:4C:306:PGV:H152 | 1.86                     | 0.56              |
| 55:8A:104:LEU:HD12 | 55:8A:152:LEU:CD1  | 2.35                     | 0.56              |
| 55:8A:476:PHE:HB3  | 66:8L:21:LEU:HD21  | 1.87                     | 0.56              |
| 56:8B:95:LEU:HD12  | 56:8B:96:THR:H     | 1.69                     | 0.56              |
| 87:8B:301:PGV:H312 | 75:8D:201:CDL:H462 | 1.88                     | 0.56              |
| 75:8C:306:CDL:H581 | 75:8C:306:CDL:H761 | 1.87                     | 0.56              |
| 58:8D:76:ASN:HB3   | 58:8D:79:LYS:HE2   | 1.88                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:8E:33:MET:HE2   | 59:8E:67:ILE:HG22  | 1.86                     | 0.56              |
| 64:8J:28:ASP:OD1   | 64:8J:29:ASN:N     | 2.39                     | 0.56              |
| 67:8M:20:SER:O     | 67:8M:24:LEU:HD23  | 2.06                     | 0.56              |
| 7:1G:105:CYS:HA    | 7:1G:108:CYS:CB    | 2.33                     | 0.56              |
| 12:1L:606:GLU:OE1  | 12:1L:606:GLU:N    | 2.39                     | 0.56              |
| 16:1P:179:LEU:H    | 16:1P:179:LEU:HD23 | 1.71                     | 0.56              |
| 58:4D:118:LYS:HE3  | 65:4K:53:TRP:HA    | 1.88                     | 0.56              |
| 55:8A:428:GLN:HA   | 55:8A:431:LEU:HD12 | 1.88                     | 0.56              |
| 55:8A:460:ILE:HG12 | 58:8D:92:THR:HG21  | 1.86                     | 0.56              |
| 57:8C:247:VAL:O    | 57:8C:251:PHE:HD1  | 1.88                     | 0.56              |
| 63:8I:43:ARG:O     | 63:8I:47:TYR:HD1   | 1.89                     | 0.56              |
| 68:8N:8:GLN:HA     | 68:8N:11:LYS:HZ1   | 1.69                     | 0.56              |
| 4:1D:237:ASN:HB3   | 8:1H:284:GLN:NE2   | 2.21                     | 0.56              |
| 6:1F:384:ALA:HB1   | 6:1F:388:GLU:HG3   | 1.88                     | 0.56              |
| 8:1H:189:THR:HG22  | 8:1H:270:PHE:HZ    | 1.69                     | 0.56              |
| 12:1L:341:MET:HE1  | 12:1L:457:LEU:HD12 | 1.86                     | 0.56              |
| 14:1N:237:MET:HE1  | 14:1N:319:HIS:CD2  | 2.41                     | 0.56              |
| 15:1O:232:GLU:O    | 15:1O:236:GLU:HG2  | 2.05                     | 0.56              |
| 38:1m:117:GLU:N    | 38:1m:117:GLU:CD   | 2.63                     | 0.56              |
| 46:3B:46:ARG:NH2   | 46:3B:110:GLU:OE1  | 2.39                     | 0.56              |
| 56:4B:37:LEU:O     | 56:4B:41:ILE:HD12  | 2.06                     | 0.56              |
| 56:4B:62:GLU:HB3   | 56:4B:65:TRP:CH2   | 2.40                     | 0.56              |
| 55:8A:333:LYS:CE   | 55:8A:335:SER:HB3  | 2.36                     | 0.56              |
| 57:8C:179:SER:OG   | 57:8C:180:GLU:OE1  | 2.24                     | 0.56              |
| 61:8G:15:THR:C     | 61:8G:19:LEU:HD12  | 2.30                     | 0.56              |
| 65:8K:42:LEU:HD11  | 87:8K:101:PGV:H202 | 1.88                     | 0.56              |
| 66:8L:28:TYR:CE2   | 87:8L:101:PGV:H302 | 2.41                     | 0.56              |
| 7:1G:252:PRO:HB3   | 7:1G:263:ILE:HG23  | 1.87                     | 0.55              |
| 12:1L:209:PRO:HB2  | 12:1L:213:LEU:HG   | 1.88                     | 0.55              |
| 13:1M:90:THR:HG21  | 69:1M:504:3PE:H12  | 1.87                     | 0.55              |
| 48:3D:204:ILE:HG12 | 86:3D:501:HEC:HMA3 | 1.87                     | 0.55              |
| 48:3D:247:ILE:HG12 | 48:3D:249:MET:H    | 1.71                     | 0.55              |
| 59:4E:37:VAL:HG13  | 59:4E:74:LYS:HD3   | 1.89                     | 0.55              |
| 55:8A:232:GLN:C    | 55:8A:292:MET:HE1  | 2.31                     | 0.55              |
| 56:8B:3:TYR:CZ     | 56:8B:6:GLN:HG3    | 2.41                     | 0.55              |
| 62:8H:30:TRP:NE1   | 94:8H:101:PO4:O2   | 2.37                     | 0.55              |
| 66:8L:33:PHE:O     | 66:8L:37:PHE:CE2   | 2.60                     | 0.55              |
| 7:1G:228:ILE:H     | 7:1G:583:THR:HG22  | 1.70                     | 0.55              |
| 7:1G:359:ARG:O     | 7:1G:363:LEU:HG    | 2.06                     | 0.55              |
| 10:1J:74:MET:HE1   | 10:1J:75:ALA:HB2   | 1.86                     | 0.55              |
| 12:1L:327:LEU:O    | 12:1L:331:MET:HG2  | 2.06                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:366:MET:HB3  | 12:1L:369:THR:HB   | 1.86                     | 0.55              |
| 69:1M:502:3PE:H391 | 69:1M:502:3PE:H291 | 1.89                     | 0.55              |
| 14:1N:95:MET:CE    | 14:1N:149:ILE:HG12 | 2.36                     | 0.55              |
| 18:1R:42:ASP:O     | 18:1R:46:GLU:HG3   | 2.05                     | 0.55              |
| 24:1Y:78:GLN:HE22  | 51:3T:60:THR:HG21  | 1.70                     | 0.55              |
| 24:1Y:128:GLN:HG2  | 69:1Y:204:3PE:N    | 2.21                     | 0.55              |
| 24:1Y:140:VAL:O    | 33:1h:115:ARG:NH1  | 2.38                     | 0.55              |
| 32:1g:28:GLU:HA    | 32:1g:28:GLU:OE2   | 2.06                     | 0.55              |
| 45:3A:91:THR:HG23  | 45:3A:93:GLU:H     | 1.72                     | 0.55              |
| 47:3C:196:HIS:HE1  | 85:3C:502:HEM:ND   | 2.03                     | 0.55              |
| 46:3O:365:LYS:HG2  | 46:3O:399:LEU:HD22 | 1.88                     | 0.55              |
| 52:3U:34:ARG:O     | 52:3U:38:GLU:HG3   | 2.06                     | 0.55              |
| 55:4A:52:GLN:O     | 55:4A:56:VAL:HG13  | 2.07                     | 0.55              |
| 55:4A:117:MET:SD   | 66:4L:39:ILE:HG12  | 2.47                     | 0.55              |
| 75:4C:305:CDL:H581 | 75:4C:305:CDL:H761 | 1.88                     | 0.55              |
| 59:4E:64:ALA:O     | 59:4E:67:ILE:HG12  | 2.07                     | 0.55              |
| 60:4F:22:MET:O     | 60:4F:26:LYS:HG2   | 2.05                     | 0.55              |
| 55:8A:80:ASN:OD1   | 55:8A:98:ASN:ND2   | 2.36                     | 0.55              |
| 55:8A:377:PHE:O    | 55:8A:381:LEU:HB2  | 2.06                     | 0.55              |
| 57:8C:182:TYR:O    | 61:8G:72:ASN:ND2   | 2.39                     | 0.55              |
| 6:1F:261:HIS:CE1   | 6:1F:341:THR:OG1   | 2.59                     | 0.55              |
| 7:1G:216:THR:CG2   | 7:1G:248:MET:HE3   | 2.36                     | 0.55              |
| 7:1G:283:MET:HB2   | 7:1G:560:ILE:HB    | 1.88                     | 0.55              |
| 47:3P:215:MET:HB2  | 51:3T:10:MET:CE    | 2.37                     | 0.55              |
| 49:3R:209:GLU:HG2  | 49:3R:210:TRP:CE3  | 2.41                     | 0.55              |
| 58:4D:63:LYS:HB3   | 58:4D:64:PHE:CD1   | 2.41                     | 0.55              |
| 63:8I:17:LEU:O     | 63:8I:21:ILE:HG12  | 2.06                     | 0.55              |
| 10:1J:23:LYS:HE3   | 11:1K:21:MET:O     | 2.07                     | 0.55              |
| 13:1M:66:LEU:O     | 13:1M:70:THR:HG23  | 2.06                     | 0.55              |
| 28:1c:33:LYS:O     | 28:1c:37:GLU:HG2   | 2.07                     | 0.55              |
| 33:1h:13:PRO:HD3   | 39:1n:98:VAL:HG21  | 1.87                     | 0.55              |
| 35:1j:32:MET:O     | 35:1j:36:ILE:HG12  | 2.06                     | 0.55              |
| 55:4A:508:PRO:HG2  | 60:4F:32:ASN:HD22  | 1.71                     | 0.55              |
| 56:4B:134:ARG:HB2  | 58:4D:110:THR:HG21 | 1.88                     | 0.55              |
| 6:1F:250:ASN:HD21  | 6:1F:318:ASP:CB    | 2.11                     | 0.55              |
| 7:1G:366:THR:HG21  | 7:1G:450:MET:CE    | 2.35                     | 0.55              |
| 23:1X:33:ALA:HB2   | 23:1X:119:PRO:HG3  | 1.88                     | 0.55              |
| 23:1X:63:ASN:OD1   | 25:1Z:81:ARG:NH2   | 2.40                     | 0.55              |
| 49:3E:136:PHE:O    | 49:3E:139:SER:OG   | 2.21                     | 0.55              |
| 1:1A:3:ILE:HG21    | 70:1H:403:PC1:H221 | 1.89                     | 0.55              |
| 4:1D:209:ASP:O     | 4:1D:213:GLU:HG2   | 2.07                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:282:GLU:O     | 4:1D:313:GLN:NE2   | 2.27                     | 0.55              |
| 5:1E:111:ARG:HB2   | 5:1E:152:PRO:HD3   | 1.89                     | 0.55              |
| 5:1E:146:GLY:HA3   | 6:1F:142:PHE:HZ    | 1.71                     | 0.55              |
| 7:1G:160:ILE:HD11  | 7:1G:183:VAL:HG13  | 1.89                     | 0.55              |
| 7:1G:216:THR:HG22  | 7:1G:248:MET:HE3   | 1.89                     | 0.55              |
| 11:1K:47:ILE:HD11  | 14:1N:79:LEU:HB2   | 1.87                     | 0.55              |
| 12:1L:49:VAL:HG13  | 41:1p:32:LEU:HD13  | 1.87                     | 0.55              |
| 27:1b:26:GLY:O     | 27:1b:30:ILE:HG23  | 2.06                     | 0.55              |
| 34:1i:85:LEU:HA    | 34:1i:89:VAL:HB    | 1.88                     | 0.55              |
| 46:3B:109:VAL:HB   | 46:3B:119:LEU:HD12 | 1.89                     | 0.55              |
| 47:3C:266:PRO:HG3  | 49:3R:220:LEU:HD21 | 1.89                     | 0.55              |
| 45:3N:86:LEU:HD13  | 45:3N:99:ILE:HG12  | 1.87                     | 0.55              |
| 57:4C:121:ILE:HG21 | 57:4C:193:TYR:CD2  | 2.41                     | 0.55              |
| 56:8B:9:PHE:HE1    | 56:8B:24:HIS:CD2   | 2.23                     | 0.55              |
| 56:8B:118:PHE:HD2  | 56:8B:226:MET:HE1  | 1.72                     | 0.55              |
| 62:8H:6:THR:CA     | 62:8H:9:LYS:HZ1    | 2.18                     | 0.55              |
| 13:1M:65:LEU:O     | 13:1M:69:THR:HG23  | 2.06                     | 0.55              |
| 36:1k:48:GLU:HG2   | 39:1n:33:ARG:HB3   | 1.88                     | 0.55              |
| 43:1r:101:LYS:N    | 43:1r:101:LYS:HD2  | 2.22                     | 0.55              |
| 75:3A:501:CDL:H132 | 69:3A:503:3PE:H372 | 1.89                     | 0.55              |
| 45:3N:412:SER:HB3  | 53:3W:15:ARG:HH22  | 1.71                     | 0.55              |
| 57:4C:157:LYS:O    | 57:4C:161:GLN:HG3  | 2.07                     | 0.55              |
| 58:4D:64:PHE:CE2   | 59:4E:66:ARG:HD3   | 2.41                     | 0.55              |
| 55:8A:264:LYS:NZ   | 55:8A:326:THR:O    | 2.33                     | 0.55              |
| 87:8A:602:PGV:H71  | 58:8D:84:THR:HG21  | 1.89                     | 0.55              |
| 59:8E:72:LYS:HB2   | 59:8E:82:TYR:CD2   | 2.28                     | 0.55              |
| 61:8G:61:SER:O     | 61:8G:61:SER:OG    | 2.24                     | 0.55              |
| 68:8N:36:LEU:HA    | 68:8N:40:ASN:OD1   | 2.07                     | 0.55              |
| 70:1M:503:PC1:H282 | 69:1M:506:3PE:H262 | 1.88                     | 0.55              |
| 33:1h:84:GLU:O     | 33:1h:88:GLU:HG2   | 2.07                     | 0.55              |
| 48:3Q:118:ARG:HG3  | 48:3Q:194:SER:HB3  | 1.87                     | 0.55              |
| 55:4A:383:MET:HE3  | 55:4A:421:VAL:HG22 | 1.87                     | 0.55              |
| 8:1H:146:LEU:HD11  | 8:1H:192:GLU:HG3   | 1.89                     | 0.55              |
| 20:1T:12:LYS:HZ1   | 20:1T:32:VAL:HA    | 1.72                     | 0.55              |
| 25:1Z:103:ASP:OD1  | 25:1Z:103:ASP:N    | 2.40                     | 0.55              |
| 55:4A:37:ILE:HD11  | 55:4A:58:VAL:HA    | 1.89                     | 0.55              |
| 55:8A:144:ASP:OD2  | 57:8C:36:HIS:NE2   | 2.40                     | 0.55              |
| 12:1L:213:LEU:HB3  | 12:1L:273:VAL:HG11 | 1.87                     | 0.55              |
| 13:1M:195:MET:HB2  | 69:1M:501:3PE:H221 | 1.88                     | 0.55              |
| 69:1M:502:3PE:H2E2 | 69:1M:504:3PE:H2C2 | 1.89                     | 0.55              |
| 70:1M:505:PC1:H322 | 75:1h:202:CDL:H111 | 1.88                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:14:MET:O     | 14:1N:18:MET:HG2   | 2.07                     | 0.55              |
| 15:1O:37:ARG:NH2   | 15:1O:40:ARG:HD2   | 2.22                     | 0.55              |
| 20:1U:22:TYR:HB3   | 20:1U:25:ILE:HD12  | 1.89                     | 0.55              |
| 29:1d:3:SER:HB2    | 70:1d:202:PC1:H131 | 1.89                     | 0.55              |
| 35:1j:69:ASP:OD1   | 40:1o:110:ARG:HG3  | 2.07                     | 0.55              |
| 41:1p:105:ILE:HG13 | 41:1p:134:VAL:HG21 | 1.87                     | 0.55              |
| 46:3B:107:TYR:HB3  | 46:3B:123:LEU:HD11 | 1.88                     | 0.55              |
| 49:3I:49:VAL:HG11  | 49:3I:55:LEU:HD13  | 1.88                     | 0.55              |
| 49:3R:239:HIS:HD2  | 49:3R:240:GLY:N    | 2.04                     | 0.55              |
| 50:3S:52:GLU:OE2   | 51:3T:11:ARG:NH1   | 2.40                     | 0.55              |
| 56:4B:49:LYS:HZ1   | 59:4E:76:GLY:C     | 2.15                     | 0.55              |
| 55:8A:44:PRO:HD3   | 55:8A:448:THR:HG23 | 1.88                     | 0.55              |
| 56:8B:59:GLN:HE21  | 68:8N:13:PRO:CD    | 2.20                     | 0.55              |
| 58:8D:144:GLU:N    | 58:8D:144:GLU:OE1  | 2.40                     | 0.55              |
| 4:1D:257:GLY:HA3   | 4:1D:372:GLY:HA2   | 1.90                     | 0.54              |
| 54:3X:1:MET:HA     | 54:3X:5:PHE:CE2    | 2.42                     | 0.54              |
| 59:4E:25:ASP:OD1   | 59:4E:28:GLU:CD    | 2.50                     | 0.54              |
| 70:1A:202:PC1:H11  | 8:1H:62:ARG:HH22   | 1.72                     | 0.54              |
| 4:1D:279:ASP:OD1   | 4:1D:279:ASP:N     | 2.40                     | 0.54              |
| 4:1D:336:ALA:O     | 4:1D:340:THR:HG23  | 2.06                     | 0.54              |
| 13:1M:2:LEU:HD21   | 75:1X:201:CDL:H552 | 1.88                     | 0.54              |
| 13:1M:16:TRP:CE2   | 69:1M:502:3PE:H281 | 2.42                     | 0.54              |
| 20:1U:46:ASP:OD1   | 39:1n:44:ARG:NH1   | 2.40                     | 0.54              |
| 34:1i:86:LYS:HG2   | 34:1i:87:TYR:CD1   | 2.42                     | 0.54              |
| 49:3E:179:ARG:HE   | 49:3E:211:VAL:HB   | 1.71                     | 0.54              |
| 56:4B:52:HIS:CD2   | 59:4E:40:ASP:HB2   | 2.42                     | 0.54              |
| 57:4C:250:LEU:O    | 57:4C:254:VAL:HG23 | 2.07                     | 0.54              |
| 55:8A:90:PRO:HG3   | 57:8C:6:HIS:CD2    | 2.41                     | 0.54              |
| 55:8A:417:MET:O    | 55:8A:421:VAL:HG22 | 2.07                     | 0.54              |
| 55:8A:447:TYR:O    | 55:8A:451:ASN:ND2  | 2.41                     | 0.54              |
| 92:8B:305:PSC:H251 | 63:8I:21:ILE:HG13  | 1.89                     | 0.54              |
| 67:8M:38:ASP:C     | 67:8M:38:ASP:OD1   | 2.50                     | 0.54              |
| 6:1F:99:GLU:O      | 6:1F:139:ARG:NH1   | 2.39                     | 0.54              |
| 7:1G:601:ARG:NH1   | 7:1G:605:GLU:OE1   | 2.39                     | 0.54              |
| 16:1P:147:ARG:NH1  | 59:8E:9:GLU:H      | 1.99                     | 0.54              |
| 29:1d:86:ARG:O     | 29:1d:90:MET:HB2   | 2.06                     | 0.54              |
| 49:3E:176:VAL:HG22 | 49:3E:212:ILE:HD12 | 1.89                     | 0.54              |
| 48:3Q:223:LYS:NZ   | 75:3T:101:CDL:OB4  | 2.37                     | 0.54              |
| 55:4A:275:TRP:CE3  | 87:4A:603:PGV:H12  | 2.42                     | 0.54              |
| 59:4E:82:TYR:O     | 59:4E:86:ILE:HG12  | 2.07                     | 0.54              |
| 55:8A:52:GLN:O     | 55:8A:56:VAL:HG13  | 2.07                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:8D:48:TRP:HH2   | 59:8E:61:PHE:HA    | 1.71                     | 0.54              |
| 4:1D:354:GLU:OE2   | 4:1D:357:GLN:NE2   | 2.40                     | 0.54              |
| 6:1F:107:ASP:OD1   | 6:1F:108:ARG:N     | 2.40                     | 0.54              |
| 7:1G:110:GLN:HG3   | 7:1G:113:GLU:HG3   | 1.90                     | 0.54              |
| 10:1J:86:ASN:OD1   | 10:1J:86:ASN:C     | 2.49                     | 0.54              |
| 13:1M:126:LEU:HD23 | 13:1M:150:LEU:HD12 | 1.87                     | 0.54              |
| 33:1h:110:VAL:HG12 | 33:1h:114:MET:CE   | 2.37                     | 0.54              |
| 55:4A:468:MET:CE   | 55:4A:468:MET:CA   | 2.73                     | 0.54              |
| 1:1A:55:PHE:CD1    | 10:1J:70:TYR:OH    | 2.61                     | 0.54              |
| 4:1D:3:GLN:NE2     | 13:1M:135:ARG:O    | 2.33                     | 0.54              |
| 4:1D:100:LEU:HD22  | 4:1D:195:ARG:HD3   | 1.89                     | 0.54              |
| 4:1D:151:ILE:HD11  | 4:1D:218:PHE:CZ    | 2.43                     | 0.54              |
| 7:1G:189:LYS:HD3   | 7:1G:190:MET:O     | 2.08                     | 0.54              |
| 13:1M:5:ILE:HG23   | 13:1M:104:LEU:HD11 | 1.88                     | 0.54              |
| 13:1M:306:PRO:O    | 13:1M:310:MET:HG3  | 2.07                     | 0.54              |
| 34:1i:52:ASP:HB3   | 34:1i:57:LYS:HE3   | 1.88                     | 0.54              |
| 37:1l:68:ASP:OD1   | 37:1l:68:ASP:N     | 2.39                     | 0.54              |
| 92:8B:305:PSC:H011 | 63:8I:17:LEU:HD21  | 1.90                     | 0.54              |
| 1:1A:21:ALA:HB1    | 8:1H:218:GLY:HA3   | 1.88                     | 0.54              |
| 15:1O:22:SER:OG    | 15:1O:119:GLY:O    | 2.25                     | 0.54              |
| 75:1X:201:CDL:H531 | 75:1X:201:CDL:H352 | 1.88                     | 0.54              |
| 46:3B:197:ASN:HB3  | 46:3B:232:LEU:HB2  | 1.89                     | 0.54              |
| 47:3C:149:LEU:HD21 | 47:3C:281:LEU:HD13 | 1.90                     | 0.54              |
| 49:3E:165:MET:HA   | 49:3E:165:MET:CE   | 2.30                     | 0.54              |
| 55:4A:1:FME:SD     | 87:4A:601:PGV:H211 | 2.47                     | 0.54              |
| 55:4A:483:SER:HB3  | 67:4M:4:LYS:HG3    | 1.89                     | 0.54              |
| 58:4D:77:GLU:HG3   | 65:4K:10:HIS:CE1   | 2.40                     | 0.54              |
| 68:4N:24:ALA:HA    | 68:4N:27:THR:HG22  | 1.89                     | 0.54              |
| 55:8A:298:ASP:OD2  | 55:8A:301:THR:N    | 2.38                     | 0.54              |
| 57:8C:63:ARG:HD3   | 64:8J:12:PHE:CE2   | 2.43                     | 0.54              |
| 58:8D:114:GLU:OE2  | 58:8D:114:GLU:N    | 2.26                     | 0.54              |
| 7:1G:551:ASP:OD2   | 7:1G:679:ARG:NE    | 2.41                     | 0.54              |
| 46:3B:286:LYS:HG2  | 46:3B:287:ARG:HG3  | 1.90                     | 0.54              |
| 46:3B:312:PHE:HA   | 49:3I:61:GLY:HA2   | 1.89                     | 0.54              |
| 48:3Q:216:LEU:HB3  | 75:3T:101:CDL:H562 | 1.90                     | 0.54              |
| 55:8A:406:ASN:HD22 | 55:8A:409:TRP:HD1  | 1.56                     | 0.54              |
| 62:8H:20:PHE:CB    | 62:8H:28:ASN:HD21  | 2.21                     | 0.54              |
| 2:1B:173:LEU:HD11  | 70:1B:202:PC1:H252 | 1.90                     | 0.54              |
| 12:1L:13:ILE:HD11  | 75:1h:202:CDL:H401 | 1.89                     | 0.54              |
| 13:1M:364:LEU:HD13 | 13:1M:369:LEU:HD22 | 1.89                     | 0.54              |
| 14:1N:213:LEU:HD13 | 14:1N:329:MET:HE3  | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:1V:36:GLN:OE1   | 21:1V:94:LEU:HD21  | 2.07                     | 0.54              |
| 22:1W:47:VAL:HA    | 22:1W:52:LEU:HD12  | 1.89                     | 0.54              |
| 69:1d:201:3PE:O13  | 69:1d:201:3PE:H31  | 2.08                     | 0.54              |
| 42:1q:25:ARG:HD2   | 42:1q:74:PHE:HZ    | 1.71                     | 0.54              |
| 53:3J:12:ARG:O     | 53:3J:16:LEU:HG    | 2.08                     | 0.54              |
| 55:4A:191:THR:HG23 | 55:4A:245:ILE:HG23 | 1.88                     | 0.54              |
| 75:4C:305:CDL:H191 | 75:4C:305:CDL:H322 | 1.90                     | 0.54              |
| 62:4H:31:GLN:HA    | 62:4H:31:GLN:HE21  | 1.72                     | 0.54              |
| 55:8A:242:GLU:O    | 55:8A:246:LEU:HG   | 2.07                     | 0.54              |
| 56:8B:104:TRP:CG   | 56:8B:203:ASN:HB2  | 2.43                     | 0.54              |
| 10:1J:14:VAL:HA    | 10:1J:17:PHE:HB2   | 1.90                     | 0.54              |
| 12:1L:407:TRP:HE1  | 37:1l:112:MET:HE3  | 1.73                     | 0.54              |
| 75:1L:702:CDL:H142 | 13:1M:361:MET:HE1  | 1.89                     | 0.54              |
| 25:1Z:105:LYS:HB2  | 25:1Z:108:GLU:HB2  | 1.89                     | 0.54              |
| 34:1i:83:TYR:HE1   | 41:1p:48:ARG:HD3   | 1.73                     | 0.54              |
| 42:1q:8:ARG:O      | 42:1q:12:GLN:HG3   | 2.08                     | 0.54              |
| 47:3C:237:LEU:HD13 | 48:3D:301:MET:HG3  | 1.90                     | 0.54              |
| 51:3G:21:SER:HB2   | 51:3G:24:GLU:HG2   | 1.90                     | 0.54              |
| 46:3O:29:LEU:HD12  | 46:3O:33:LEU:HB3   | 1.89                     | 0.54              |
| 57:4C:27:MET:HE1   | 57:4C:50:ASN:ND2   | 2.23                     | 0.54              |
| 57:4C:138:LEU:O    | 57:4C:142:VAL:HG23 | 2.08                     | 0.54              |
| 60:4F:51:SER:HB3   | 60:4F:91:LEU:HD21  | 1.88                     | 0.54              |
| 62:4H:27:ARG:HG2   | 62:4H:27:ARG:HH11  | 1.73                     | 0.54              |
| 55:8A:28:MET:HG3   | 66:8L:29:PHE:HD1   | 1.73                     | 0.54              |
| 58:8D:99:GLU:OE1   | 58:8D:103:VAL:HG21 | 2.07                     | 0.54              |
| 59:8E:52:LEU:HD22  | 59:8E:98:ILE:HD13  | 1.89                     | 0.54              |
| 59:8E:52:LEU:HD23  | 59:8E:67:ILE:HD11  | 1.89                     | 0.54              |
| 62:8H:5:GLN:HG2    | 62:8H:6:THR:HG23   | 1.89                     | 0.54              |
| 6:1F:134:ALA:HB3   | 6:1F:175:VAL:HG12  | 1.90                     | 0.54              |
| 7:1G:356:THR:HG22  | 7:1G:503:LEU:HG    | 1.89                     | 0.54              |
| 21:1V:34:LEU:HD13  | 21:1V:48:GLU:HG2   | 1.90                     | 0.54              |
| 30:1e:37:LYS:O     | 30:1e:41:GLU:HG3   | 2.07                     | 0.54              |
| 47:3C:229:ILE:HG21 | 70:3J:101:PC1:H351 | 1.89                     | 0.54              |
| 48:3D:235:LEU:HD11 | 49:3R:238:CYS:HA   | 1.89                     | 0.54              |
| 55:4A:8:TYR:OH     | 64:4J:36:MET:HE3   | 2.08                     | 0.54              |
| 66:4L:17:ASN:HB3   | 66:4L:20:ARG:HB3   | 1.90                     | 0.54              |
| 55:8A:86:MET:HE1   | 55:8A:184:PHE:HB3  | 1.89                     | 0.54              |
| 55:8A:333:LYS:HZ1  | 55:8A:335:SER:CB   | 2.21                     | 0.54              |
| 57:8C:54:MET:HE1   | 87:8C:303:PGV:H181 | 1.89                     | 0.54              |
| 3:1C:53:HIS:ND1    | 3:1C:55:ASP:OD1    | 2.41                     | 0.53              |
| 4:1D:165:THR:HG23  | 8:1H:32:GLN:HG2    | 1.90                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:1G:324:ASP:OD1   | 7:1G:324:ASP:N    | 2.38                     | 0.53              |
| 12:1L:140:LEU:CD2  | 12:1L:182:PHE:CE2 | 2.91                     | 0.53              |
| 12:1L:175:ASN:O    | 12:1L:179:ASP:OD2 | 2.25                     | 0.53              |
| 12:1L:591:PHE:CE1  | 14:1N:111:PHE:HA  | 2.42                     | 0.53              |
| 14:1N:20:VAL:HG11  | 14:1N:137:ALA:HB1 | 1.91                     | 0.53              |
| 16:1P:46:ILE:O     | 16:1P:46:ILE:HG22 | 2.07                     | 0.53              |
| 45:3A:412:SER:HB3  | 53:3J:19:ARG:NH2  | 2.23                     | 0.53              |
| 45:3N:412:SER:O    | 53:3W:15:ARG:NH2  | 2.41                     | 0.53              |
| 49:3R:173:PRO:CD   | 49:3R:215:GLY:O   | 2.57                     | 0.53              |
| 55:4A:273:MET:CE   | 55:4A:319:LYS:HE3 | 2.37                     | 0.53              |
| 55:8A:307:SER:O    | 55:8A:311:ILE:CD1 | 2.56                     | 0.53              |
| 55:8A:499:PRO:HG3  | 66:8L:10:ASN:HD21 | 1.73                     | 0.53              |
| 2:1B:48:MET:HE2    | 2:1B:80:PRO:CG    | 2.37                     | 0.53              |
| 13:1M:220:HIS:CE1  | 13:1M:231:LEU:HB3 | 2.44                     | 0.53              |
| 15:1O:303:LYS:H    | 15:1O:309:ASN:ND2 | 2.06                     | 0.53              |
| 21:1V:49:GLN:HE22  | 43:1r:92:LYS:HB3  | 1.72                     | 0.53              |
| 22:1W:56:VAL:HG12  | 22:1W:60:ARG:HD2  | 1.88                     | 0.53              |
| 30:1e:64:GLU:O     | 30:1e:68:ARG:HD2  | 2.08                     | 0.53              |
| 32:1g:41:ASN:HB3   | 32:1g:44:SER:HB2  | 1.89                     | 0.53              |
| 75:1h:202:CDL:H562 | 34:1i:79:TRP:HB3  | 1.91                     | 0.53              |
| 47:3P:108:MET:HA   | 47:3P:108:MET:HE3 | 1.90                     | 0.53              |
| 48:3Q:203:ARG:HH22 | 53:3W:53:LYS:NZ   | 2.06                     | 0.53              |
| 3:1C:33:LEU:HD13   | 21:1V:98:PRO:HB3  | 1.91                     | 0.53              |
| 8:1H:307:LEU:HD12  | 8:1H:310:MET:HE2  | 1.89                     | 0.53              |
| 9:1I:84:GLU:HB2    | 9:1I:94:ILE:HD12  | 1.89                     | 0.53              |
| 37:1l:124:SER:O    | 37:1l:124:SER:OG  | 2.22                     | 0.53              |
| 47:3P:345:HIS:CE1  | 51:3T:65:GLU:OE2  | 2.61                     | 0.53              |
| 54:3X:8:PRO:O      | 54:3X:12:GLU:HG3  | 2.07                     | 0.53              |
| 57:4C:129:VAL:HG11 | 57:4C:180:GLU:CD  | 2.34                     | 0.53              |
| 56:8B:188:ARG:HG2  | 63:8I:54:TYR:CE2  | 2.43                     | 0.53              |
| 57:8C:203:PHE:O    | 57:8C:207:HIS:ND1 | 2.28                     | 0.53              |
| 64:8J:11:ILE:HG22  | 64:8J:12:PHE:CD1  | 2.44                     | 0.53              |
| 14:1N:95:MET:HE3   | 14:1N:99:THR:OG1  | 2.08                     | 0.53              |
| 16:1P:203:GLN:OE1  | 16:1P:235:ARG:NH1 | 2.42                     | 0.53              |
| 19:1S:50:LEU:O     | 19:1S:52:ILE:HD12 | 2.08                     | 0.53              |
| 41:1p:31:TYR:O     | 41:1p:35:ILE:HG12 | 2.08                     | 0.53              |
| 46:3B:56:ARG:HD2   | 46:3B:103:GLU:HG2 | 1.89                     | 0.53              |
| 46:3B:76:THR:HG23  | 46:3B:81:SER:HA   | 1.91                     | 0.53              |
| 48:3Q:16:GLY:O     | 48:3Q:202:LYS:NZ  | 2.33                     | 0.53              |
| 48:3Q:195:GLU:OE2  | 48:3Q:201:ARG:NE  | 2.41                     | 0.53              |
| 49:3R:195:LEU:HD22 | 49:3R:250:ARG:HA  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:4L:15:VAL:HG12  | 66:4L:21:LEU:HD22  | 1.91                     | 0.53              |
| 56:8B:152:MET:HE2  | 56:8B:152:MET:HA   | 1.89                     | 0.53              |
| 59:8E:52:LEU:HD21  | 59:8E:68:LEU:HD11  | 1.91                     | 0.53              |
| 63:8I:55:ASP:HB3   | 63:8I:58:LYS:HB3   | 1.90                     | 0.53              |
| 5:1E:147:ALA:HB3   | 5:1E:153:MET:HE3   | 1.90                     | 0.53              |
| 13:1M:61:LEU:HD22  | 13:1M:244:MET:HE2  | 1.89                     | 0.53              |
| 14:1N:40:MET:HE1   | 14:1N:129:LEU:HB3  | 1.91                     | 0.53              |
| 32:1g:108:MET:HE1  | 41:1p:98:ASP:HB3   | 1.90                     | 0.53              |
| 46:3B:222:ARG:CD   | 46:3B:223:PHE:CE1  | 2.92                     | 0.53              |
| 87:4G:101:PGV:H102 | 87:4G:101:PGV:H282 | 1.91                     | 0.53              |
| 55:8A:5:ARG:HD2    | 66:8L:3:TYR:CD2    | 2.43                     | 0.53              |
| 55:8A:328:HIS:CE1  | 63:8I:13:LEU:HD21  | 2.43                     | 0.53              |
| 12:1L:483:PRO:HG3  | 35:1j:53:TYR:CZ    | 2.44                     | 0.53              |
| 14:1N:149:ILE:CD1  | 14:1N:154:MET:HE1  | 2.34                     | 0.53              |
| 19:1S:82:SER:O     | 19:1S:86:VAL:HG23  | 2.08                     | 0.53              |
| 69:1Y:202:3PE:H342 | 69:1Y:203:3PE:H231 | 1.91                     | 0.53              |
| 45:3A:304:CYS:HB3  | 45:3A:334:MET:HE2  | 1.89                     | 0.53              |
| 45:3N:171:SER:OG   | 49:3R:82:ASP:OD2   | 2.25                     | 0.53              |
| 55:4A:100:MET:HE2  | 57:4C:57:TRP:CH2   | 2.44                     | 0.53              |
| 58:4D:100:LYS:HA   | 58:4D:104:TYR:HD2  | 1.72                     | 0.53              |
| 55:8A:307:SER:O    | 55:8A:311:ILE:HD11 | 2.08                     | 0.53              |
| 56:8B:70:ALA:HA    | 56:8B:73:LEU:HD23  | 1.90                     | 0.53              |
| 70:1A:202:PC1:O22  | 16:1P:187:TRP:CH2  | 2.62                     | 0.53              |
| 6:1F:102:PRO:HD2   | 6:1F:302:SER:HB3   | 1.91                     | 0.53              |
| 6:1F:292:ASP:O     | 6:1F:339:ARG:NH1   | 2.41                     | 0.53              |
| 7:1G:672:TYR:HD1   | 7:1G:684:MET:CE    | 2.20                     | 0.53              |
| 8:1H:46:LEU:HD23   | 8:1H:49:ILE:HD12   | 1.90                     | 0.53              |
| 12:1L:526:LEU:HD12 | 12:1L:530:PRO:HG2  | 1.90                     | 0.53              |
| 69:1M:506:3PE:H332 | 69:1M:506:3PE:H241 | 1.90                     | 0.53              |
| 15:1O:25:ILE:HG23  | 15:1O:168:VAL:HB   | 1.90                     | 0.53              |
| 23:1X:136:LEU:HD23 | 23:1X:137:PRO:HD2  | 1.91                     | 0.53              |
| 25:1Z:10:MET:HE3   | 25:1Z:11:PRO:HD2   | 1.91                     | 0.53              |
| 39:1n:94:GLU:HA    | 39:1n:97:LYS:HG3   | 1.91                     | 0.53              |
| 41:1p:47:ALA:O     | 41:1p:51:ILE:HG13  | 2.09                     | 0.53              |
| 41:1p:50:PHE:O     | 41:1p:54:GLN:HG2   | 2.08                     | 0.53              |
| 43:1r:91:LYS:HD3   | 43:1r:92:LYS:N     | 2.23                     | 0.53              |
| 47:3C:221:HIS:O    | 47:3C:225:THR:OG1  | 2.24                     | 0.53              |
| 47:3P:128:PHE:CD1  | 47:3P:146:ILE:HD11 | 2.43                     | 0.53              |
| 55:4A:447:TYR:O    | 55:4A:451:ASN:ND2  | 2.42                     | 0.53              |
| 56:4B:160:LEU:HB3  | 56:4B:198:GLU:HG2  | 1.91                     | 0.53              |
| 57:4C:88:ILE:O     | 57:4C:92:LEU:HD23  | 2.08                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:4C:221:ARG:HB3  | 57:4C:226:HIS:HB2  | 1.91                     | 0.53              |
| 87:4C:303:PGV:H221 | 87:4C:303:PGV:H31  | 1.91                     | 0.53              |
| 57:8C:172:TYR:HE2  | 93:8G:102:PEK:H181 | 1.74                     | 0.53              |
| 58:8D:53:MET:H     | 58:8D:53:MET:CE    | 2.22                     | 0.53              |
| 62:8H:39:CYS:O     | 62:8H:43:MET:HG2   | 2.08                     | 0.53              |
| 64:8J:35:THR:O     | 64:8J:39:CYS:SG    | 2.67                     | 0.53              |
| 7:1G:295:THR:HG23  | 7:1G:298:ASP:H     | 1.74                     | 0.53              |
| 9:1I:60:ARG:HG2    | 9:1I:172:ASP:OD2   | 2.09                     | 0.53              |
| 16:1P:201:VAL:HG12 | 16:1P:290:SER:HB3  | 1.90                     | 0.53              |
| 41:1p:98:ASP:OD2   | 41:1p:142:TYR:OH   | 2.24                     | 0.53              |
| 45:3A:304:CYS:CB   | 45:3A:334:MET:HE2  | 2.39                     | 0.53              |
| 48:3D:185:ASN:OD1  | 48:3D:187:GLU:N    | 2.42                     | 0.53              |
| 51:3G:42:ARG:HD2   | 75:3G:102:CDL:OB3  | 2.09                     | 0.53              |
| 45:3N:140:GLU:O    | 45:3N:143:SER:OG   | 2.25                     | 0.53              |
| 58:4D:145:TRP:CD1  | 58:4D:145:TRP:H    | 2.24                     | 0.53              |
| 55:8A:65:MET:SD    | 55:8A:69:MET:SD    | 3.07                     | 0.53              |
| 56:8B:60:GLU:CD    | 56:8B:60:GLU:H     | 2.17                     | 0.53              |
| 57:8C:138:LEU:O    | 57:8C:142:VAL:HG23 | 2.08                     | 0.53              |
| 58:8D:48:TRP:CD1   | 59:8E:56:ARG:HD3   | 2.44                     | 0.53              |
| 75:8D:201:CDL:H371 | 75:8D:201:CDL:H561 | 1.90                     | 0.53              |
| 6:1F:96:ASN:OD1    | 6:1F:192:LEU:HD13  | 2.09                     | 0.53              |
| 6:1F:164:LYS:HB2   | 44:1s:63:MET:HE1   | 1.89                     | 0.53              |
| 13:1M:123:GLU:OE1  | 13:1M:123:GLU:HA   | 2.09                     | 0.53              |
| 21:1V:46:TYR:O     | 21:1V:50:ILE:HG13  | 2.09                     | 0.53              |
| 22:1W:23:ARG:O     | 22:1W:23:ARG:CD    | 2.53                     | 0.53              |
| 48:3D:106:LEU:HD22 | 48:3D:295:LEU:HB2  | 1.90                     | 0.53              |
| 46:3O:240:ARG:O    | 46:3O:421:ARG:NH1  | 2.42                     | 0.53              |
| 48:3Q:152:TYR:OH   | 52:3U:66:ASP:OD2   | 2.20                     | 0.53              |
| 49:3V:49:VAL:O     | 49:3V:49:VAL:HG23  | 2.09                     | 0.53              |
| 55:4A:100:MET:HE2  | 57:4C:57:TRP:CZ3   | 2.43                     | 0.53              |
| 57:4C:117:PRO:HG2  | 57:4C:123:PRO:HG3  | 1.89                     | 0.53              |
| 75:4C:305:CDL:H401 | 75:4C:305:CDL:H342 | 1.91                     | 0.53              |
| 63:4I:22:VAL:O     | 63:4I:26:ILE:HG12  | 2.09                     | 0.53              |
| 56:8B:59:GLN:CD    | 68:8N:14:SER:HG    | 2.04                     | 0.53              |
| 56:8B:150:ILE:HB   | 56:8B:184:LEU:HB3  | 1.90                     | 0.53              |
| 58:8D:48:TRP:CE3   | 59:8E:61:PHE:CD2   | 2.96                     | 0.53              |
| 1:1A:53:MET:O      | 1:1A:57:LEU:HD23   | 2.09                     | 0.53              |
| 2:1B:86:MET:CE     | 2:1B:103:VAL:HG23  | 2.39                     | 0.53              |
| 7:1G:544:ILE:HG23  | 7:1G:559:VAL:HG23  | 1.91                     | 0.53              |
| 8:1H:2:PHE:O       | 8:1H:6:ILE:HG13    | 2.09                     | 0.53              |
| 8:1H:70:MET:HA     | 8:1H:73:ILE:HG22   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:213:LEU:HB2  | 12:1L:273:VAL:HG21 | 1.91                     | 0.53              |
| 13:1M:282:LEU:HG   | 13:1M:342:MET:HG3  | 1.91                     | 0.53              |
| 42:1q:6:VAL:HG12   | 75:1q:203:CDL:HA61 | 1.90                     | 0.53              |
| 48:3Q:134:TYR:OH   | 48:3Q:160:MET:HB3  | 2.09                     | 0.53              |
| 49:3R:173:PRO:CG   | 49:3R:215:GLY:O    | 2.56                     | 0.53              |
| 55:8A:186:TRP:O    | 55:8A:190:ILE:HG12 | 2.09                     | 0.53              |
| 55:8A:187:SER:O    | 55:8A:191:THR:OG1  | 2.17                     | 0.53              |
| 58:8D:48:TRP:CH2   | 59:8E:61:PHE:HA    | 2.44                     | 0.53              |
| 65:8K:31:TYR:HA    | 65:8K:35:GLN:HG3   | 1.91                     | 0.53              |
| 4:1D:258:VAL:HG12  | 4:1D:296:ARG:HG2   | 1.91                     | 0.52              |
| 6:1F:312:CYS:HA    | 6:1F:315:VAL:HG22  | 1.90                     | 0.52              |
| 7:1G:122:MET:HA    | 43:1r:60:ARG:HH22  | 1.74                     | 0.52              |
| 7:1G:237:ASN:H     | 7:1G:259:ASN:ND2   | 2.07                     | 0.52              |
| 37:1l:96:VAL:HB    | 37:1l:101:MET:HE3  | 1.91                     | 0.52              |
| 47:3C:11:MET:HA    | 47:3C:11:MET:HE3   | 1.91                     | 0.52              |
| 75:4B:303:CDL:H321 | 63:4l:34:PHE:CE1   | 2.43                     | 0.52              |
| 55:8A:165:ILE:O    | 55:8A:169:ILE:HG13 | 2.09                     | 0.52              |
| 55:8A:333:LYS:NZ   | 55:8A:335:SER:CB   | 2.72                     | 0.52              |
| 9:1I:28:THR:HG22   | 70:1I:203:PC1:H221 | 1.91                     | 0.52              |
| 9:1I:148:LEU:HD23  | 17:1Q:70:MET:HG3   | 1.91                     | 0.52              |
| 10:1J:86:ASN:ND2   | 11:1K:23:ARG:HH12  | 2.07                     | 0.52              |
| 14:1N:298:TYR:O    | 14:1N:303:THR:OG1  | 2.19                     | 0.52              |
| 16:1P:260:HIS:O    | 16:1P:264:ARG:HG2  | 2.08                     | 0.52              |
| 25:1Z:59:ARG:HA    | 25:1Z:62:ILE:HG22  | 1.92                     | 0.52              |
| 39:1n:91:GLU:HB2   | 39:1n:94:GLU:HG3   | 1.91                     | 0.52              |
| 50:3F:108:GLU:OE2  | 50:3F:111:ARG:NH1  | 2.42                     | 0.52              |
| 55:4A:264:LYS:NZ   | 55:4A:326:THR:O    | 2.37                     | 0.52              |
| 64:4J:21:HIS:CD2   | 64:4J:22:LEU:CD1   | 2.90                     | 0.52              |
| 55:8A:69:MET:HE1   | 88:8A:604:HEA:H18  | 1.91                     | 0.52              |
| 67:8M:31:GLY:O     | 67:8M:35:SER:OG    | 2.19                     | 0.52              |
| 5:1E:194:GLU:HG3   | 6:1F:26:TYR:CD2    | 2.44                     | 0.52              |
| 12:1L:188:TRP:CE3  | 12:1L:212:PRO:HG3  | 2.44                     | 0.52              |
| 12:1L:375:ILE:HD12 | 12:1L:458:LEU:HD11 | 1.90                     | 0.52              |
| 13:1M:11:LEU:HB3   | 13:1M:100:ILE:HD13 | 1.90                     | 0.52              |
| 16:1P:173:GLY:H    | 16:1P:176:ASP:HB3  | 1.73                     | 0.52              |
| 16:1P:268:ARG:HH12 | 16:1P:272:VAL:HG22 | 1.74                     | 0.52              |
| 25:1Z:62:ILE:O     | 25:1Z:66:GLU:HG3   | 2.09                     | 0.52              |
| 33:1h:39:GLY:HA3   | 70:1h:203:PC1:H2E1 | 1.91                     | 0.52              |
| 49:3E:249:ILE:HG23 | 49:3E:249:ILE:O    | 2.09                     | 0.52              |
| 45:3N:279:HIS:ND1  | 45:3N:284:TYR:OH   | 2.24                     | 0.52              |
| 58:4D:95:LEU:HD21  | 67:4M:27:LEU:CD1   | 2.39                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:4H:8:ILE:HG13   | 62:4H:9:LYS:N      | 2.24                     | 0.52              |
| 55:8A:338:MET:HE3  | 55:8A:341:ALA:HB3  | 1.90                     | 0.52              |
| 58:8D:24:LEU:CD1   | 59:8E:33:MET:HE2   | 2.39                     | 0.52              |
| 58:8D:48:TRP:HE1   | 59:8E:56:ARG:HD3   | 1.74                     | 0.52              |
| 58:8D:78:TRP:CD1   | 75:8D:201:CDL:H202 | 2.45                     | 0.52              |
| 61:8G:56:ARG:HH21  | 61:8G:60:TYR:HE2   | 1.56                     | 0.52              |
| 4:1D:155:THR:HB    | 4:1D:167:PHE:HA    | 1.91                     | 0.52              |
| 4:1D:183:ARG:NH1   | 4:1D:210:ASP:OD2   | 2.29                     | 0.52              |
| 6:1F:406:ALA:HB3   | 73:1F:501:FMN:HM82 | 1.90                     | 0.52              |
| 8:1H:197:PRO:HD2   | 8:1H:198:PHE:CD2   | 2.44                     | 0.52              |
| 14:1N:143:CYS:SG   | 14:1N:198:THR:HG23 | 2.49                     | 0.52              |
| 14:1N:190:MET:HG3  | 14:1N:204:ASN:HD22 | 1.75                     | 0.52              |
| 15:1O:268:GLU:HA   | 15:1O:271:ASN:HB2  | 1.91                     | 0.52              |
| 16:1P:97:ARG:NH2   | 78:1P:402:NDP:O1A  | 2.40                     | 0.52              |
| 25:1Z:108:GLU:N    | 30:1e:74:ARG:HH22  | 2.07                     | 0.52              |
| 45:3N:36:THR:HG21  | 45:3N:373:THR:HA   | 1.92                     | 0.52              |
| 45:3N:276:ILE:HD11 | 45:3N:354:VAL:HA   | 1.91                     | 0.52              |
| 45:3N:298:ALA:HA   | 45:3N:303:LEU:HB2  | 1.90                     | 0.52              |
| 75:3P:504:CDL:HB22 | 51:3T:40:ARG:HH21  | 1.75                     | 0.52              |
| 87:4G:101:PGV:H011 | 87:4G:101:PGV:H51  | 1.92                     | 0.52              |
| 62:4H:57:ARG:HA    | 62:4H:60:TYR:CD1   | 2.44                     | 0.52              |
| 87:8C:304:PGV:H231 | 87:8C:304:PGV:H271 | 1.92                     | 0.52              |
| 1:1A:55:PHE:HZ     | 8:1H:134:ARG:HE    | 1.58                     | 0.52              |
| 7:1G:320:GLY:O     | 7:1G:498:SER:OG    | 2.26                     | 0.52              |
| 9:1I:69:ARG:NH1    | 9:1I:73:GLY:O      | 2.42                     | 0.52              |
| 38:1m:16:THR:O     | 38:1m:22:TYR:HE2   | 1.93                     | 0.52              |
| 46:3B:207:ILE:HG12 | 46:3B:382:VAL:HG12 | 1.92                     | 0.52              |
| 50:3F:47:ASP:OD1   | 50:3F:101:TYR:OH   | 2.27                     | 0.52              |
| 48:3Q:145:GLU:HA   | 48:3Q:145:GLU:OE2  | 2.09                     | 0.52              |
| 49:3R:205:VAL:HB   | 49:3R:211:VAL:HG23 | 1.90                     | 0.52              |
| 49:3R:225:ILE:HG12 | 49:3R:237:PRO:HG3  | 1.92                     | 0.52              |
| 50:3S:108:ALA:O    | 54:3Y:9:ARG:NE     | 2.37                     | 0.52              |
| 55:4A:126:TRP:HZ3  | 88:4A:605:HEA:HBD2 | 1.74                     | 0.52              |
| 55:4A:408:ALA:O    | 55:4A:412:ILE:HG13 | 2.09                     | 0.52              |
| 87:4A:602:PGV:H281 | 87:4C:306:PGV:H312 | 1.90                     | 0.52              |
| 58:4D:78:TRP:O     | 58:4D:82:VAL:HG23  | 2.10                     | 0.52              |
| 56:8B:160:LEU:HD11 | 56:8B:175:ILE:HG23 | 1.92                     | 0.52              |
| 57:8C:243:HIS:O    | 57:8C:247:VAL:HG23 | 2.08                     | 0.52              |
| 64:8J:43:THR:O     | 64:8J:47:LEU:HG    | 2.09                     | 0.52              |
| 2:1B:62:MET:HB2    | 2:1B:153:ALA:HB1   | 1.92                     | 0.52              |
| 4:1D:50:ASN:HB3    | 4:1D:65:VAL:HG13   | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:68:LEU:HD21   | 4:1D:411:LEU:HD21  | 1.92                     | 0.52              |
| 7:1G:43:HIS:HB3    | 7:1G:46:LEU:HB2    | 1.90                     | 0.52              |
| 8:1H:187:ILE:HD11  | 70:1H:402:PC1:H271 | 1.91                     | 0.52              |
| 9:1I:49:ASN:ND2    | 42:1q:30:ALA:O     | 2.40                     | 0.52              |
| 12:1L:407:TRP:HE1  | 37:1l:112:MET:CE   | 2.22                     | 0.52              |
| 69:1M:501:3PE:H31  | 14:1N:276:ILE:HG21 | 1.92                     | 0.52              |
| 17:1Q:27:GLU:HA    | 17:1Q:30:ILE:HG22  | 1.91                     | 0.52              |
| 49:3E:263:TYR:HB3  | 49:3E:273:VAL:HG13 | 1.92                     | 0.52              |
| 45:3N:14:THR:HG21  | 45:3N:389:ARG:HB3  | 1.90                     | 0.52              |
| 46:3O:76:THR:HG23  | 46:3O:81:SER:HA    | 1.90                     | 0.52              |
| 49:3R:125:VAL:HG21 | 70:3R:303:PC1:H361 | 1.91                     | 0.52              |
| 49:3R:209:GLU:OE1  | 49:3R:210:TRP:CZ3  | 2.63                     | 0.52              |
| 59:4E:25:ASP:C     | 59:4E:58:LEU:HD11  | 2.34                     | 0.52              |
| 65:8K:15:ASN:N     | 65:8K:15:ASN:OD1   | 2.42                     | 0.52              |
| 7:1G:252:PRO:HG3   | 7:1G:263:ILE:HG12  | 1.92                     | 0.52              |
| 12:1L:484:LEU:HD21 | 12:1L:488:MET:HE2  | 1.91                     | 0.52              |
| 15:1O:240:TYR:OH   | 21:1V:22:ARG:NH2   | 2.39                     | 0.52              |
| 16:1P:208:VAL:O    | 16:1P:212:LYS:HG3  | 2.09                     | 0.52              |
| 23:1X:82:THR:HA    | 23:1X:85:TRP:CD1   | 2.44                     | 0.52              |
| 23:1X:120:ASP:OD1  | 23:1X:121:LEU:N    | 2.41                     | 0.52              |
| 39:1n:9:LEU:HD23   | 39:1n:14:LYS:HG2   | 1.92                     | 0.52              |
| 45:3A:412:SER:HB3  | 53:3J:19:ARG:HH21  | 1.74                     | 0.52              |
| 47:3C:82:LEU:HD12  | 47:3C:243:VAL:HG21 | 1.92                     | 0.52              |
| 69:3C:504:3PE:H2A1 | 49:3R:130:LYS:HA   | 1.92                     | 0.52              |
| 46:3O:169:ARG:HG3  | 46:3O:240:ARG:HB3  | 1.91                     | 0.52              |
| 56:4B:89:GLU:HG2   | 68:4N:70:VAL:HG22  | 1.90                     | 0.52              |
| 59:4E:21:LYS:C     | 59:4E:57:ARG:HH12  | 2.03                     | 0.52              |
| 62:4H:40:GLU:O     | 62:4H:44:THR:HG23  | 2.10                     | 0.52              |
| 55:8A:94:PHE:HE1   | 57:8C:79:LEU:HD22  | 1.74                     | 0.52              |
| 57:8C:92:LEU:O     | 57:8C:95:THR:OG1   | 2.26                     | 0.52              |
| 4:1D:238:ARG:NH2   | 4:1D:412:ALA:HB1   | 2.25                     | 0.52              |
| 9:1I:150:ASN:ND2   | 42:1q:127:TYR:O    | 2.42                     | 0.52              |
| 10:1J:156:VAL:O    | 10:1J:160:SER:OG   | 2.20                     | 0.52              |
| 14:1N:25:HIS:O     | 14:1N:29:ILE:HG12  | 2.10                     | 0.52              |
| 15:1O:53:GLU:OE2   | 15:1O:126:ARG:NH1  | 2.43                     | 0.52              |
| 19:1S:94:LEU:HD12  | 19:1S:94:LEU:O     | 2.09                     | 0.52              |
| 23:1X:82:THR:HA    | 23:1X:85:TRP:NE1   | 2.25                     | 0.52              |
| 45:3A:324:PHE:HB2  | 45:3A:334:MET:CE   | 2.39                     | 0.52              |
| 49:3E:185:ASP:OD1  | 49:3E:186:GLN:N    | 2.43                     | 0.52              |
| 46:3O:35:ILE:HG23  | 46:3O:216:LEU:HD23 | 1.90                     | 0.52              |
| 49:3R:248:ARG:CZ   | 49:3R:257:ASN:HD22 | 2.23                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:86:MET:HE1   | 55:4A:184:PHE:HB3  | 1.92                     | 0.52              |
| 55:8A:287:VAL:HG21 | 55:8A:312:ILE:HD11 | 1.91                     | 0.52              |
| 55:8A:456:MET:HE1  | 65:8K:40:TRP:CH2   | 2.45                     | 0.52              |
| 87:8A:602:PGV:H261 | 87:8A:602:PGV:H102 | 1.90                     | 0.52              |
| 57:8C:119:THR:HG21 | 62:8H:82:PRO:HA    | 1.92                     | 0.52              |
| 63:8I:45:LYS:HE2   | 63:8I:49:ASP:OD2   | 2.10                     | 0.52              |
| 68:8N:62:GLN:NE2   | 68:8N:64:LYS:O     | 2.34                     | 0.52              |
| 2:1B:47:PRO:HB3    | 2:1B:85:VAL:HG13   | 1.92                     | 0.52              |
| 12:1L:249:SER:OG   | 12:1L:336:LYS:HG3  | 2.10                     | 0.52              |
| 12:1L:357:ARG:HG2  | 39:1n:31:VAL:HG22  | 1.91                     | 0.52              |
| 69:1Y:202:3PE:H391 | 69:1Y:203:3PE:H261 | 1.91                     | 0.52              |
| 80:1n:201:EHZ:O1   | 80:1n:201:EHZ:S1   | 2.68                     | 0.52              |
| 40:1o:17:ASP:O     | 40:1o:21:MET:HG2   | 2.10                     | 0.52              |
| 49:3E:219:HIS:C    | 49:3E:221:GLY:H    | 2.16                     | 0.52              |
| 45:3N:57:TYR:OH    | 45:3N:137:GLU:OE1  | 2.20                     | 0.52              |
| 45:3N:195:MET:SD   | 45:3N:219:LEU:HD21 | 2.50                     | 0.52              |
| 55:4A:115:SER:HB2  | 55:4A:145:LEU:HB2  | 1.92                     | 0.52              |
| 55:4A:278:MET:HG2  | 87:4A:603:PGV:H241 | 1.92                     | 0.52              |
| 55:4A:413:HIS:CD2  | 55:4A:468:MET:HE3  | 2.44                     | 0.52              |
| 92:4B:305:PSC:H251 | 63:4I:21:ILE:HG13  | 1.92                     | 0.52              |
| 55:8A:127:THR:HA   | 55:8A:235:PHE:CE2  | 2.45                     | 0.52              |
| 55:8A:169:ILE:HG21 | 75:8C:306:CDL:HA62 | 1.92                     | 0.52              |
| 57:8C:23:SER:HB2   | 57:8C:49:THR:HG23  | 1.91                     | 0.52              |
| 57:8C:59:ARG:HD2   | 57:8C:63:ARG:NH2   | 2.24                     | 0.52              |
| 59:8E:53:ARG:NH1   | 59:8E:92:THR:HG23  | 2.25                     | 0.52              |
| 62:8H:75:ARG:HH11  | 62:8H:75:ARG:HG3   | 1.75                     | 0.52              |
| 1:1A:68:GLU:CG     | 10:1J:161:LEU:HD13 | 2.35                     | 0.52              |
| 5:1E:14:GLU:N      | 5:1E:14:GLU:OE2    | 2.42                     | 0.52              |
| 6:1F:299:PRO:O     | 6:1F:334:VAL:HG12  | 2.10                     | 0.52              |
| 12:1L:561:ILE:HD12 | 70:1Y:207:PC1:H291 | 1.91                     | 0.52              |
| 16:1P:137:ALA:HA   | 16:1P:146:LEU:HB3  | 1.92                     | 0.52              |
| 37:1l:115:MET:HA   | 37:1l:118:VAL:HG12 | 1.91                     | 0.52              |
| 41:1p:141:ARG:HG3  | 41:1p:142:TYR:CE1  | 2.45                     | 0.52              |
| 48:3D:222:TYR:OH   | 48:3D:249:MET:HB3  | 2.09                     | 0.52              |
| 45:3N:224:VAL:CG1  | 45:3N:225:GLU:N    | 2.43                     | 0.52              |
| 50:3S:35:ASP:OD1   | 50:3S:89:TYR:OH    | 2.22                     | 0.52              |
| 59:4E:33:MET:CE    | 59:4E:67:ILE:HG21  | 2.38                     | 0.52              |
| 56:8B:44:LEU:HD11  | 63:8I:20:HIS:CD2   | 2.45                     | 0.52              |
| 56:8B:72:ILE:O     | 56:8B:76:ILE:HG13  | 2.09                     | 0.52              |
| 87:8C:301:PGV:H242 | 87:8C:301:PGV:H22  | 1.92                     | 0.52              |
| 4:1D:260:LEU:HD22  | 4:1D:265:ILE:HD13  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|----------------------|--------------------------|-------------------|
| 4:1D:410:MET:HE2   | 8:1H:283:ASP:OD1     | 2.09                     | 0.51              |
| 6:1F:120:GLU:HG3   | 6:1F:232:PRO:HG2     | 1.92                     | 0.51              |
| 6:1F:309:LYS:HA    | 6:1F:312:CYS:SG      | 2.50                     | 0.51              |
| 11:1K:26:LEU:O     | 11:1K:30:LEU:HG      | 2.10                     | 0.51              |
| 12:1L:10:THR:O     | 12:1L:14:ILE:HG23    | 2.10                     | 0.51              |
| 16:1P:203:GLN:NE2  | 16:1P:232:GLY:O      | 2.43                     | 0.51              |
| 38:1m:23:ASP:HB2   | 45:3N:230:ALA:HB3    | 1.91                     | 0.51              |
| 38:1m:82:THR:OG1   | 38:1m:83:PRO:HD2     | 2.10                     | 0.51              |
| 40:1o:51:MET:HA    | 41:1p:118:GLU:HG2    | 1.91                     | 0.51              |
| 40:1o:54:GLN:HB3   | 40:1o:62:LEU:HD13    | 1.92                     | 0.51              |
| 58:4D:44:GLU:HG3   | 58:4D:59:LEU:HD11    | 1.92                     | 0.51              |
| 55:8A:294:THR:HG22 | 55:8A:365:ILE:HD13   | 1.92                     | 0.51              |
| 55:8A:418:PHE:CE2  | 87:8B:301:PGV:H061   | 2.45                     | 0.51              |
| 56:8B:3:TYR:CE1    | 56:8B:6:GLN:HG3      | 2.44                     | 0.51              |
| 56:8B:41:ILE:O     | 56:8B:45:MET:HG2     | 2.08                     | 0.51              |
| 56:8B:116:LEU:HD21 | 56:8B:226:MET:CE     | 2.40                     | 0.51              |
| 57:8C:83:MET:O     | 57:8C:87:ILE:HG13    | 2.10                     | 0.51              |
| 1:1A:55:PHE:HD1    | 10:1J:70:TYR:OH      | 1.93                     | 0.51              |
| 3:1C:68:THR:N      | 21:1V:86:GLU:OE1     | 2.41                     | 0.51              |
| 4:1D:106:LEU:HD13  | 4:1D:391:ILE:HG21    | 1.93                     | 0.51              |
| 6:1F:140:GLY:O     | 6:1F:179:ARG:NH2     | 2.43                     | 0.51              |
| 8:1H:99:ASN:N      | 70:1H:403:PC1:O12    | 2.30                     | 0.51              |
| 70:1M:505:PC1:H341 | 75:1h:202:CDL:H311   | 1.91                     | 0.51              |
| 14:1N:291:TYR:CE2  | 69:1N:901:3PE:H322   | 2.45                     | 0.51              |
| 39:1n:96:TYR:HB2   | 39:1n:177:PRO:HG2    | 1.92                     | 0.51              |
| 43:1r:18:ASP:C     | 43:1r:18:ASP:OD1     | 2.54                     | 0.51              |
| 47:3C:262:LEU:HD11 | 49:3R:172:LYS:HA     | 1.93                     | 0.51              |
| 45:3N:204:GLU:HB2  | 45:3N:207[B]:GLN:HG2 | 1.93                     | 0.51              |
| 57:4C:47:LEU:HD22  | 87:4C:302:PGV:H12    | 1.91                     | 0.51              |
| 58:4D:72:ASN:HB3   | 75:4D:201:CDL:H832   | 1.91                     | 0.51              |
| 55:8A:211:THR:HA   | 55:8A:215:LEU:HD13   | 1.91                     | 0.51              |
| 56:8B:44:LEU:HD11  | 63:8I:20:HIS:CG      | 2.45                     | 0.51              |
| 56:8B:118:PHE:HB3  | 56:8B:226:MET:HE1    | 1.91                     | 0.51              |
| 1:1A:55:PHE:CE1    | 8:1H:134:ARG:HD3     | 2.46                     | 0.51              |
| 8:1H:156:MET:CE    | 25:1Z:50:MET:HG2     | 2.35                     | 0.51              |
| 12:1L:368:PHE:HE2  | 12:1L:454:ILE:HB     | 1.75                     | 0.51              |
| 15:1O:50:HIS:HE2   | 15:1O:125:GLU:CD     | 2.18                     | 0.51              |
| 24:1Y:13:GLU:N     | 24:1Y:13:GLU:OE1     | 2.43                     | 0.51              |
| 35:1j:65:GLY:N     | 40:1o:30:PHE:HE1     | 2.09                     | 0.51              |
| 46:3B:38:LEU:HB3   | 46:3B:209:LEU:HD12   | 1.91                     | 0.51              |
| 48:3D:309:TYR:OH   | 75:3G:103:CDL:OB3    | 2.25                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:71:MET:HA    | 55:4A:75:ILE:HD12  | 1.92                     | 0.51              |
| 55:4A:167:THR:HA   | 55:4A:171:MET:HG3  | 1.92                     | 0.51              |
| 55:4A:216:ASN:ND2  | 61:4G:58:LYS:O     | 2.32                     | 0.51              |
| 57:4C:158:HIS:HE1  | 61:4G:17:ARG:NH2   | 2.08                     | 0.51              |
| 75:4C:305:CDL:H251 | 75:4C:305:CDL:H371 | 1.93                     | 0.51              |
| 64:4J:36:MET:CG    | 87:4J:101:PGV:H182 | 2.40                     | 0.51              |
| 68:4N:38:LEU:C     | 68:4N:39:PHE:HD1   | 2.18                     | 0.51              |
| 55:8A:218:THR:HG23 | 57:8C:192:VAL:HG22 | 1.92                     | 0.51              |
| 56:8B:156:SER:OG   | 56:8B:159:VAL:O    | 2.26                     | 0.51              |
| 57:8C:163:LEU:O    | 57:8C:167:ILE:HG13 | 2.10                     | 0.51              |
| 5:1E:78:MET:HE3    | 7:1G:173:GLY:HA3   | 1.92                     | 0.51              |
| 5:1E:106:THR:O     | 5:1E:110:LEU:HG    | 2.10                     | 0.51              |
| 24:1Y:128:GLN:NE2  | 69:1Y:204:3PE:O14  | 2.43                     | 0.51              |
| 46:3B:24:LEU:HD23  | 46:3B:38:LEU:HB2   | 1.91                     | 0.51              |
| 49:3E:235:TYR:OH   | 48:3Q:144:ARG:NE   | 2.37                     | 0.51              |
| 55:4A:204:ALA:O    | 55:4A:208:MET:HG3  | 2.10                     | 0.51              |
| 55:4A:357:VAL:O    | 55:4A:360:ASN:ND2  | 2.44                     | 0.51              |
| 56:4B:133:MET:HA   | 56:4B:133:MET:HE2  | 1.93                     | 0.51              |
| 55:8A:96:ARG:HH21  | 57:8C:61:ILE:HG13  | 1.76                     | 0.51              |
| 55:8A:240:HIS:O    | 55:8A:243:VAL:HB   | 2.10                     | 0.51              |
| 56:8B:75:LEU:O     | 56:8B:75:LEU:HD23  | 2.10                     | 0.51              |
| 56:8B:102:HIS:NE2  | 56:8B:107:SER:OG   | 2.37                     | 0.51              |
| 58:8D:64:PHE:CE2   | 59:8E:62:ALA:HB1   | 2.45                     | 0.51              |
| 1:1A:48:ARG:H      | 8:1H:126:LYS:HZ1   | 1.57                     | 0.51              |
| 1:1A:50:PRO:HA     | 8:1H:130:ILE:HD11  | 1.92                     | 0.51              |
| 6:1F:151:VAL:HG23  | 6:1F:154:ARG:HH21  | 1.76                     | 0.51              |
| 8:1H:65:THR:O      | 8:1H:124:ASN:ND2   | 2.36                     | 0.51              |
| 10:1J:17:PHE:HA    | 10:1J:20:PHE:CD2   | 2.46                     | 0.51              |
| 10:1J:65:LEU:O     | 10:1J:66:VAL:HG23  | 2.10                     | 0.51              |
| 11:1K:96:LEU:HD12  | 14:1N:54:GLU:HG2   | 1.93                     | 0.51              |
| 13:1M:72:LEU:O     | 13:1M:76:MET:HG3   | 2.10                     | 0.51              |
| 13:1M:306:PRO:HA   | 13:1M:458:LEU:HD22 | 1.91                     | 0.51              |
| 14:1N:211:MET:HG2  | 14:1N:333:SER:HB2  | 1.93                     | 0.51              |
| 44:1s:43:HIS:HA    | 44:1s:46:TYR:CE1   | 2.45                     | 0.51              |
| 55:4A:18:LEU:HB3   | 55:4A:102:PHE:CZ   | 2.45                     | 0.51              |
| 59:4E:84:TYR:HA    | 59:4E:87:GLN:HG2   | 1.92                     | 0.51              |
| 60:4F:25:ARG:HG2   | 60:4F:25:ARG:HH11  | 1.76                     | 0.51              |
| 57:8C:72:THR:HG22  | 57:8C:73:SER:H     | 1.76                     | 0.51              |
| 57:8C:137:LEU:HG   | 57:8C:173:PHE:CD2  | 2.45                     | 0.51              |
| 58:8D:85:ALA:C     | 58:8D:89:ILE:HD12  | 2.34                     | 0.51              |
| 87:8G:101:PGV:H51  | 87:8G:101:PGV:H011 | 1.91                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:1C:65:ARG:NH1    | 3:1C:123:VAL:O     | 2.44                     | 0.51              |
| 8:1H:156:MET:CG    | 8:1H:174:MET:CE    | 2.89                     | 0.51              |
| 37:1I:80:ASP:CB    | 37:1I:83:MET:CE    | 2.88                     | 0.51              |
| 49:3R:199:GLN:CB   | 49:3R:248:ARG:HH21 | 2.20                     | 0.51              |
| 55:4A:428:GLN:HA   | 55:4A:431:LEU:HD12 | 1.92                     | 0.51              |
| 57:4C:163:LEU:HB3  | 57:4C:219:LEU:HD13 | 1.93                     | 0.51              |
| 57:4C:243:HIS:O    | 57:4C:247:VAL:HG23 | 2.11                     | 0.51              |
| 58:4D:129:ALA:HB3  | 58:4D:134:PHE:H    | 1.76                     | 0.51              |
| 63:4I:34:PHE:C     | 63:4I:34:PHE:CD1   | 2.89                     | 0.51              |
| 55:8A:18:LEU:HB3   | 55:8A:102:PHE:CZ   | 2.45                     | 0.51              |
| 55:8A:338:MET:HE3  | 55:8A:338:MET:O    | 2.11                     | 0.51              |
| 87:8A:602:PGV:H342 | 67:8M:23:PHE:HD2   | 1.75                     | 0.51              |
| 56:8B:162:SER:HB3  | 56:8B:197:SER:H    | 1.76                     | 0.51              |
| 58:8D:55:GLU:HA    | 58:8D:58:GLU:HG3   | 1.93                     | 0.51              |
| 2:1B:52:LEU:HB2    | 2:1B:90:GLY:HA3    | 1.91                     | 0.51              |
| 4:1D:246:THR:HB    | 4:1D:249:ASP:HB2   | 1.92                     | 0.51              |
| 8:1H:85:MET:HE2    | 8:1H:233:MET:HG3   | 1.92                     | 0.51              |
| 12:1L:9:LEU:HD12   | 34:1I:85:LEU:HD11  | 1.92                     | 0.51              |
| 13:1M:12:LEU:HB2   | 13:1M:13:PRO:HD3   | 1.91                     | 0.51              |
| 15:1O:234:VAL:O    | 15:1O:238:ILE:HG12 | 2.09                     | 0.51              |
| 37:1I:121:ILE:HG13 | 37:1I:122:TYR:CD1  | 2.46                     | 0.51              |
| 40:1O:103:ARG:HD3  | 40:1O:107:LEU:HD12 | 1.91                     | 0.51              |
| 49:3E:238:CYS:HB3  | 72:3E:301:FES:S2   | 2.50                     | 0.51              |
| 46:3O:319:SER:OG   | 46:3O:320:GLY:N    | 2.43                     | 0.51              |
| 48:3Q:131:LEU:HB3  | 48:3Q:164:ILE:HD11 | 1.93                     | 0.51              |
| 55:4A:404:THR:O    | 55:4A:480:ARG:NH1  | 2.44                     | 0.51              |
| 55:8A:202:LEU:HD22 | 55:8A:238:PHE:CE2  | 2.45                     | 0.51              |
| 56:8B:41:ILE:CG2   | 56:8B:45:MET:HE2   | 2.39                     | 0.51              |
| 11:1K:55:LEU:HD13  | 30:1E:16:TRP:CE3   | 2.45                     | 0.51              |
| 12:1L:78:LEU:HD11  | 75:1L:702:CDL:H662 | 1.93                     | 0.51              |
| 12:1L:261:ILE:HD12 | 12:1L:326:PHE:HB2  | 1.93                     | 0.51              |
| 15:1O:73:LEU:HD13  | 15:1O:299:LEU:HD11 | 1.92                     | 0.51              |
| 32:1G:90:ARG:O     | 32:1G:94:GLU:HG3   | 2.11                     | 0.51              |
| 59:4E:19:PHE:HD2   | 59:4E:51:ALA:HA    | 1.75                     | 0.51              |
| 55:8A:38:ARG:HD3   | 55:8A:455:SER:HA   | 1.92                     | 0.51              |
| 55:8A:150:LEU:HD12 | 55:8A:202:LEU:HD21 | 1.91                     | 0.51              |
| 55:8A:442:ASP:OD2  | 56:8B:134:ARG:NH1  | 2.40                     | 0.51              |
| 56:8B:52:HIS:HD2   | 56:8B:56:MET:SD    | 2.12                     | 0.51              |
| 57:8C:77:LYS:O     | 57:8C:80:ARG:HG2   | 2.10                     | 0.51              |
| 3:1C:77:ASP:OD1    | 3:1C:78:LEU:N      | 2.44                     | 0.51              |
| 4:1D:233:ARG:NH2   | 9:1I:23:GLN:O      | 2.44                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:337:MET:HB3   | 6:1F:341:THR:HG21  | 1.93                     | 0.51              |
| 10:1J:167:VAL:HG13 | 14:1N:42:PRO:HG3   | 1.92                     | 0.51              |
| 12:1L:253:VAL:HB   | 12:1L:310:LEU:HD11 | 1.92                     | 0.51              |
| 16:1P:95:VAL:HG11  | 16:1P:113:ILE:HG21 | 1.92                     | 0.51              |
| 45:3A:172:GLU:OE1  | 45:3A:172:GLU:C    | 2.54                     | 0.51              |
| 49:3V:77:ARG:C     | 49:3V:77:ARG:NE    | 2.69                     | 0.51              |
| 55:4A:254:ILE:HD12 | 55:4A:341:ALA:HA   | 1.93                     | 0.51              |
| 60:4F:26:LYS:HB2   | 60:4F:28:LEU:HD12  | 1.93                     | 0.51              |
| 65:4K:31:TYR:O     | 65:4K:35:GLN:HB2   | 2.11                     | 0.51              |
| 55:8A:349:THR:O    | 55:8A:353:LEU:HG   | 2.10                     | 0.51              |
| 57:8C:34:TRP:HZ3   | 93:8C:308:PEK:H272 | 1.74                     | 0.51              |
| 57:8C:231:HIS:CD2  | 87:8C:307:PGV:H042 | 2.46                     | 0.51              |
| 59:8E:16:VAL:HG23  | 59:8E:47:ILE:HG22  | 1.92                     | 0.51              |
| 7:1G:140:LYS:O     | 7:1G:148:THR:OG1   | 2.29                     | 0.51              |
| 8:1H:33:LEU:HD22   | 9:1I:40:TYR:HE2    | 1.76                     | 0.51              |
| 24:1Y:134:VAL:HG11 | 69:1Y:205:3PE:H222 | 1.92                     | 0.51              |
| 32:1g:24:ILE:HG12  | 32:1g:26:LEU:O     | 2.11                     | 0.51              |
| 44:1s:43:HIS:HA    | 44:1s:46:TYR:CD1   | 2.45                     | 0.51              |
| 45:3A:97:TYR:HH    | 45:3A:190:TYR:HH   | 1.59                     | 0.51              |
| 69:3C:504:3PE:H11  | 49:3R:137:VAL:HG12 | 1.93                     | 0.51              |
| 48:3Q:180:SER:HB2  | 52:3U:77:LEU:HD11  | 1.92                     | 0.51              |
| 49:3R:243:TYR:HA   | 49:3R:248:ARG:O    | 2.11                     | 0.51              |
| 49:3R:260:VAL:HG13 | 49:3R:263:TYR:HE1  | 1.76                     | 0.51              |
| 87:4B:302:PGV:H62  | 68:4N:29:ALA:HB1   | 1.92                     | 0.51              |
| 75:4C:305:CDL:H311 | 75:4C:305:CDL:H212 | 1.91                     | 0.51              |
| 60:4F:70:ILE:HG21  | 60:4F:83:PRO:HD3   | 1.92                     | 0.51              |
| 55:8A:240:HIS:HA   | 55:8A:243:VAL:HB   | 1.92                     | 0.51              |
| 65:8K:38:ILE:CD1   | 65:8K:40:TRP:CE2   | 2.86                     | 0.51              |
| 4:1D:64:LEU:HD11   | 4:1D:418:ILE:HD11  | 1.93                     | 0.50              |
| 5:1E:100:ILE:HB    | 5:1E:139:LEU:HA    | 1.93                     | 0.50              |
| 6:1F:300:GLY:O     | 6:1F:304:THR:OG1   | 2.18                     | 0.50              |
| 7:1G:673:MET:SD    | 7:1G:679:ARG:HA    | 2.51                     | 0.50              |
| 15:1O:165:PRO:O    | 15:1O:248:TRP:NE1  | 2.38                     | 0.50              |
| 16:1P:45:VAL:HB    | 16:1P:68:ILE:HG13  | 1.94                     | 0.50              |
| 16:1P:176:ASP:OD1  | 16:1P:178:PHE:N    | 2.37                     | 0.50              |
| 21:1V:89:LEU:O     | 21:1V:93:MET:HG2   | 2.10                     | 0.50              |
| 22:1W:88:MET:O     | 22:1W:92:GLU:HG3   | 2.11                     | 0.50              |
| 32:1g:68:ILE:HG23  | 32:1g:72:LEU:HD12  | 1.93                     | 0.50              |
| 34:1i:15:ARG:HD2   | 34:1i:19:ARG:HH22  | 1.76                     | 0.50              |
| 37:1l:80:ASP:CB    | 37:1l:83:MET:HE2   | 2.30                     | 0.50              |
| 44:1s:46:TYR:HD2   | 44:1s:50:THR:HG21  | 1.76                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:3B:109:VAL:HG13 | 46:3B:123:LEU:HD13 | 1.92                     | 0.50              |
| 45:3N:443:TRP:HB3  | 45:3N:445:ARG:HG2  | 1.92                     | 0.50              |
| 47:3P:186:PRO:HA   | 47:3P:189:ILE:HD12 | 1.93                     | 0.50              |
| 55:8A:473:TRP:CD1  | 66:8L:22:LEU:HD13  | 2.46                     | 0.50              |
| 56:8B:118:PHE:CD2  | 56:8B:226:MET:HE1  | 2.46                     | 0.50              |
| 57:8C:119:THR:HG22 | 61:8G:50:TYR:HE2   | 1.72                     | 0.50              |
| 57:8C:182:TYR:CE2  | 87:8C:305:PGV:C04  | 2.92                     | 0.50              |
| 5:1E:105:THR:O     | 5:1E:109:MET:N     | 2.36                     | 0.50              |
| 10:1J:45:LEU:HD23  | 10:1J:50:SER:HA    | 1.93                     | 0.50              |
| 12:1L:73:THR:HG22  | 12:1L:73:THR:O     | 2.10                     | 0.50              |
| 17:1Q:77:ASP:OD1   | 17:1Q:77:ASP:O     | 2.29                     | 0.50              |
| 19:1S:88:ARG:NH1   | 19:1S:88:ARG:C     | 2.67                     | 0.50              |
| 20:1T:22:TYR:HE2   | 20:1T:24:LYS:HB2   | 1.76                     | 0.50              |
| 24:1Y:68:ILE:HG13  | 24:1Y:99:THR:HG21  | 1.93                     | 0.50              |
| 34:1i:67:SER:O     | 34:1i:71:VAL:HG22  | 2.11                     | 0.50              |
| 39:1n:56:MET:HE2   | 45:3N:228:VAL:HG11 | 1.93                     | 0.50              |
| 42:1q:88:ARG:HG2   | 42:1q:93:MET:HB2   | 1.94                     | 0.50              |
| 46:3B:264:THR:HB   | 46:3B:315:SER:HB3  | 1.92                     | 0.50              |
| 56:4B:104:TRP:NE1  | 56:4B:200:CYS:O    | 2.42                     | 0.50              |
| 58:4D:54:ASP:OD1   | 58:4D:54:ASP:O     | 2.29                     | 0.50              |
| 59:4E:78:HIS:CE1   | 63:4I:12:LEU:HD23  | 2.46                     | 0.50              |
| 57:8C:244:PHE:CD1  | 57:8C:244:PHE:C    | 2.90                     | 0.50              |
| 58:8D:68:PHE:HZ    | 59:8E:66:ARG:HG3   | 1.76                     | 0.50              |
| 13:1M:114:GLU:OE1  | 23:1X:168:PHE:HB3  | 2.12                     | 0.50              |
| 13:1M:373:ILE:HA   | 13:1M:376:ILE:HD12 | 1.92                     | 0.50              |
| 15:1O:34:GLY:N     | 76:1O:401:GTP:O3G  | 2.32                     | 0.50              |
| 43:1r:57:ASP:OD1   | 43:1r:57:ASP:C     | 2.54                     | 0.50              |
| 45:3A:276:ILE:HD11 | 45:3A:354:VAL:HA   | 1.93                     | 0.50              |
| 46:3B:276:GLN:HG2  | 46:3B:281:ALA:HB2  | 1.93                     | 0.50              |
| 75:3N:502:CDL:HB32 | 75:3N:502:CDL:H112 | 1.93                     | 0.50              |
| 49:3R:222:CYS:HB2  | 72:3R:301:FES:S2   | 2.51                     | 0.50              |
| 55:8A:165:ILE:CG2  | 55:8A:169:ILE:HD11 | 2.41                     | 0.50              |
| 56:8B:155:SER:HB3  | 56:8B:179:LEU:HD12 | 1.94                     | 0.50              |
| 75:8C:306:CDL:H631 | 75:8C:306:CDL:H821 | 1.93                     | 0.50              |
| 8:1H:272:TRP:CZ2   | 9:1I:38:LEU:HB2    | 2.47                     | 0.50              |
| 14:1N:190:MET:HG3  | 14:1N:204:ASN:ND2  | 2.26                     | 0.50              |
| 69:1Y:203:3PE:H262 | 70:1Y:207:PC1:H3E2 | 1.93                     | 0.50              |
| 25:1Z:58:ARG:NH2   | 27:1b:48:THR:OG1   | 2.39                     | 0.50              |
| 47:3P:240:LEU:HB3  | 48:3Q:208:MET:HE2  | 1.93                     | 0.50              |
| 56:4B:223:SER:O    | 56:4B:227:LEU:HG   | 2.12                     | 0.50              |
| 65:4K:22:ALA:O     | 65:4K:26:VAL:HG23  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:8A:24:ALA:O     | 55:8A:28:MET:HG2   | 2.10                     | 0.50              |
| 55:8A:269:GLY:O    | 55:8A:273:MET:HG3  | 2.11                     | 0.50              |
| 57:8C:87:ILE:HG23  | 57:8C:244:PHE:CD2  | 2.46                     | 0.50              |
| 5:1E:51:LEU:HD23   | 5:1E:69:VAL:HG21   | 1.92                     | 0.50              |
| 6:1F:31:TRP:HH2    | 6:1F:151:VAL:HG13  | 1.77                     | 0.50              |
| 6:1F:191:ALA:HB2   | 6:1F:203:PRO:HG3   | 1.94                     | 0.50              |
| 7:1G:623:LEU:HD22  | 7:1G:630:LEU:HD22  | 1.93                     | 0.50              |
| 8:1H:267:THR:O     | 8:1H:271:LEU:HG    | 2.12                     | 0.50              |
| 10:1J:71:THR:HG21  | 11:1K:75:LEU:HD22  | 1.94                     | 0.50              |
| 12:1L:529:TYR:HB3  | 12:1L:530:PRO:HD3  | 1.93                     | 0.50              |
| 15:1O:128:ILE:HG21 | 15:1O:160:ALA:HB2  | 1.94                     | 0.50              |
| 23:1X:19:VAL:HG23  | 23:1X:24:LEU:HG    | 1.93                     | 0.50              |
| 23:1X:46:ARG:NH1   | 25:1Z:80:ASP:OD2   | 2.45                     | 0.50              |
| 23:1X:139:ASN:OD1  | 23:1X:139:ASN:O    | 2.30                     | 0.50              |
| 32:1g:52:ILE:HG23  | 32:1g:53:VAL:HG13  | 1.94                     | 0.50              |
| 40:1o:45:MET:SD    | 40:1o:55:ARG:HG2   | 2.52                     | 0.50              |
| 43:1r:92:LYS:N     | 43:1r:92:LYS:HD2   | 2.26                     | 0.50              |
| 47:3C:24:PRO:HB2   | 47:3C:27:ILE:HG23  | 1.93                     | 0.50              |
| 53:3J:12:ARG:HH22  | 61:8G:14:ARG:HE    | 1.59                     | 0.50              |
| 46:3O:197:ASN:HB3  | 46:3O:232:LEU:HB2  | 1.91                     | 0.50              |
| 55:8A:43:GLN:HG3   | 55:8A:44:PRO:HD2   | 1.93                     | 0.50              |
| 55:8A:362:SER:CA   | 56:8B:87:MET:HE1   | 2.40                     | 0.50              |
| 58:8D:89:ILE:HG22  | 65:8K:29:TRP:HE1   | 1.77                     | 0.50              |
| 58:8D:145:TRP:H    | 58:8D:145:TRP:CD1  | 2.28                     | 0.50              |
| 59:8E:43:PRO:HB2   | 59:8E:48:ILE:HD11  | 1.94                     | 0.50              |
| 59:8E:78:HIS:ND1   | 63:8I:12:LEU:CD1   | 2.65                     | 0.50              |
| 67:8M:24:LEU:O     | 67:8M:28:ILE:HG13  | 2.11                     | 0.50              |
| 1:1A:113:TRP:CZ2   | 8:1H:286:MET:HG3   | 2.47                     | 0.50              |
| 2:1B:69:MET:HA     | 2:1B:72:PHE:HD2    | 1.77                     | 0.50              |
| 2:1B:154:GLU:HG2   | 9:1I:50:TYR:CE1    | 2.45                     | 0.50              |
| 5:1E:146:GLY:HA3   | 6:1F:142:PHE:CZ    | 2.45                     | 0.50              |
| 6:1F:342:ASP:HB3   | 6:1F:345:LYS:HB3   | 1.94                     | 0.50              |
| 12:1L:21:MET:HE3   | 12:1L:24:SER:OG    | 2.12                     | 0.50              |
| 12:1L:149:ILE:HG13 | 13:1M:369:LEU:HD13 | 1.94                     | 0.50              |
| 16:1P:192:PRO:HB2  | 16:1P:263:TYR:OH   | 2.12                     | 0.50              |
| 20:1U:26:ASP:OD1   | 20:1U:28:GLU:HG3   | 2.11                     | 0.50              |
| 24:1Y:48:PHE:HA    | 69:1Y:206:3PE:H222 | 1.93                     | 0.50              |
| 25:1Z:95:ALA:HB2   | 25:1Z:106:VAL:HG21 | 1.94                     | 0.50              |
| 25:1Z:98:MET:HE2   | 30:1e:78:ILE:HA    | 1.93                     | 0.50              |
| 69:1d:201:3PE:H252 | 69:1d:201:3PE:H362 | 1.93                     | 0.50              |
| 34:1i:44:GLN:HA    | 34:1i:47:ASN:HD21  | 1.77                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:3B:95:LYS:HG3   | 49:3I:32:ALA:HB2   | 1.92                     | 0.50              |
| 52:3H:100:PHE:HA   | 52:3H:103:LEU:HB2  | 1.93                     | 0.50              |
| 49:3R:179:ARG:HH21 | 49:3R:184:ILE:HG23 | 1.76                     | 0.50              |
| 58:4D:89:ILE:HG22  | 65:4K:29:TRP:NE1   | 2.20                     | 0.50              |
| 56:8B:6:GLN:NE2    | 56:8B:8:GLY:O      | 2.44                     | 0.50              |
| 56:8B:59:GLN:OE1   | 56:8B:59:GLN:HA    | 2.11                     | 0.50              |
| 57:8C:187:THR:N    | 57:8C:190:ASP:OD2  | 2.30                     | 0.50              |
| 58:8D:123:MET:HE2  | 58:8D:134:PHE:CE2  | 2.46                     | 0.50              |
| 58:8D:137:LYS:HD2  | 65:8K:45:VAL:HG21  | 1.94                     | 0.50              |
| 58:8D:141:ASP:O    | 58:8D:143:ASN:N    | 2.44                     | 0.50              |
| 1:1A:54:LYS:HG2    | 1:1A:114:ALA:H     | 1.77                     | 0.50              |
| 6:1F:110:ILE:HD12  | 6:1F:114:ASP:HB2   | 1.94                     | 0.50              |
| 7:1G:231:MET:HE3   | 7:1G:270:ALA:HB3   | 1.94                     | 0.50              |
| 7:1G:409:ILE:HD11  | 7:1G:422:LEU:HD12  | 1.93                     | 0.50              |
| 10:1J:119:PHE:CE1  | 11:1K:1:FME:HE2    | 2.46                     | 0.50              |
| 12:1L:118:PHE:O    | 12:1L:122:VAL:HG23 | 2.11                     | 0.50              |
| 69:1L:701:3PE:H242 | 69:1L:701:3PE:H322 | 1.93                     | 0.50              |
| 15:1O:24:VAL:HG23  | 15:1O:166:PRO:HA   | 1.94                     | 0.50              |
| 20:1T:8:LEU:HD23   | 20:1T:88:GLU:HB3   | 1.93                     | 0.50              |
| 24:1Y:28:GLY:HA2   | 69:1Y:203:3PE:H2B2 | 1.93                     | 0.50              |
| 25:1Z:125:TYR:HB3  | 25:1Z:133:ILE:HG22 | 1.93                     | 0.50              |
| 37:1I:125:TYR:OH   | 40:1O:7:ARG:HD3    | 2.12                     | 0.50              |
| 46:3O:52:LYS:O     | 46:3O:203:ARG:NH2  | 2.36                     | 0.50              |
| 49:3R:204:ARG:HH22 | 49:3R:213:LEU:HD23 | 1.77                     | 0.50              |
| 55:8A:110:LEU:CD1  | 87:8A:601:PGV:H181 | 2.41                     | 0.50              |
| 1:1A:53:MET:HE2    | 10:1J:172:THR:HG23 | 1.93                     | 0.50              |
| 6:1F:254:LYS:HD3   | 6:1F:332:ALA:HB2   | 1.93                     | 0.50              |
| 10:1J:167:VAL:O    | 10:1J:171:ILE:HG13 | 2.11                     | 0.50              |
| 12:1L:473:PRO:HG2  | 12:1L:475:MET:HE3  | 1.94                     | 0.50              |
| 69:1Y:202:3PE:H31  | 69:1Y:202:3PE:H242 | 1.93                     | 0.50              |
| 25:1Z:121:MET:HG3  | 25:1Z:137:THR:HG22 | 1.94                     | 0.50              |
| 32:1g:95:ARG:HH11  | 32:1g:95:ARG:HG3   | 1.77                     | 0.50              |
| 46:3B:369:LEU:HD11 | 46:3B:399:LEU:HD11 | 1.94                     | 0.50              |
| 45:3N:34:THR:HG22  | 45:3N:102:LEU:HD23 | 1.94                     | 0.50              |
| 47:3P:234:PHE:HD2  | 75:3T:101:CDL:H762 | 1.75                     | 0.50              |
| 55:4A:265:LYS:HB3  | 55:4A:490:THR:HG21 | 1.94                     | 0.50              |
| 87:4C:303:PGV:H231 | 87:4C:303:PGV:H271 | 1.94                     | 0.50              |
| 63:4I:29:LEU:O     | 63:4I:33:THR:OG1   | 2.22                     | 0.50              |
| 56:8B:12:ALA:HB2   | 56:8B:21:LEU:HD12  | 1.93                     | 0.50              |
| 57:8C:147:ALA:HB2  | 57:8C:162:ALA:HB3  | 1.94                     | 0.50              |
| 62:8H:55:TRP:O     | 62:8H:59:VAL:HG12  | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:134:ASP:OD1   | 5:1E:136:LEU:HB2   | 2.12                     | 0.50              |
| 5:1E:194:GLU:HG2   | 6:1F:28:ARG:NH2    | 2.23                     | 0.50              |
| 7:1G:229:ASP:OD2   | 7:1G:267:THR:HG23  | 2.12                     | 0.50              |
| 15:1O:104:ARG:NH2  | 76:1O:401:GTP:N7   | 2.59                     | 0.50              |
| 16:1P:139:ILE:HD12 | 59:8E:9:GLU:OE1    | 2.11                     | 0.50              |
| 34:1i:14:LEU:HD22  | 39:1n:169:ILE:HD11 | 1.93                     | 0.50              |
| 50:3S:14:GLU:OE1   | 50:3S:14:GLU:N     | 2.38                     | 0.50              |
| 56:4B:110:TYR:HE2  | 56:4B:118:PHE:HE2  | 1.59                     | 0.50              |
| 55:8A:69:MET:HE3   | 88:8A:604:HEA:C27  | 2.40                     | 0.50              |
| 55:8A:155:VAL:C    | 55:8A:159:LEU:HD12 | 2.35                     | 0.50              |
| 55:8A:483:SER:N    | 67:8M:4:LYS:HZ1    | 2.05                     | 0.50              |
| 55:8A:496:HIS:CE1  | 60:8F:57:ILE:CD1   | 2.95                     | 0.50              |
| 69:1A:201:3PE:H3A2 | 27:1b:19:VAL:HG23  | 1.94                     | 0.49              |
| 7:1G:385:ARG:HE    | 7:1G:416:THR:HG23  | 1.77                     | 0.49              |
| 7:1G:624:GLU:HB2   | 7:1G:631:VAL:HG21  | 1.94                     | 0.49              |
| 10:1J:129:ASP:OD2  | 11:1K:52:HIS:NE2   | 2.45                     | 0.49              |
| 11:1K:27:MET:HE1   | 11:1K:78:LEU:HD22  | 1.94                     | 0.49              |
| 69:1L:701:3PE:H221 | 37:1l:88:ARG:HA    | 1.92                     | 0.49              |
| 13:1M:92:LYS:O     | 13:1M:96:ILE:HG12  | 2.12                     | 0.49              |
| 13:1M:131:ILE:HD12 | 14:1N:302:LEU:HD21 | 1.94                     | 0.49              |
| 16:1P:113:ILE:O    | 16:1P:117:ILE:HG12 | 2.12                     | 0.49              |
| 20:1T:11:ILE:HG23  | 20:1T:58:PHE:HE2   | 1.77                     | 0.49              |
| 27:1b:34:LEU:O     | 27:1b:34:LEU:HD12  | 2.11                     | 0.49              |
| 30:1e:83:ASP:OD1   | 30:1e:84:LYS:N     | 2.45                     | 0.49              |
| 35:1j:42:HIS:NE2   | 36:1k:84:GLU:OE1   | 2.45                     | 0.49              |
| 48:3D:240:TYR:OH   | 52:3H:92:ASP:OD2   | 2.26                     | 0.49              |
| 46:3O:51:ILE:HG12  | 46:3O:204:MET:HG2  | 1.94                     | 0.49              |
| 46:3O:109:VAL:HG13 | 46:3O:123:LEU:HD13 | 1.93                     | 0.49              |
| 48:3Q:200:HIS:O    | 48:3Q:204:MET:HG3  | 2.12                     | 0.49              |
| 75:4B:303:CDL:H321 | 63:4I:34:PHE:HE1   | 1.76                     | 0.49              |
| 59:4E:93:LEU:HB3   | 59:4E:98:ILE:O     | 2.11                     | 0.49              |
| 55:8A:35:LEU:HG    | 55:8A:462:LEU:HD22 | 1.94                     | 0.49              |
| 56:8B:105:TYR:HE2  | 56:8B:119:ASP:OD2  | 1.95                     | 0.49              |
| 56:8B:139:ASP:N    | 56:8B:139:ASP:OD1  | 2.43                     | 0.49              |
| 56:8B:161:HIS:HB2  | 56:8B:174:ALA:HB3  | 1.94                     | 0.49              |
| 57:8C:59:ARG:HG2   | 57:8C:63:ARG:HE    | 1.77                     | 0.49              |
| 57:8C:210:ILE:HG21 | 87:8C:307:PGV:H281 | 1.93                     | 0.49              |
| 64:8J:28:ASP:HA    | 64:8J:31:LEU:CD1   | 2.42                     | 0.49              |
| 1:1A:111:LEU:HD13  | 8:1H:290:TRP:HB3   | 1.94                     | 0.49              |
| 7:1G:350:PRO:HD3   | 7:1G:458:LEU:HD13  | 1.94                     | 0.49              |
| 7:1G:366:THR:HG22  | 7:1G:370:GLY:HA3   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:44:GLU:OE1    | 81:1q:202:AYA:HM3  | 2.12                     | 0.49              |
| 10:1J:99:MET:SD    | 10:1J:99:MET:O     | 2.70                     | 0.49              |
| 11:1K:48:ILE:HG23  | 11:1K:53:PHE:HB3   | 1.94                     | 0.49              |
| 13:1M:14:MET:HE1   | 13:1M:30:HIS:CG    | 2.47                     | 0.49              |
| 20:1T:72:CYS:O     | 20:1T:76:ILE:HG13  | 2.12                     | 0.49              |
| 34:1i:114:GLU:OE1  | 34:1i:114:GLU:N    | 2.41                     | 0.49              |
| 35:1j:65:GLY:N     | 40:1o:30:PHE:CE1   | 2.80                     | 0.49              |
| 47:3C:29:SER:HB2   | 75:3G:103:CDL:H731 | 1.94                     | 0.49              |
| 49:3E:164:ASN:HA   | 49:3E:177:ARG:HB2  | 1.94                     | 0.49              |
| 47:3P:67:THR:HG22  | 48:3Q:115:TYR:HE2  | 1.77                     | 0.49              |
| 49:3R:179:ARG:HG3  | 49:3R:184:ILE:HG12 | 1.93                     | 0.49              |
| 87:4A:602:PGV:H242 | 87:4A:602:PGV:H22  | 1.94                     | 0.49              |
| 57:4C:118:PRO:HB2  | 57:4C:121:ILE:HD12 | 1.94                     | 0.49              |
| 58:4D:111:PHE:HE2  | 65:4K:41:ASN:HB2   | 1.77                     | 0.49              |
| 55:8A:338:MET:HE2  | 55:8A:342:LEU:HG   | 1.93                     | 0.49              |
| 55:8A:449:ALA:O    | 55:8A:453:ILE:HG12 | 2.12                     | 0.49              |
| 56:8B:188:ARG:NH1  | 63:8I:51:TYR:OH    | 2.45                     | 0.49              |
| 68:8N:18:LEU:CD1   | 68:8N:22:ILE:HD11  | 2.42                     | 0.49              |
| 5:1E:150:ASN:HA    | 5:1E:190:ARG:HH12  | 1.77                     | 0.49              |
| 14:1N:152:ASN:ND2  | 69:1Y:205:3PE:O12  | 2.45                     | 0.49              |
| 40:1o:102:GLU:OE2  | 40:1o:105:ARG:NH1  | 2.45                     | 0.49              |
| 45:3A:273:ALA:HB1  | 45:3A:345:LEU:HD13 | 1.94                     | 0.49              |
| 46:3B:366:ALA:O    | 46:3B:370:MET:HG3  | 2.11                     | 0.49              |
| 47:3C:267:HIS:ND1  | 47:3C:267:HIS:O    | 2.45                     | 0.49              |
| 47:3C:310:SER:HB2  | 47:3C:370:SER:HB3  | 1.94                     | 0.49              |
| 55:4A:23:GLY:HA3   | 55:4A:73:ILE:HG13  | 1.94                     | 0.49              |
| 55:4A:240:HIS:O    | 55:4A:243:VAL:HB   | 2.12                     | 0.49              |
| 57:4C:244:PHE:HA   | 75:4C:305:CDL:H832 | 1.93                     | 0.49              |
| 55:8A:242:GLU:HA   | 55:8A:245:ILE:CD1  | 2.40                     | 0.49              |
| 57:8C:244:PHE:HA   | 75:8C:306:CDL:H832 | 1.94                     | 0.49              |
| 68:8N:22:ILE:HD12  | 68:8N:22:ILE:H     | 1.78                     | 0.49              |
| 1:1A:85:LYS:HG3    | 1:1A:86:THR:H      | 1.78                     | 0.49              |
| 7:1G:444:LYS:NZ    | 7:1G:480:SER:HB2   | 2.27                     | 0.49              |
| 9:1I:132:VAL:HG21  | 9:1I:165:ILE:HD12  | 1.94                     | 0.49              |
| 10:1J:135:PHE:CD2  | 25:1Z:68:ARG:HD3   | 2.47                     | 0.49              |
| 23:1X:124:LEU:HD21 | 25:1Z:70:ALA:HB2   | 1.94                     | 0.49              |
| 34:1i:92:LYS:HD3   | 34:1i:95:THR:CG2   | 2.43                     | 0.49              |
| 38:1m:47:LEU:HB3   | 39:1n:165:LEU:HD13 | 1.94                     | 0.49              |
| 40:1o:68:CYS:SG    | 40:1o:79:CYS:HB2   | 2.51                     | 0.49              |
| 46:3B:137:VAL:O    | 46:3B:141:GLN:HG2  | 2.12                     | 0.49              |
| 48:3D:185:ASN:OD1  | 48:3D:185:ASN:C    | 2.56                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 45:3N:8:LEU:HD22   | 45:3N:392:LEU:HB3  | 1.94                     | 0.49              |
| 45:3N:358:LYS:O    | 45:3N:362:ARG:HG3  | 2.13                     | 0.49              |
| 55:4A:362:SER:HA   | 56:4B:87:MET:HE3   | 1.94                     | 0.49              |
| 57:4C:15:PRO:HB2   | 64:4J:36:MET:HE1   | 1.94                     | 0.49              |
| 75:4D:201:CDL:H371 | 75:4D:201:CDL:H561 | 1.94                     | 0.49              |
| 59:4E:52:LEU:CD2   | 59:4E:67:ILE:HD11  | 2.42                     | 0.49              |
| 55:8A:274:VAL:O    | 55:8A:278:MET:HG3  | 2.12                     | 0.49              |
| 55:8A:445:ASP:OD1  | 55:8A:446:ALA:N    | 2.45                     | 0.49              |
| 57:8C:79:LEU:HB3   | 57:8C:233:PHE:CE2  | 2.46                     | 0.49              |
| 57:8C:121:ILE:HG21 | 57:8C:193:TYR:HD2  | 1.77                     | 0.49              |
| 58:8D:34:SER:OG    | 58:8D:37:GLN:OE1   | 2.30                     | 0.49              |
| 3:1C:49:GLU:HG2    | 3:1C:106:ARG:HE    | 1.78                     | 0.49              |
| 5:1E:216:GLY:O     | 5:1E:217:LEU:HD23  | 2.13                     | 0.49              |
| 6:1F:261:HIS:HE1   | 6:1F:341:THR:OG1   | 1.93                     | 0.49              |
| 10:1J:120:ASN:OD1  | 10:1J:122:LEU:N    | 2.45                     | 0.49              |
| 13:1M:216:LEU:HB3  | 13:1M:217:PRO:HD3  | 1.94                     | 0.49              |
| 15:1O:49:ARG:HH21  | 15:1O:51:PHE:HE1   | 1.60                     | 0.49              |
| 15:1O:139:TYR:CZ   | 15:1O:146:LYS:HD3  | 2.47                     | 0.49              |
| 39:1n:161:ASP:OD1  | 39:1n:161:ASP:C    | 2.55                     | 0.49              |
| 45:3A:8:LEU:HD22   | 45:3A:392:LEU:HB3  | 1.94                     | 0.49              |
| 46:3B:156:GLN:NE2  | 49:3I:58:GLN:O     | 2.46                     | 0.49              |
| 48:3D:121:TYR:CZ   | 48:3D:131:MET:HG3  | 2.47                     | 0.49              |
| 48:3D:316:TRP:O    | 48:3D:320:LYS:HG2  | 2.13                     | 0.49              |
| 49:3E:194:GLN:NE2  | 49:3E:194:GLN:O    | 2.45                     | 0.49              |
| 46:3O:137:VAL:O    | 46:3O:141:GLN:HG2  | 2.13                     | 0.49              |
| 55:4A:468:MET:CE   | 55:4A:471:ILE:HD11 | 2.36                     | 0.49              |
| 87:4A:602:PGV:O14  | 57:4C:57:TRP:NE1   | 2.39                     | 0.49              |
| 56:4B:148:MET:HE1  | 56:4B:216:LEU:HD21 | 1.94                     | 0.49              |
| 55:8A:445:ASP:O    | 55:8A:448:THR:OG1  | 2.24                     | 0.49              |
| 62:8H:8:ILE:HD11   | 62:8H:55:TRP:HB2   | 1.94                     | 0.49              |
| 4:1D:357:GLN:O     | 43:1r:59:ARG:NH1   | 2.45                     | 0.49              |
| 8:1H:100:LEU:HD13  | 8:1H:103:LEU:HD12  | 1.93                     | 0.49              |
| 11:1K:27:MET:HE2   | 11:1K:78:LEU:HD13  | 1.94                     | 0.49              |
| 13:1M:385:SER:OG   | 13:1M:396:MET:HE1  | 2.13                     | 0.49              |
| 16:1P:21:ALA:HA    | 16:1P:90:VAL:O     | 2.11                     | 0.49              |
| 20:1T:11:ILE:HG23  | 20:1T:58:PHE:CE2   | 2.47                     | 0.49              |
| 21:1V:75:GLN:O     | 21:1V:78:GLU:HG2   | 2.13                     | 0.49              |
| 28:1c:19:LEU:HB3   | 75:1d:203:CDL:H122 | 1.95                     | 0.49              |
| 35:1j:53:TYR:CE1   | 40:1o:98:MET:HE1   | 2.47                     | 0.49              |
| 46:3O:312:PHE:HA   | 49:3V:61:GLY:HA2   | 1.93                     | 0.49              |
| 56:4B:160:LEU:HD11 | 56:4B:175:ILE:HG23 | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:4C:58:TRP:CZ3   | 87:4C:306:PGV:H71  | 2.48                     | 0.49              |
| 63:4I:57:MET:O     | 63:4I:57:MET:HE3   | 2.11                     | 0.49              |
| 55:8A:29:VAL:HG13  | 66:8L:36:PRO:HG3   | 1.94                     | 0.49              |
| 1:1A:48:ARG:HE     | 10:1J:78:MET:HA    | 1.78                     | 0.49              |
| 6:1F:202:LYS:HE2   | 6:1F:361:GLN:HB2   | 1.94                     | 0.49              |
| 13:1M:122:PHE:CE1  | 13:1M:206:LYS:HD3  | 2.46                     | 0.49              |
| 16:1P:165:ILE:HB   | 16:1P:227:THR:HG23 | 1.95                     | 0.49              |
| 16:1P:172:PHE:HB2  | 16:1P:179:LEU:CD2  | 2.43                     | 0.49              |
| 19:1S:49:ASP:N     | 19:1S:49:ASP:OD1   | 2.45                     | 0.49              |
| 20:1U:13:ASP:O     | 20:1U:17:TYR:HB2   | 2.13                     | 0.49              |
| 23:1X:38:PRO:HG3   | 23:1X:65:CYS:SG    | 2.53                     | 0.49              |
| 28:1c:44:ARG:C     | 28:1c:44:ARG:HD3   | 2.38                     | 0.49              |
| 47:3P:157:GLY:O    | 47:3P:161:VAL:HG23 | 2.13                     | 0.49              |
| 56:4B:25:ASP:OD2   | 63:4I:43:ARG:NE    | 2.42                     | 0.49              |
| 59:4E:11:PHE:CE2   | 59:4E:41:LEU:HD21  | 2.47                     | 0.49              |
| 60:4F:93:SER:O     | 60:4F:94:HIS:HB3   | 2.11                     | 0.49              |
| 56:8B:59:GLN:HE21  | 68:8N:13:PRO:N     | 2.10                     | 0.49              |
| 59:8E:9:GLU:HA     | 59:8E:12:ASP:HB2   | 1.94                     | 0.49              |
| 2:1B:71:ARG:HH21   | 8:1H:38:ASN:HD21   | 1.60                     | 0.49              |
| 4:1D:269:LEU:HB2   | 4:1D:368:GLU:HB2   | 1.94                     | 0.49              |
| 6:1F:98:ASP:OD1    | 6:1F:139:ARG:HD2   | 2.13                     | 0.49              |
| 7:1G:194:GLU:OE1   | 7:1G:194:GLU:N     | 2.29                     | 0.49              |
| 9:1I:114:THR:HG21  | 9:1I:144:HIS:CE1   | 2.47                     | 0.49              |
| 70:1M:503:PC1:H2   | 70:1M:503:PC1:H221 | 1.53                     | 0.49              |
| 20:1U:48:VAL:HG12  | 20:1U:52:MET:SD    | 2.53                     | 0.49              |
| 22:1W:69:LYS:NZ    | 22:1W:69:LYS:HB3   | 2.28                     | 0.49              |
| 22:1W:98:LYS:HB3   | 22:1W:102:HIS:HB2  | 1.93                     | 0.49              |
| 75:3A:501:CDL:H152 | 69:3A:503:3PE:H381 | 1.95                     | 0.49              |
| 49:3E:197:ASP:N    | 49:3E:197:ASP:OD1  | 2.44                     | 0.49              |
| 75:3G:103:CDL:H522 | 75:3G:103:CDL:H562 | 1.93                     | 0.49              |
| 45:3N:80:GLU:OE2   | 46:3O:292:THR:OG1  | 2.21                     | 0.49              |
| 49:3R:121:THR:O    | 49:3R:125:VAL:HG23 | 2.12                     | 0.49              |
| 87:4C:304:PGV:H222 | 87:4C:304:PGV:H21  | 1.94                     | 0.49              |
| 55:8A:54:TYR:O     | 55:8A:58:VAL:HG23  | 2.13                     | 0.49              |
| 59:8E:18:TYR:HE2   | 59:8E:32:GLY:HA3   | 1.77                     | 0.49              |
| 61:8G:14:ARG:HD2   | 61:8G:17:ARG:HD3   | 1.95                     | 0.49              |
| 63:8I:27:VAL:O     | 63:8I:31:VAL:HG13  | 2.13                     | 0.49              |
| 66:8L:21:LEU:O     | 66:8L:25:MET:HG3   | 2.12                     | 0.49              |
| 5:1E:217:LEU:HD23  | 5:1E:217:LEU:N     | 2.28                     | 0.49              |
| 10:1J:120:ASN:OD1  | 10:1J:120:ASN:C    | 2.56                     | 0.49              |
| 75:1N:902:CDL:OA4  | 75:1N:902:CDL:O1   | 2.27                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:1R:49:VAL:HG22  | 18:1R:90:GLN:HB2   | 1.95                     | 0.49              |
| 23:1X:84:TYR:CZ    | 23:1X:88:ILE:HD11  | 2.48                     | 0.49              |
| 33:1h:110:VAL:CG1  | 33:1h:114:MET:HE2  | 2.42                     | 0.49              |
| 37:1l:91:THR:HG22  | 38:1m:10:LEU:HA    | 1.95                     | 0.49              |
| 49:3E:241:SER:HA   | 49:3E:252:GLY:HA3  | 1.94                     | 0.49              |
| 46:3O:258:VAL:HA   | 46:3O:323:GLY:HA3  | 1.94                     | 0.49              |
| 46:3O:299:VAL:HG11 | 46:3O:336:VAL:HG13 | 1.95                     | 0.49              |
| 56:4B:150:ILE:HB   | 56:4B:184:LEU:HB3  | 1.95                     | 0.49              |
| 63:4I:41:GLU:OE1   | 63:4I:41:GLU:CA    | 2.60                     | 0.49              |
| 63:4I:41:GLU:OE1   | 63:4I:41:GLU:HA    | 2.11                     | 0.49              |
| 55:8A:63:PHE:CE1   | 55:8A:150:LEU:HD21 | 2.48                     | 0.49              |
| 4:1D:223:ASP:HB3   | 4:1D:305:ARG:HH22  | 1.78                     | 0.49              |
| 6:1F:74:PRO:HB2    | 6:1F:77:LEU:HB2    | 1.94                     | 0.49              |
| 7:1G:20:VAL:HG21   | 7:1G:73:VAL:HG21   | 1.95                     | 0.49              |
| 8:1H:92:PRO:HD3    | 8:1H:255:TYR:CD1   | 2.48                     | 0.49              |
| 10:1J:120:ASN:OD1  | 10:1J:122:LEU:HB2  | 2.12                     | 0.49              |
| 13:1M:2:LEU:HD13   | 31:1f:26:LEU:HD23  | 1.93                     | 0.49              |
| 14:1N:44:LEU:HD22  | 14:1N:122:ILE:HD13 | 1.94                     | 0.49              |
| 14:1N:172:GLN:NE2  | 14:1N:177:LYS:HD3  | 2.28                     | 0.49              |
| 15:1O:77:CYS:HB3   | 15:1O:95:ARG:HG2   | 1.95                     | 0.49              |
| 19:1S:17:GLU:OE1   | 19:1S:19:ARG:HD3   | 2.12                     | 0.49              |
| 23:1X:126:LYS:HE3  | 27:1b:66:PRO:HG3   | 1.95                     | 0.49              |
| 27:1b:56:LEU:HD11  | 27:1b:65:VAL:HG21  | 1.95                     | 0.49              |
| 46:3B:204:MET:HE1  | 46:3B:224:LEU:HD22 | 1.95                     | 0.49              |
| 46:3O:203:ARG:NH1  | 46:3O:232:LEU:O    | 2.46                     | 0.49              |
| 56:4B:61:VAL:C     | 56:4B:65:TRP:CZ3   | 2.91                     | 0.49              |
| 57:4C:90:GLU:OE1   | 87:4C:306:PGV:H321 | 2.12                     | 0.49              |
| 59:4E:96:LEU:CD1   | 59:4E:98:ILE:HD11  | 2.43                     | 0.49              |
| 55:8A:275:TRP:CE3  | 87:8A:603:PGV:H12  | 2.48                     | 0.49              |
| 55:8A:443:TYR:O    | 56:8B:134:ARG:NH2  | 2.46                     | 0.49              |
| 57:8C:95:THR:HA    | 57:8C:98:PHE:HD2   | 1.78                     | 0.49              |
| 57:8C:102:TYR:HE2  | 87:8C:304:PGV:H12  | 1.76                     | 0.49              |
| 69:1A:201:3PE:H2A2 | 69:1A:201:3PE:H2E1 | 1.94                     | 0.48              |
| 10:1J:163:ILE:HG21 | 14:1N:12:THR:HG21  | 1.95                     | 0.48              |
| 12:1L:332:HIS:HA   | 12:1L:335:PHE:CE2  | 2.48                     | 0.48              |
| 26:1a:50:ARG:O     | 26:1a:54:ILE:HG23  | 2.12                     | 0.48              |
| 36:1k:48:GLU:N     | 36:1k:48:GLU:OE2   | 2.46                     | 0.48              |
| 47:3P:246:SER:HB2  | 47:3P:249:LEU:HB2  | 1.95                     | 0.48              |
| 48:3Q:203:ARG:NH2  | 53:3W:53:LYS:HZ1   | 2.11                     | 0.48              |
| 49:3R:172:LYS:CB   | 49:3R:214:ILE:HD12 | 2.43                     | 0.48              |
| 55:4A:92:MET:HE2   | 55:4A:163:ASN:ND2  | 2.27                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:4B:303:CDL:H631 | 75:4B:303:CDL:H141 | 1.95                     | 0.48              |
| 55:8A:333:LYS:HZ2  | 55:8A:335:SER:CA   | 2.22                     | 0.48              |
| 56:8B:29:MET:CE    | 63:8I:36:LYS:HG3   | 2.43                     | 0.48              |
| 59:8E:13:ALA:O     | 59:8E:17:THR:HG22  | 2.13                     | 0.48              |
| 61:8G:32:THR:OG1   | 87:8G:101:PGV:C30  | 2.61                     | 0.48              |
| 2:1B:65:PRO:HA     | 8:1H:34:ARG:HG2    | 1.94                     | 0.48              |
| 2:1B:68:ASP:OD2    | 8:1H:34:ARG:HB3    | 2.13                     | 0.48              |
| 5:1E:160:TYR:O     | 5:1E:185:GLY:N     | 2.44                     | 0.48              |
| 6:1F:93:LEU:O      | 6:1F:134:ALA:HA    | 2.14                     | 0.48              |
| 7:1G:218:ARG:HD2   | 7:1G:220:TRP:CH2   | 2.48                     | 0.48              |
| 7:1G:241:SER:HB2   | 7:1G:249:ARG:HG3   | 1.95                     | 0.48              |
| 8:1H:316:PRO:HG3   | 25:1Z:57:ARG:HB3   | 1.94                     | 0.48              |
| 20:1T:52:MET:SD    | 22:1W:37:ARG:HD3   | 2.54                     | 0.48              |
| 22:1W:89:GLU:O     | 22:1W:93:THR:HG22  | 2.13                     | 0.48              |
| 38:1m:32:GLN:HA    | 38:1m:35:ARG:HD2   | 1.95                     | 0.48              |
| 39:1n:10:THR:O     | 39:1n:14:LYS:HG3   | 2.12                     | 0.48              |
| 39:1n:89:SER:O     | 39:1n:89:SER:OG    | 2.31                     | 0.48              |
| 45:3A:142:ASP:OD2  | 49:3E:79:SER:OG    | 2.27                     | 0.48              |
| 45:3A:324:PHE:CG   | 45:3A:334:MET:HE3  | 2.48                     | 0.48              |
| 45:3A:358:LYS:O    | 45:3A:362:ARG:HG3  | 2.13                     | 0.48              |
| 69:3C:504:3PE:H322 | 70:3X:101:PC1:H252 | 1.95                     | 0.48              |
| 51:3G:21:SER:O     | 51:3G:25:GLN:HG2   | 2.12                     | 0.48              |
| 45:3N:444:LEU:HB3  | 75:3N:502:CDL:H712 | 1.95                     | 0.48              |
| 49:3R:191:GLU:HG3  | 49:3R:194:GLN:H    | 1.78                     | 0.48              |
| 50:3S:82:LYS:HB2   | 50:3S:85:GLU:HG3   | 1.94                     | 0.48              |
| 55:8A:69:MET:HG2   | 55:8A:70:VAL:N     | 2.28                     | 0.48              |
| 55:8A:313:ALA:HB2  | 55:8A:356:ILE:HD11 | 1.95                     | 0.48              |
| 75:8D:201:CDL:H171 | 75:8D:201:CDL:H721 | 1.95                     | 0.48              |
| 59:8E:72:LYS:HB2   | 59:8E:82:TYR:HE2   | 0.81                     | 0.48              |
| 65:8K:17:ILE:HD12  | 65:8K:17:ILE:H     | 1.78                     | 0.48              |
| 68:8N:35:ARG:HE    | 68:8N:65:PHE:HE1   | 1.61                     | 0.48              |
| 2:1B:57:VAL:HA     | 2:1B:60:MET:HG2    | 1.95                     | 0.48              |
| 4:1D:62:LEU:HD11   | 4:1D:78:PRO:HB3    | 1.95                     | 0.48              |
| 12:1L:127:THR:HG21 | 12:1L:146:GLY:HA3  | 1.94                     | 0.48              |
| 12:1L:237:MET:HB3  | 12:1L:299:LYS:HE2  | 1.95                     | 0.48              |
| 13:1M:41:LEU:HD13  | 13:1M:66:LEU:HD13  | 1.96                     | 0.48              |
| 16:1P:63:GLY:HA3   | 16:1P:68:ILE:HD13  | 1.94                     | 0.48              |
| 19:1S:43:LEU:HD12  | 19:1S:47:ASN:ND2   | 2.27                     | 0.48              |
| 25:1Z:87:LEU:HD11  | 25:1Z:119:PRO:HG3  | 1.94                     | 0.48              |
| 45:3A:240:GLU:OE1  | 45:3A:242:ARG:NH1  | 2.45                     | 0.48              |
| 45:3N:29:GLN:NE2   | 45:3N:204:GLU:OE1  | 2.45                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:3O:276:GLN:HB2  | 46:3O:322:PHE:HE1  | 1.78                     | 0.48              |
| 58:4D:60:TYR:CD1   | 58:4D:60:TYR:C     | 2.91                     | 0.48              |
| 58:4D:61:ARG:NH1   | 58:4D:65:ASN:O     | 2.47                     | 0.48              |
| 66:8L:19:TRP:CH2   | 67:8M:14:GLU:OE1   | 2.66                     | 0.48              |
| 68:8N:11:LYS:HD3   | 68:8N:11:LYS:H     | 1.78                     | 0.48              |
| 2:1B:71:ARG:HA     | 8:1H:37:PRO:HA     | 1.95                     | 0.48              |
| 8:1H:197:PRO:HB2   | 8:1H:280:PHE:HD2   | 1.78                     | 0.48              |
| 12:1L:367:PRO:O    | 12:1L:371:THR:HG23 | 2.13                     | 0.48              |
| 13:1M:6:ILE:HD12   | 31:1f:23:GLY:HA2   | 1.94                     | 0.48              |
| 13:1M:220:HIS:HD2  | 13:1M:232:ALA:HB2  | 1.77                     | 0.48              |
| 14:1N:107:GLY:O    | 14:1N:187:MET:CE   | 2.60                     | 0.48              |
| 15:1O:9:VAL:HG12   | 15:1O:10:LEU:HD23  | 1.96                     | 0.48              |
| 15:1O:306:PRO:HB2  | 28:1c:7:PRO:HB3    | 1.96                     | 0.48              |
| 15:1O:318:TRP:CD1  | 15:1O:318:TRP:H    | 2.31                     | 0.48              |
| 16:1P:317:VAL:HG23 | 16:1P:318:LEU:HD22 | 1.94                     | 0.48              |
| 24:1Y:80:ARG:HB3   | 24:1Y:82:LYS:HE2   | 1.95                     | 0.48              |
| 33:1h:41:THR:HG22  | 75:1h:202:CDL:H711 | 1.94                     | 0.48              |
| 46:3B:37:SER:HB3   | 46:3B:216:LEU:HD12 | 1.94                     | 0.48              |
| 47:3C:119:LEU:HD22 | 85:3C:502:HEM:HBB2 | 1.95                     | 0.48              |
| 49:3E:155:LYS:NZ   | 49:3E:274:GLY:OXT  | 2.39                     | 0.48              |
| 49:3R:243:TYR:HB3  | 49:3R:247:GLY:HA2  | 1.94                     | 0.48              |
| 57:4C:25:LEU:HD23  | 64:4J:43:THR:HG22  | 1.96                     | 0.48              |
| 57:4C:47:LEU:HD13  | 87:4C:302:PGV:H12  | 1.96                     | 0.48              |
| 55:8A:244:TYR:O    | 55:8A:248:LEU:HD12 | 2.14                     | 0.48              |
| 58:8D:23:PRO:O     | 59:8E:66:ARG:NH1   | 2.46                     | 0.48              |
| 59:8E:53:ARG:HH12  | 59:8E:92:THR:HG23  | 1.78                     | 0.48              |
| 2:1B:150:PRO:HD3   | 4:1D:190:HIS:CD2   | 2.49                     | 0.48              |
| 5:1E:78:MET:HE3    | 7:1G:173:GLY:CA    | 2.44                     | 0.48              |
| 6:1F:21:ILE:CG2    | 6:1F:117:LYS:HZ1   | 2.27                     | 0.48              |
| 6:1F:32:ARG:HH12   | 44:1s:42:GLN:NE2   | 2.11                     | 0.48              |
| 6:1F:308:PRO:HD2   | 6:1F:311:VAL:HB    | 1.94                     | 0.48              |
| 9:1I:144:HIS:CE1   | 16:1P:65:LEU:HD21  | 2.48                     | 0.48              |
| 11:1K:22:TYR:CD2   | 11:1K:90:VAL:HG21  | 2.48                     | 0.48              |
| 12:1L:156:GLY:HA3  | 13:1M:416:ARG:HH12 | 1.78                     | 0.48              |
| 12:1L:419:THR:HA   | 12:1L:422:TYR:CE2  | 2.48                     | 0.48              |
| 13:1M:237:LYS:HD2  | 13:1M:316:MET:HB3  | 1.95                     | 0.48              |
| 69:1M:502:3PE:H2B2 | 69:1M:504:3PE:H252 | 1.94                     | 0.48              |
| 24:1Y:72:THR:HB    | 24:1Y:92:GLY:HA2   | 1.95                     | 0.48              |
| 25:1Z:140:PHE:HB2  | 26:1a:45:TRP:CD1   | 2.49                     | 0.48              |
| 31:1f:2:ASN:O      | 31:1f:6:ILE:HG13   | 2.13                     | 0.48              |
| 46:3B:222:ARG:HD2  | 46:3B:223:PHE:CE1  | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:3C:100:ARG:HA   | 69:3C:503:3PE:H252 | 1.95                     | 0.48              |
| 56:4B:49:LYS:NZ    | 59:4E:76:GLY:C     | 2.71                     | 0.48              |
| 55:8A:21:LEU:HB3   | 87:8L:101:PGV:H271 | 1.95                     | 0.48              |
| 55:8A:181:THR:O    | 55:8A:270:TYR:OH   | 2.24                     | 0.48              |
| 55:8A:266:GLU:HB3  | 60:8F:68:THR:HG21  | 1.95                     | 0.48              |
| 56:8B:112:ASP:OD1  | 62:8H:62:SER:OG    | 2.31                     | 0.48              |
| 56:8B:132:GLU:HB3  | 56:8B:137:GLU:HG3  | 1.95                     | 0.48              |
| 58:8D:52:SER:N     | 58:8D:55:GLU:OE2   | 2.45                     | 0.48              |
| 2:1B:50:PHE:HE2    | 2:1B:96:MET:CE     | 2.26                     | 0.48              |
| 2:1B:69:MET:HG3    | 2:1B:74:VAL:O      | 2.14                     | 0.48              |
| 6:1F:90:PRO:O      | 6:1F:218:CYS:HB2   | 2.14                     | 0.48              |
| 8:1H:9:LEU:O       | 8:1H:13:ILE:HG12   | 2.13                     | 0.48              |
| 10:1J:10:SER:O     | 10:1J:14:VAL:HG23  | 2.14                     | 0.48              |
| 12:1L:154:LEU:HD13 | 12:1L:243:VAL:HG22 | 1.95                     | 0.48              |
| 17:1Q:89:LYS:NZ    | 17:1Q:107:GLU:OE2  | 2.47                     | 0.48              |
| 22:1W:62:LYS:HD3   | 22:1W:62:LYS:HA    | 1.74                     | 0.48              |
| 32:1g:48:ASP:C     | 32:1g:48:ASP:OD1   | 2.57                     | 0.48              |
| 75:1h:202:CDL:HA4  | 75:1h:202:CDL:H722 | 1.95                     | 0.48              |
| 37:1l:3:HIS:ND1    | 37:1l:4:VAL:HG23   | 2.28                     | 0.48              |
| 41:1p:98:ASP:HA    | 41:1p:101:ILE:HD12 | 1.95                     | 0.48              |
| 47:3C:307:LEU:HD11 | 47:3C:363:LEU:HD23 | 1.95                     | 0.48              |
| 55:4A:54:TYR:O     | 55:4A:58:VAL:HG23  | 2.13                     | 0.48              |
| 55:4A:127:THR:HA   | 55:4A:235:PHE:CE2  | 2.48                     | 0.48              |
| 57:4C:109:THR:HG21 | 57:4C:111:GLU:OE2  | 2.14                     | 0.48              |
| 58:4D:141:ASP:O    | 58:4D:143:ASN:N    | 2.47                     | 0.48              |
| 60:4F:43:LYS:HG3   | 60:4F:44:GLU:OE2   | 2.13                     | 0.48              |
| 62:4H:4:ILE:HG21   | 62:4H:52:VAL:HG13  | 1.95                     | 0.48              |
| 62:4H:5:GLN:CD     | 62:4H:5:GLN:H      | 2.20                     | 0.48              |
| 66:4L:37:PHE:HB3   | 67:4M:33:VAL:HG21  | 1.95                     | 0.48              |
| 55:8A:413:HIS:CE1  | 55:8A:468:MET:HE3  | 2.49                     | 0.48              |
| 6:1F:369:VAL:HA    | 6:1F:372:MET:HE2   | 1.95                     | 0.48              |
| 7:1G:168:GLY:HA3   | 7:1G:416:THR:HB    | 1.95                     | 0.48              |
| 8:1H:152:SER:HA    | 8:1H:155:LEU:HD12  | 1.96                     | 0.48              |
| 9:1I:65:HIS:ND1    | 9:1I:113:MET:HE1   | 2.28                     | 0.48              |
| 12:1L:273:VAL:O    | 12:1L:277:THR:HG23 | 2.13                     | 0.48              |
| 12:1L:349:SER:HB2  | 12:1L:366:MET:CE   | 2.43                     | 0.48              |
| 13:1M:287:ALA:O    | 13:1M:291:VAL:HG23 | 2.13                     | 0.48              |
| 14:1N:102:LEU:HD13 | 14:1N:142:LEU:HG   | 1.96                     | 0.48              |
| 14:1N:270:MET:HE1  | 14:1N:282:MET:HE1  | 1.95                     | 0.48              |
| 16:1P:45:VAL:HG12  | 16:1P:47:VAL:HG23  | 1.95                     | 0.48              |
| 20:1T:31:SER:OG    | 20:1T:34:SER:OG    | 2.27                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1T:60:PHE:CZ    | 20:1T:80:ILE:HG23  | 2.49                     | 0.48              |
| 20:1U:44:SER:O     | 20:1U:48:VAL:HG23  | 2.13                     | 0.48              |
| 23:1X:8:THR:O      | 23:1X:12:LEU:HG    | 2.14                     | 0.48              |
| 69:1d:201:3PE:H2A2 | 70:1d:202:PC1:H332 | 1.96                     | 0.48              |
| 34:1i:69:PHE:O     | 34:1i:73:HIS:HB2   | 2.13                     | 0.48              |
| 45:3A:40:TRP:HB3   | 45:3A:384:LEU:HD11 | 1.95                     | 0.48              |
| 46:3O:70:ARG:HD3   | 46:3O:100:SER:OG   | 2.13                     | 0.48              |
| 48:3Q:224:ARG:NH1  | 75:3T:101:CDL:OB3  | 2.46                     | 0.48              |
| 52:3U:68:CYS:O     | 52:3U:72:LYS:HG2   | 2.13                     | 0.48              |
| 55:4A:345:ILE:O    | 55:4A:349:THR:OG1  | 2.26                     | 0.48              |
| 88:4A:604:HEA:H132 | 88:4A:604:HEA:HHC  | 1.96                     | 0.48              |
| 57:4C:22:LEU:HD22  | 64:4J:43:THR:HG21  | 1.94                     | 0.48              |
| 87:4L:101:PGV:H131 | 87:4L:101:PGV:H311 | 1.96                     | 0.48              |
| 59:8E:24:ILE:HD12  | 59:8E:25:ASP:N     | 2.27                     | 0.48              |
| 68:8N:52:GLU:HB2   | 68:8N:54:TRP:CE2   | 2.48                     | 0.48              |
| 2:1B:162:GLN:HE21  | 9:1I:142:GLU:HG2   | 1.77                     | 0.48              |
| 3:1C:79:THR:HB     | 4:1D:390:LYS:HG2   | 1.96                     | 0.48              |
| 6:1F:164:LYS:CA    | 44:1s:63:MET:HE1   | 2.42                     | 0.48              |
| 6:1F:275:PRO:HB2   | 6:1F:278:GLU:HG2   | 1.95                     | 0.48              |
| 7:1G:426:PRO:HB2   | 7:1G:656:LEU:HD23  | 1.96                     | 0.48              |
| 9:1I:169:ILE:O     | 9:1I:173:TYR:HB3   | 2.13                     | 0.48              |
| 11:1K:44:SER:HB2   | 11:1K:59:MET:HE1   | 1.96                     | 0.48              |
| 12:1L:140:LEU:HD22 | 12:1L:182:PHE:CE2  | 2.44                     | 0.48              |
| 13:1M:196:TRP:CD1  | 13:1M:250:LEU:HB3  | 2.47                     | 0.48              |
| 14:1N:65:THR:O     | 14:1N:69:MET:HG3   | 2.14                     | 0.48              |
| 15:1O:70:ASP:OD2   | 15:1O:72:GLN:NE2   | 2.46                     | 0.48              |
| 16:1P:89:ASN:OD1   | 16:1P:89:ASN:C     | 2.57                     | 0.48              |
| 16:1P:94:LEU:HD13  | 16:1P:132:ILE:HG13 | 1.95                     | 0.48              |
| 20:1T:65:ILE:H     | 20:1T:65:ILE:HD12  | 1.78                     | 0.48              |
| 75:1X:201:CDL:H273 | 75:1X:201:CDL:H322 | 1.96                     | 0.48              |
| 34:1i:44:GLN:HA    | 34:1i:47:ASN:ND2   | 2.29                     | 0.48              |
| 46:3B:226:MET:HG3  | 46:3B:227:ARG:N    | 2.29                     | 0.48              |
| 47:3C:120:LEU:O    | 47:3C:124:MET:HG3  | 2.14                     | 0.48              |
| 46:3O:395:PRO:O    | 46:3O:399:LEU:HG   | 2.14                     | 0.48              |
| 55:4A:3:VAL:HA     | 55:4A:7:LEU:HB2    | 1.94                     | 0.48              |
| 55:4A:254:ILE:HG13 | 55:4A:344:PHE:CD2  | 2.48                     | 0.48              |
| 58:4D:28:ALA:HB1   | 58:4D:63:LYS:HA    | 1.95                     | 0.48              |
| 62:4H:57:ARG:HA    | 62:4H:60:TYR:HD1   | 1.78                     | 0.48              |
| 87:4K:101:PGV:H21  | 87:4K:101:PGV:H62  | 1.96                     | 0.48              |
| 68:4N:3:ARG:HG3    | 68:4N:4:GLN:N      | 2.28                     | 0.48              |
| 57:8C:103:HIS:HA   | 87:8C:304:PGV:O02  | 2.14                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:8E:81:ILE:HG23  | 63:8I:9:MET:SD     | 2.54                     | 0.48              |
| 87:8G:101:PGV:H02  | 87:8G:101:PGV:H21  | 1.52                     | 0.48              |
| 1:1A:51:PHE:O      | 1:1A:52:SER:HB3    | 2.14                     | 0.48              |
| 4:1D:62:LEU:HD22   | 4:1D:425:PHE:HZ    | 1.79                     | 0.48              |
| 4:1D:148:LEU:HD23  | 4:1D:174:ARG:HG2   | 1.95                     | 0.48              |
| 4:1D:284:ASP:O     | 4:1D:306:GLN:HG3   | 2.14                     | 0.48              |
| 12:1L:574:SER:OG   | 14:1N:171:ASN:HB2  | 2.14                     | 0.48              |
| 14:1N:118:VAL:O    | 14:1N:122:ILE:HG23 | 2.14                     | 0.48              |
| 16:1P:112:LYS:HD3  | 16:1P:112:LYS:N    | 2.29                     | 0.48              |
| 37:1l:10:PRO:HD3   | 38:1m:66:ARG:HG2   | 1.96                     | 0.48              |
| 49:3E:204:ARG:NH2  | 49:3E:246:SER:OG   | 2.40                     | 0.48              |
| 50:3F:61:ARG:NH2   | 50:3F:112:GLU:OE1  | 2.36                     | 0.48              |
| 45:3N:224:VAL:CG1  | 45:3N:225:GLU:OE1  | 2.61                     | 0.48              |
| 75:3P:504:CDL:OB4  | 51:3T:40:ARG:NE    | 2.38                     | 0.48              |
| 49:3R:169:TRP:CD1  | 49:3R:174:LEU:HD22 | 2.48                     | 0.48              |
| 56:4B:165:VAL:HG11 | 56:4B:168:LEU:HD12 | 1.96                     | 0.48              |
| 59:4E:42:VAL:HG21  | 59:4E:81:ILE:HG21  | 1.95                     | 0.48              |
| 55:8A:86:MET:HE1   | 55:8A:184:PHE:HD2  | 1.78                     | 0.48              |
| 57:8C:175:LEU:HD22 | 87:8C:305:PGV:H221 | 1.96                     | 0.48              |
| 4:1D:94:LYS:HD2    | 4:1D:102:TYR:HE2   | 1.79                     | 0.48              |
| 4:1D:121:ALA:HA    | 4:1D:365:THR:HG21  | 1.95                     | 0.48              |
| 4:1D:424:VAL:O     | 4:1D:428:VAL:HG23  | 2.13                     | 0.48              |
| 6:1F:261:HIS:ND1   | 6:1F:338:ASP:OD1   | 2.37                     | 0.48              |
| 6:1F:279:LEU:HD12  | 6:1F:317:MET:HG3   | 1.95                     | 0.48              |
| 7:1G:522:LEU:HD22  | 7:1G:537:LEU:HD11  | 1.96                     | 0.48              |
| 7:1G:534:ARG:HH22  | 42:1q:145:LYS:HE3  | 1.79                     | 0.48              |
| 69:1M:504:3PE:H272 | 14:1N:246:VAL:HG21 | 1.96                     | 0.48              |
| 15:1O:49:ARG:HD3   | 15:1O:114:HIS:CD2  | 2.48                     | 0.48              |
| 16:1P:118:ALA:HA   | 16:1P:129:LEU:HD21 | 1.95                     | 0.48              |
| 16:1P:258:LEU:HD23 | 16:1P:263:TYR:CE1  | 2.49                     | 0.48              |
| 17:1Q:49:VAL:O     | 17:1Q:49:VAL:HG22  | 2.13                     | 0.48              |
| 23:1X:56:LEU:O     | 23:1X:60:LYS:HG2   | 2.14                     | 0.48              |
| 29:1d:14:LEU:HD11  | 29:1d:77:LYS:HB3   | 1.95                     | 0.48              |
| 39:1n:126:ARG:O    | 39:1n:130:GLU:HG2  | 2.14                     | 0.48              |
| 41:1p:98:ASP:O     | 41:1p:102:VAL:HG23 | 2.14                     | 0.48              |
| 46:3B:36:ALA:HB3   | 46:3B:207:ILE:HG13 | 1.95                     | 0.48              |
| 48:3D:135:ALA:HA   | 48:3D:178:TYR:HA   | 1.95                     | 0.48              |
| 48:3Q:212:MET:SD   | 69:3R:302:3PE:H352 | 2.54                     | 0.48              |
| 49:3R:211:VAL:HG11 | 49:3R:245:ALA:O    | 2.13                     | 0.48              |
| 55:4A:3:VAL:HG11   | 87:4A:601:PGV:H31  | 1.95                     | 0.48              |
| 55:4A:62:ALA:HB2   | 88:4A:604:HEA:HBD1 | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:125:THR:HG22 | 56:4B:134:ARG:HG3  | 1.96                     | 0.48              |
| 64:4J:51:GLY:O     | 64:4J:54:SER:OG    | 2.31                     | 0.48              |
| 55:8A:455:SER:O    | 55:8A:458:SER:OG   | 2.29                     | 0.48              |
| 75:8B:303:CDL:H182 | 75:8B:303:CDL:H442 | 1.96                     | 0.48              |
| 64:8J:46:SER:O     | 64:8J:50:LEU:HG    | 2.14                     | 0.48              |
| 2:1B:179:ARG:HH12  | 78:1P:402:NDP:P2B  | 2.37                     | 0.47              |
| 5:1E:78:MET:HA     | 5:1E:81:TYR:CD2    | 2.49                     | 0.47              |
| 6:1F:154:ARG:HD2   | 44:1s:57:GLU:OE1   | 2.14                     | 0.47              |
| 6:1F:404:ILE:HG22  | 7:1G:53:ARG:NH1    | 2.29                     | 0.47              |
| 12:1L:245:ALA:HB2  | 12:1L:340:PHE:HB3  | 1.96                     | 0.47              |
| 13:1M:250:LEU:O    | 13:1M:254:THR:OG1  | 2.26                     | 0.47              |
| 32:1g:114:ASP:HB3  | 32:1g:117:LYS:HD2  | 1.95                     | 0.47              |
| 34:1i:99:ARG:HA    | 41:1p:115:ARG:HA   | 1.96                     | 0.47              |
| 45:3A:349:ALA:O    | 45:3A:350:THR:HB   | 2.14                     | 0.47              |
| 47:3C:63:PHE:O     | 47:3C:67:THR:HG23  | 2.14                     | 0.47              |
| 47:3C:181:PHE:CZ   | 47:3P:53:MET:HE2   | 2.49                     | 0.47              |
| 49:3E:159:ILE:HG12 | 49:3E:165:MET:CG   | 2.42                     | 0.47              |
| 45:3N:272:VAL:O    | 45:3N:276:ILE:HG13 | 2.14                     | 0.47              |
| 55:4A:282:PHE:HA   | 87:4A:603:PGV:H292 | 1.95                     | 0.47              |
| 63:4I:23:GLY:O     | 63:4I:26:ILE:HG13  | 2.14                     | 0.47              |
| 55:8A:44:PRO:HG3   | 58:8D:111:PHE:CZ   | 2.49                     | 0.47              |
| 57:8C:176:LEU:O    | 57:8C:180:GLU:OE1  | 2.31                     | 0.47              |
| 58:8D:86:LEU:HA    | 58:8D:89:ILE:CD1   | 2.44                     | 0.47              |
| 7:1G:144:PRO:HD2   | 7:1G:192:MET:HE1   | 1.96                     | 0.47              |
| 7:1G:344:CYS:HB3   | 7:1G:510:GLY:O     | 2.14                     | 0.47              |
| 7:1G:511:VAL:HG22  | 7:1G:514:ILE:HB    | 1.96                     | 0.47              |
| 8:1H:63:PRO:HG2    | 8:1H:66:SER:HB3    | 1.96                     | 0.47              |
| 8:1H:85:MET:CE     | 8:1H:233:MET:HG3   | 2.44                     | 0.47              |
| 12:1L:178:GLY:HA2  | 12:1L:218:LEU:HG   | 1.96                     | 0.47              |
| 12:1L:593:ILE:O    | 12:1L:597:ILE:HG13 | 2.14                     | 0.47              |
| 13:1M:243:MET:HE3  | 13:1M:301:ILE:CG2  | 2.44                     | 0.47              |
| 15:1O:75:GLY:HA2   | 15:1O:99:TRP:CD2   | 2.49                     | 0.47              |
| 15:1O:180:GLN:O    | 15:1O:183:ILE:HG13 | 2.14                     | 0.47              |
| 21:1V:17:GLU:HG2   | 21:1V:18:THR:HG23  | 1.96                     | 0.47              |
| 23:1X:165:ARG:O    | 33:1h:104:ARG:NH1  | 2.44                     | 0.47              |
| 29:1d:113:LEU:HD22 | 32:1g:121:PRO:HG3  | 1.96                     | 0.47              |
| 39:1n:12:GLN:O     | 39:1n:16:LEU:HG    | 2.14                     | 0.47              |
| 39:1n:153:LEU:HD13 | 39:1n:165:LEU:HB2  | 1.96                     | 0.47              |
| 45:3A:121:SER:O    | 45:3A:179:ARG:NH1  | 2.47                     | 0.47              |
| 48:3D:304:LEU:HD21 | 49:3E:124:GLY:HA3  | 1.97                     | 0.47              |
| 49:3R:128:ALA:HB1  | 69:3R:302:3PE:H361 | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:129:TYR:OH   | 55:4A:236:TRP:NE1  | 2.46                     | 0.47              |
| 55:8A:217:THR:HB   | 57:8C:195:SER:HB3  | 1.96                     | 0.47              |
| 57:8C:77:LYS:CD    | 57:8C:80:ARG:HD3   | 2.43                     | 0.47              |
| 59:8E:73:ASP:C     | 59:8E:73:ASP:OD1   | 2.57                     | 0.47              |
| 61:8G:15:THR:O     | 61:8G:19:LEU:CD1   | 2.53                     | 0.47              |
| 1:1A:22:PHE:CD1    | 8:1H:60:PRO:HG2    | 2.49                     | 0.47              |
| 1:1A:54:LYS:NZ     | 4:1D:71:GLU:HB2    | 2.29                     | 0.47              |
| 4:1D:115:GLU:HG3   | 4:1D:194:ILE:HB    | 1.96                     | 0.47              |
| 6:1F:15:LEU:HD13   | 6:1F:271:GLU:HB2   | 1.95                     | 0.47              |
| 6:1F:115:PRO:O     | 6:1F:119:VAL:HG23  | 2.14                     | 0.47              |
| 6:1F:261:HIS:CD2   | 6:1F:261:HIS:N     | 2.78                     | 0.47              |
| 7:1G:386:PHE:CE1   | 7:1G:668:ILE:HD13  | 2.49                     | 0.47              |
| 8:1H:92:PRO:HD3    | 8:1H:255:TYR:HD1   | 1.80                     | 0.47              |
| 9:1I:54:LYS:HD3    | 42:1q:91:HIS:CE1   | 2.49                     | 0.47              |
| 12:1L:63:ILE:O     | 12:1L:79:SER:HA    | 2.14                     | 0.47              |
| 16:1P:153:GLU:OE2  | 16:1P:167:LYS:NZ   | 2.46                     | 0.47              |
| 18:1R:20:ASP:OD1   | 18:1R:21:GLY:N     | 2.46                     | 0.47              |
| 41:1p:139:GLN:O    | 41:1p:143:SER:HB2  | 2.13                     | 0.47              |
| 41:1p:141:ARG:HG3  | 41:1p:142:TYR:CD1  | 2.50                     | 0.47              |
| 45:3A:280:TYR:HA   | 45:3A:284:TYR:CE2  | 2.49                     | 0.47              |
| 48:3D:313:ARG:HD3  | 51:3G:28:PHE:CE2   | 2.50                     | 0.47              |
| 48:3Q:47:ALA:HA    | 48:3Q:90:TYR:HA    | 1.95                     | 0.47              |
| 75:4D:201:CDL:OB4  | 75:4D:201:CDL:HA4  | 2.14                     | 0.47              |
| 55:8A:499:PRO:HG3  | 66:8L:10:ASN:ND2   | 2.29                     | 0.47              |
| 56:8B:221:LYS:HD2  | 56:8B:221:LYS:O    | 2.14                     | 0.47              |
| 58:8D:94:LEU:HD23  | 58:8D:97:ILE:HD11  | 1.96                     | 0.47              |
| 1:1A:23:TRP:HZ2    | 70:1A:202:PC1:H222 | 1.79                     | 0.47              |
| 70:1B:203:PC1:H2   | 70:1B:203:PC1:H221 | 1.36                     | 0.47              |
| 4:1D:52:GLY:H      | 4:1D:53:PRO:CD     | 2.24                     | 0.47              |
| 10:1J:39:VAL:O     | 10:1J:43:ILE:HG13  | 2.14                     | 0.47              |
| 12:1L:297:ASP:O    | 12:1L:301:ILE:HG13 | 2.14                     | 0.47              |
| 21:1V:48:GLU:O     | 21:1V:52:ASN:ND2   | 2.47                     | 0.47              |
| 75:1X:201:CDL:HA21 | 75:1X:201:CDL:H541 | 1.96                     | 0.47              |
| 34:1i:79:TRP:HD1   | 41:1p:40:VAL:HG13  | 1.79                     | 0.47              |
| 49:3I:32:ALA:N     | 49:3I:71:ASN:OD1   | 2.47                     | 0.47              |
| 45:3N:279:HIS:HD1  | 45:3N:284:TYR:HH   | 1.54                     | 0.47              |
| 75:3N:502:CDL:OA9  | 47:3P:221:HIS:NE2  | 2.47                     | 0.47              |
| 47:3P:116:GLY:C    | 85:3P:502:HEM:HBC2 | 2.38                     | 0.47              |
| 47:3P:119:LEU:HD22 | 85:3P:502:HEM:HBB2 | 1.97                     | 0.47              |
| 57:4C:156:ARG:NH2  | 57:4C:222:GLN:O    | 2.46                     | 0.47              |
| 63:4I:41:GLU:O     | 63:4I:41:GLU:CD    | 2.56                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:8A:378:HIS:O    | 55:8A:382:SER:OG   | 2.31                     | 0.47              |
| 55:8A:412:ILE:HG13 | 58:8D:81:ILE:HG23  | 1.97                     | 0.47              |
| 56:8B:68:LEU:O     | 56:8B:72:ILE:HG13  | 2.14                     | 0.47              |
| 1:1A:53:MET:HE1    | 11:1K:79:VAL:HG13  | 1.95                     | 0.47              |
| 4:1D:241:ASP:OD1   | 4:1D:290:ARG:NH1   | 2.47                     | 0.47              |
| 6:1F:308:PRO:HD3   | 6:1F:421:HIS:CD2   | 2.50                     | 0.47              |
| 7:1G:453:LEU:HD21  | 7:1G:458:LEU:HD21  | 1.96                     | 0.47              |
| 34:1i:94:TYR:OH    | 41:1p:10:PRO:O     | 2.26                     | 0.47              |
| 45:3A:6:GLN:HA     | 45:3A:9:GLN:HG2    | 1.96                     | 0.47              |
| 46:3B:370:MET:HA   | 46:3B:373:GLU:HG3  | 1.95                     | 0.47              |
| 47:3C:316:MET:HG2  | 47:3C:317:PHE:CE1  | 2.49                     | 0.47              |
| 49:3R:187:GLU:OE2  | 49:3R:244:ASP:HB2  | 2.15                     | 0.47              |
| 55:4A:469:ILE:HD13 | 67:4M:26:PHE:CE1   | 2.50                     | 0.47              |
| 56:4B:12:ALA:N     | 63:4I:47:TYR:OH    | 2.39                     | 0.47              |
| 60:4F:79:THR:HG21  | 60:4F:88:HIS:HB3   | 1.97                     | 0.47              |
| 55:8A:243:VAL:HG13 | 88:8A:605:HEA:C3C  | 2.44                     | 0.47              |
| 55:8A:251:PHE:HB3  | 55:8A:319:LYS:NZ   | 2.30                     | 0.47              |
| 57:8C:51:THR:HG22  | 87:8C:303:PGV:H172 | 1.95                     | 0.47              |
| 1:1A:37:TYR:HB2    | 2:1B:81:ARG:HH11   | 1.79                     | 0.47              |
| 6:1F:154:ARG:HB2   | 44:1s:58:LEU:HD11  | 1.95                     | 0.47              |
| 14:1N:69:MET:HE3   | 14:1N:97:MET:HE3   | 1.95                     | 0.47              |
| 49:3E:264:GLU:H    | 49:3E:272:ILE:HG12 | 1.78                     | 0.47              |
| 55:4A:117:MET:O    | 66:4L:46:LYS:NZ    | 2.47                     | 0.47              |
| 55:4A:334:TRP:CZ3  | 75:4D:201:CDL:H121 | 2.50                     | 0.47              |
| 56:4B:60:GLU:H     | 56:4B:60:GLU:CD    | 2.22                     | 0.47              |
| 57:4C:83:MET:HG2   | 57:4C:237:ALA:HB1  | 1.97                     | 0.47              |
| 58:4D:78:TRP:HB3   | 75:4D:201:CDL:H182 | 1.95                     | 0.47              |
| 63:4I:57:MET:O     | 63:4I:61:GLU:HG2   | 2.15                     | 0.47              |
| 55:8A:31:THR:HG21  | 55:8A:465:VAL:HG11 | 1.96                     | 0.47              |
| 55:8A:277:MET:O    | 55:8A:280:ILE:HG13 | 2.15                     | 0.47              |
| 55:8A:342:LEU:HD22 | 56:8B:46:LEU:HD11  | 1.97                     | 0.47              |
| 75:8C:306:CDL:O1   | 75:8C:306:CDL:OA7  | 2.31                     | 0.47              |
| 1:1A:4:MET:HE2     | 70:1H:403:PC1:H261 | 1.96                     | 0.47              |
| 2:1B:30:VAL:HG13   | 2:1B:173:LEU:HB3   | 1.97                     | 0.47              |
| 2:1B:36:LEU:HD22   | 70:1B:203:PC1:H2C2 | 1.97                     | 0.47              |
| 2:1B:179:ARG:NH2   | 70:1B:202:PC1:H111 | 2.29                     | 0.47              |
| 4:1D:312:SER:O     | 4:1D:316:ASN:ND2   | 2.48                     | 0.47              |
| 5:1E:78:MET:O      | 5:1E:82:GLU:HG3    | 2.14                     | 0.47              |
| 6:1F:92:TYR:CD1    | 6:1F:133:ALA:HB3   | 2.50                     | 0.47              |
| 7:1G:16:GLN:OE1    | 7:1G:17:SER:N      | 2.48                     | 0.47              |
| 7:1G:110:GLN:NE2   | 17:1Q:45:MET:HB3   | 2.25                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:655:GLN:OE1   | 7:1G:655:GLN:N     | 2.47                     | 0.47              |
| 11:1K:62:ILE:HG21  | 14:1N:31:ILE:HD11  | 1.97                     | 0.47              |
| 12:1L:11:THR:O     | 12:1L:15:LEU:HD13  | 2.14                     | 0.47              |
| 12:1L:83:ASP:OD1   | 12:1L:85:PHE:N     | 2.47                     | 0.47              |
| 12:1L:536:LEU:HB3  | 12:1L:537:PRO:HD3  | 1.97                     | 0.47              |
| 13:1M:237:LYS:NZ   | 13:1M:316:MET:O    | 2.41                     | 0.47              |
| 13:1M:328:CYS:HB3  | 13:1M:437:MET:HE1  | 1.96                     | 0.47              |
| 16:1P:109:VAL:HA   | 16:1P:113:ILE:HD12 | 1.97                     | 0.47              |
| 20:1U:55:GLU:OE1   | 39:1n:24:ARG:NH1   | 2.31                     | 0.47              |
| 20:1U:72:CYS:N     | 20:1U:75:GLU:OE1   | 2.47                     | 0.47              |
| 26:1a:59:ARG:NH2   | 26:1a:61:HIS:NE2   | 2.63                     | 0.47              |
| 26:1a:61:HIS:HD1   | 26:1a:62:VAL:N     | 2.13                     | 0.47              |
| 31:1f:8:ARG:HA     | 31:1f:8:ARG:HD2    | 1.77                     | 0.47              |
| 36:1k:62:PHE:O     | 36:1k:66:LEU:HD23  | 2.15                     | 0.47              |
| 42:1q:94:THR:OG1   | 42:1q:96:ASP:OD1   | 2.30                     | 0.47              |
| 44:1s:74:ARG:NH1   | 44:1s:74:ARG:HB2   | 2.30                     | 0.47              |
| 45:3A:329:MET:HE3  | 45:3A:430:GLN:HE22 | 1.80                     | 0.47              |
| 46:3B:100:SER:OG   | 46:3B:105:MET:HG2  | 2.15                     | 0.47              |
| 69:3C:503:3PE:H281 | 69:3C:503:3PE:H242 | 1.97                     | 0.47              |
| 48:3D:253:ILE:HD11 | 86:3D:501:HEC:HBB2 | 1.96                     | 0.47              |
| 52:3H:60:GLU:OE1   | 52:3H:60:GLU:N     | 2.41                     | 0.47              |
| 45:3N:40:TRP:HB3   | 45:3N:384:LEU:HD11 | 1.96                     | 0.47              |
| 49:3R:210:TRP:CD1  | 49:3R:268:ASP:HB3  | 2.50                     | 0.47              |
| 55:4A:93:ALA:HA    | 55:4A:171:MET:HE3  | 1.83                     | 0.47              |
| 55:4A:147:ILE:HG23 | 55:4A:206:ILE:HB   | 1.95                     | 0.47              |
| 55:4A:449:ALA:O    | 55:4A:453:ILE:HG12 | 2.15                     | 0.47              |
| 56:4B:40:TYR:CD2   | 63:4I:24:ALA:HA    | 2.50                     | 0.47              |
| 57:4C:132:LEU:HD22 | 57:4C:176:LEU:CD2  | 2.44                     | 0.47              |
| 64:4J:16:ASN:O     | 64:4J:18:LEU:HD12  | 2.14                     | 0.47              |
| 64:4J:37:THR:HG23  | 87:4J:101:PGV:H152 | 1.96                     | 0.47              |
| 66:4L:41:ARG:CB    | 67:4M:40:TYR:HE2   | 2.26                     | 0.47              |
| 67:4M:14:GLU:HA    | 67:4M:17:ILE:HG22  | 1.95                     | 0.47              |
| 55:8A:104:LEU:HB2  | 55:8A:156:SER:HB3  | 1.97                     | 0.47              |
| 55:8A:155:VAL:HG12 | 55:8A:159:LEU:HD11 | 1.96                     | 0.47              |
| 57:8C:165:ILE:HD13 | 87:8C:302:PGV:H11  | 1.97                     | 0.47              |
| 57:8C:251:PHE:HA   | 57:8C:254:VAL:HG22 | 1.96                     | 0.47              |
| 62:8H:20:PHE:CG    | 62:8H:28:ASN:ND2   | 2.83                     | 0.47              |
| 62:8H:36:PHE:CE1   | 62:8H:40:GLU:OE2   | 2.68                     | 0.47              |
| 68:8N:41:PRO:O     | 68:8N:54:TRP:HE3   | 1.98                     | 0.47              |
| 7:1G:199:ILE:HD13  | 7:1G:202:ILE:HD11  | 1.96                     | 0.47              |
| 10:1J:86:ASN:ND2   | 10:1J:88:THR:HB    | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:1M:183:SER:O    | 41:1p:152:ARG:NH2  | 2.43                     | 0.47              |
| 14:1N:131:LEU:HA   | 14:1N:135:LYS:HE2  | 1.96                     | 0.47              |
| 15:1O:40:ARG:NH2   | 15:1O:50:HIS:HE1   | 2.12                     | 0.47              |
| 20:1U:69:LYS:NZ    | 34:1i:7:GLU:OE1    | 2.45                     | 0.47              |
| 29:1d:11:LEU:O     | 30:1e:8:ARG:NH2    | 2.47                     | 0.47              |
| 40:1o:40:ALA:HB3   | 40:1o:45:MET:HE2   | 1.97                     | 0.47              |
| 45:3A:238:GLY:O    | 51:3G:21:SER:OG    | 2.27                     | 0.47              |
| 69:3A:503:3PE:C35  | 47:3C:11:MET:HE2   | 2.37                     | 0.47              |
| 48:3Q:203:ARG:HH22 | 53:3W:53:LYS:HZ2   | 1.62                     | 0.47              |
| 55:4A:22:PHE:HE2   | 55:4A:105:LEU:HB3  | 1.77                     | 0.47              |
| 55:4A:172:LYS:HG3  | 55:4A:176:MET:HE2  | 1.96                     | 0.47              |
| 55:4A:405:LEU:HD22 | 55:4A:471:ILE:HD12 | 1.97                     | 0.47              |
| 56:4B:198:GLU:O    | 56:4B:204:HIS:CE1  | 2.68                     | 0.47              |
| 68:4N:53:PRO:HD2   | 68:4N:54:TRP:CE3   | 2.49                     | 0.47              |
| 55:8A:202:LEU:O    | 55:8A:206:ILE:HG12 | 2.14                     | 0.47              |
| 55:8A:209:LEU:HA   | 55:8A:212:ASP:OD2  | 2.15                     | 0.47              |
| 87:8A:601:PGV:H341 | 87:8L:101:PGV:H152 | 1.96                     | 0.47              |
| 4:1D:302:GLU:HG2   | 9:1I:3:LYS:HD3     | 1.97                     | 0.47              |
| 5:1E:27:ASN:ND2    | 5:1E:57:GLN:OE1    | 2.48                     | 0.47              |
| 5:1E:73:LEU:HB2    | 5:1E:75:VAL:HG12   | 1.97                     | 0.47              |
| 6:1F:84:LYS:HB2    | 6:1F:84:LYS:HE3    | 1.63                     | 0.47              |
| 6:1F:395:ILE:O     | 6:1F:399:ILE:HG23  | 2.14                     | 0.47              |
| 7:1G:627:SER:HB3   | 7:1G:630:LEU:HD13  | 1.96                     | 0.47              |
| 10:1J:86:ASN:HD22  | 11:1K:23:ARG:NH2   | 2.13                     | 0.47              |
| 11:1K:27:MET:HE2   | 11:1K:78:LEU:CD1   | 2.45                     | 0.47              |
| 14:1N:317:PHE:HZ   | 15:1O:106:LEU:HD21 | 1.80                     | 0.47              |
| 19:1S:21:HIS:O     | 19:1S:62:PRO:HA    | 2.14                     | 0.47              |
| 32:1g:50:ASP:HB3   | 32:1g:53:VAL:HG22  | 1.97                     | 0.47              |
| 32:1g:111:ASN:OD1  | 41:1p:161:ARG:NH1  | 2.47                     | 0.47              |
| 42:1q:2:GLU:O      | 42:1q:6:VAL:HG23   | 2.14                     | 0.47              |
| 47:3C:11:MET:CE    | 47:3C:11:MET:HA    | 2.45                     | 0.47              |
| 46:3O:101:THR:HG22 | 49:3V:65:VAL:HG12  | 1.97                     | 0.47              |
| 48:3Q:27:ARG:HB2   | 48:3Q:55:CYS:HB2   | 1.96                     | 0.47              |
| 49:3R:198:PRO:O    | 49:3R:199:GLN:HG2  | 2.15                     | 0.47              |
| 49:3R:224:PRO:HA   | 49:3R:237:PRO:HD3  | 1.97                     | 0.47              |
| 55:4A:271:MET:CA   | 55:4A:271:MET:CE   | 2.90                     | 0.47              |
| 57:4C:151:LEU:HD21 | 57:4C:159:MET:HE1  | 1.97                     | 0.47              |
| 63:4I:41:GLU:OE1   | 63:4I:41:GLU:O     | 2.33                     | 0.47              |
| 64:4J:36:MET:HG2   | 87:4J:101:PGV:H182 | 1.97                     | 0.47              |
| 57:8C:58:TRP:HD1   | 57:8C:61:ILE:HD12  | 1.80                     | 0.47              |
| 60:8F:13:ALA:O     | 60:8F:18:ARG:NH2   | 2.47                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:8G:13:ALA:O     | 61:8G:17:ARG:HG2   | 2.15                     | 0.47              |
| 87:8G:101:PGV:H261 | 87:8G:101:PGV:H92  | 1.96                     | 0.47              |
| 68:8N:41:PRO:HA    | 68:8N:53:PRO:O     | 2.14                     | 0.47              |
| 4:1D:110:SER:HA    | 4:1D:145:THR:HG22  | 1.97                     | 0.47              |
| 5:1E:172:ILE:HG12  | 5:1E:187:ARG:HH21  | 1.80                     | 0.47              |
| 5:1E:191:PHE:N     | 5:1E:194:GLU:OE1   | 2.47                     | 0.47              |
| 7:1G:455:SER:O     | 7:1G:459:GLN:HG2   | 2.15                     | 0.47              |
| 12:1L:486:MET:HA   | 12:1L:489:THR:OG1  | 2.15                     | 0.47              |
| 75:1L:702:CDL:H562 | 75:1L:702:CDL:H601 | 1.97                     | 0.47              |
| 20:1U:31:SER:OG    | 20:1U:32:VAL:N     | 2.48                     | 0.47              |
| 39:1n:34:ASP:OD1   | 39:1n:35:LYS:N     | 2.46                     | 0.47              |
| 43:1r:53:TYR:CE2   | 43:1r:57:ASP:HB2   | 2.50                     | 0.47              |
| 46:3B:109:VAL:HG22 | 46:3B:123:LEU:HD22 | 1.97                     | 0.47              |
| 47:3C:215:MET:HB2  | 51:3G:12:MET:HE2   | 1.97                     | 0.47              |
| 45:3N:100:LYS:O    | 46:3O:370:MET:HE1  | 2.15                     | 0.47              |
| 47:3P:344:GLU:HA   | 47:3P:344:GLU:OE2  | 2.15                     | 0.47              |
| 49:3R:239:HIS:HE1  | 49:3R:253:PRO:HD2  | 1.80                     | 0.47              |
| 55:4A:243:VAL:HG13 | 88:4A:605:HEA:C3C  | 2.44                     | 0.47              |
| 58:4D:60:TYR:OH    | 58:4D:67:SER:HA    | 2.15                     | 0.47              |
| 75:4D:201:CDL:H512 | 75:4D:201:CDL:HB4  | 1.39                     | 0.47              |
| 63:4I:55:ASP:OD1   | 63:4I:55:ASP:O     | 2.33                     | 0.47              |
| 55:8A:349:THR:HG23 | 88:8A:605:HEA:H272 | 1.97                     | 0.47              |
| 62:8H:17:ASP:OD1   | 62:8H:17:ASP:C     | 2.57                     | 0.47              |
| 1:1A:1:FME:O1      | 1:1A:2:ASN:N       | 2.47                     | 0.46              |
| 2:1B:134:ARG:HE    | 3:1C:173:GLU:CD    | 2.23                     | 0.46              |
| 4:1D:306:GLN:O     | 4:1D:310:ILE:HG13  | 2.15                     | 0.46              |
| 7:1G:242:THR:HG21  | 7:1G:586:ALA:HB1   | 1.96                     | 0.46              |
| 7:1G:703:ILE:HB    | 18:1R:83:THR:OG1   | 2.14                     | 0.46              |
| 8:1H:165:LEU:HD13  | 8:1H:241:LEU:HA    | 1.98                     | 0.46              |
| 10:1J:173:ARG:HH12 | 15:1O:254:ARG:HD3  | 1.80                     | 0.46              |
| 14:1N:187:MET:HB2  | 14:1N:187:MET:HE2  | 1.55                     | 0.46              |
| 15:1O:236:GLU:HG3  | 21:1V:29:LYS:NZ    | 2.30                     | 0.46              |
| 16:1P:111:VAL:HB   | 16:1P:112:LYS:HD3  | 1.97                     | 0.46              |
| 20:1T:49:GLU:OE2   | 22:1W:40:TYR:OH    | 2.32                     | 0.46              |
| 22:1W:43:VAL:HG11  | 22:1W:60:ARG:HG3   | 1.96                     | 0.46              |
| 30:1e:88:GLU:HB2   | 30:1e:90:LYS:NZ    | 2.30                     | 0.46              |
| 45:3A:329:MET:HE3  | 45:3A:430:GLN:NE2  | 2.30                     | 0.46              |
| 46:3B:274:VAL:O    | 46:3B:278:VAL:HG23 | 2.15                     | 0.46              |
| 47:3C:272:TRP:HA   | 47:3C:275:LEU:HG   | 1.98                     | 0.46              |
| 48:3D:297:MET:HE3  | 48:3D:297:MET:HB3  | 1.88                     | 0.46              |
| 46:3O:56:ARG:HD2   | 46:3O:103:GLU:HG2  | 1.96                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:102:HIS:O    | 56:4B:207:MET:HE1  | 2.15                     | 0.46              |
| 56:8B:28:LEU:HD21  | 75:8B:303:CDL:H561 | 1.97                     | 0.46              |
| 57:8C:221:ARG:HH21 | 57:8C:226:HIS:HB3  | 1.80                     | 0.46              |
| 75:8D:201:CDL:H581 | 75:8D:201:CDL:H621 | 1.98                     | 0.46              |
| 7:1G:190:MET:SD    | 7:1G:690:ALA:HB1   | 2.54                     | 0.46              |
| 11:1K:95:LEU:HD23  | 11:1K:95:LEU:H     | 1.80                     | 0.46              |
| 13:1M:114:GLU:HG2  | 13:1M:117:LEU:H    | 1.79                     | 0.46              |
| 69:1M:501:3PE:H332 | 69:1M:501:3PE:H291 | 1.96                     | 0.46              |
| 16:1P:191:VAL:O    | 16:1P:255:PRO:HA   | 2.14                     | 0.46              |
| 19:1S:23:CYS:HA    | 19:1S:57:CYS:O     | 2.15                     | 0.46              |
| 23:1X:84:TYR:CE2   | 23:1X:88:ILE:HD11  | 2.50                     | 0.46              |
| 32:1g:66:PHE:O     | 32:1g:71:VAL:HG23  | 2.14                     | 0.46              |
| 37:1l:82:ASP:OD1   | 37:1l:82:ASP:N     | 2.46                     | 0.46              |
| 37:1l:111:PHE:O    | 37:1l:115:MET:HG2  | 2.15                     | 0.46              |
| 37:1l:128:VAL:HG22 | 37:1l:129:GLY:O    | 2.15                     | 0.46              |
| 45:3N:156:THR:O    | 45:3N:239:SER:OG   | 2.32                     | 0.46              |
| 69:3N:501:3PE:H332 | 75:3N:502:CDL:H111 | 1.96                     | 0.46              |
| 46:3O:342:ASP:O    | 46:3O:346:THR:HG23 | 2.16                     | 0.46              |
| 49:3R:162:GLY:N    | 49:3R:178:HIS:HB3  | 2.29                     | 0.46              |
| 49:3R:248:ARG:NH1  | 49:3R:257:ASN:HD22 | 2.13                     | 0.46              |
| 67:4M:33:VAL:O     | 67:4M:37:LEU:HG    | 2.15                     | 0.46              |
| 55:8A:340:TRP:HZ2  | 55:8A:413:HIS:CE1  | 2.33                     | 0.46              |
| 56:8B:24:HIS:HE1   | 56:8B:28:LEU:HD22  | 1.80                     | 0.46              |
| 57:8C:94:PHE:HB3   | 57:8C:98:PHE:CE2   | 2.50                     | 0.46              |
| 3:1C:53:HIS:HD1    | 3:1C:55:ASP:H      | 1.61                     | 0.46              |
| 4:1D:342:MET:HE2   | 4:1D:346:ILE:HG13  | 1.97                     | 0.46              |
| 9:1I:44:GLU:HG3    | 26:1a:1:MET:CE     | 2.39                     | 0.46              |
| 9:1I:160:LYS:HD2   | 9:1I:161:TRP:NE1   | 2.30                     | 0.46              |
| 12:1L:434:LYS:HG3  | 36:1k:52:TYR:CD2   | 2.50                     | 0.46              |
| 13:1M:24:TRP:CD2   | 13:1M:81:GLN:HB3   | 2.51                     | 0.46              |
| 14:1N:112:HIS:CE1  | 14:1N:164:ILE:HG21 | 2.50                     | 0.46              |
| 14:1N:278:MET:O    | 14:1N:282:MET:HG3  | 2.16                     | 0.46              |
| 14:1N:326:LEU:O    | 14:1N:330:ILE:HG12 | 2.15                     | 0.46              |
| 23:1X:137:PRO:HB2  | 23:1X:140:PRO:HG3  | 1.98                     | 0.46              |
| 25:1Z:89:GLU:OE1   | 30:1e:96:HIS:ND1   | 2.46                     | 0.46              |
| 31:1f:5:GLN:O      | 31:1f:9:ASP:CB     | 2.60                     | 0.46              |
| 45:3A:80:GLU:HG2   | 46:3B:284:HIS:HB2  | 1.97                     | 0.46              |
| 45:3A:191:LYS:O    | 45:3A:195:MET:HG3  | 2.16                     | 0.46              |
| 48:3D:121:TYR:HA   | 48:3D:125:CYS:SG   | 2.56                     | 0.46              |
| 49:3E:201:ASP:HB2  | 49:3E:248:ARG:NH2  | 2.30                     | 0.46              |
| 55:4A:470:PHE:CG   | 67:4M:19:LEU:HD13  | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:138:VAL:HG12 | 56:4B:140:ASN:H    | 1.81                     | 0.46              |
| 58:8D:56:LYS:HB2   | 59:8E:104:LEU:HD21 | 1.98                     | 0.46              |
| 63:8I:14:ALA:O     | 63:8I:18:ARG:HG2   | 2.15                     | 0.46              |
| 66:8L:18:LYS:HZ3   | 67:8M:14:GLU:CD    | 2.10                     | 0.46              |
| 3:1C:133:GLU:OE2   | 4:1D:430:ARG:NH2   | 2.49                     | 0.46              |
| 5:1E:214:GLN:CD    | 5:1E:214:GLN:N     | 2.73                     | 0.46              |
| 6:1F:133:ALA:HB1   | 6:1F:176:PHE:HE1   | 1.81                     | 0.46              |
| 8:1H:312:ALA:HB3   | 25:1Z:55:ARG:HH21  | 1.80                     | 0.46              |
| 10:1J:41:CYS:HA    | 10:1J:44:VAL:HG22  | 1.98                     | 0.46              |
| 11:1K:76:SER:HA    | 11:1K:79:VAL:HG12  | 1.96                     | 0.46              |
| 12:1L:205:ASN:O    | 12:1L:207:GLU:N    | 2.49                     | 0.46              |
| 12:1L:291:CYS:O    | 12:1L:295:GLN:HG2  | 2.15                     | 0.46              |
| 15:1O:310:GLU:HA   | 15:1O:314:ASP:HB2  | 1.96                     | 0.46              |
| 17:1Q:11:ILE:O     | 22:1W:16:SER:OG    | 2.29                     | 0.46              |
| 75:1X:201:CDL:H512 | 31:1f:26:LEU:HD21  | 1.96                     | 0.46              |
| 28:1c:46:ASN:C     | 28:1c:46:ASN:OD1   | 2.57                     | 0.46              |
| 30:1e:50:ARG:O     | 30:1e:54:GLU:HG3   | 2.15                     | 0.46              |
| 39:1n:107:HIS:CD2  | 39:1n:108:PRO:HD2  | 2.50                     | 0.46              |
| 43:1r:5:ARG:HA     | 43:1r:8:GLN:HB2    | 1.97                     | 0.46              |
| 50:3F:79:ASP:OD1   | 50:3F:82:MET:CE    | 2.63                     | 0.46              |
| 46:3O:306:PRO:HA   | 49:3V:52:ARG:HD3   | 1.96                     | 0.46              |
| 47:3P:300:ILE:HA   | 47:3P:303:LEU:HD23 | 1.97                     | 0.46              |
| 47:3P:310:SER:HB2  | 47:3P:370:SER:HB2  | 1.96                     | 0.46              |
| 55:4A:96:ARG:HB3   | 57:4C:57:TRP:CZ2   | 2.49                     | 0.46              |
| 55:4A:189:LEU:HD21 | 87:4A:603:PGV:H212 | 1.98                     | 0.46              |
| 57:4C:43:LEU:HD21  | 87:4C:302:PGV:H262 | 1.97                     | 0.46              |
| 58:4D:93:ALA:HB2   | 65:4K:29:TRP:CE2   | 2.50                     | 0.46              |
| 55:8A:32:ALA:HB3   | 66:8L:36:PRO:HG2   | 1.97                     | 0.46              |
| 58:8D:48:TRP:CZ3   | 59:8E:61:PHE:HD2   | 2.26                     | 0.46              |
| 65:8K:42:LEU:HD11  | 87:8K:101:PGV:H012 | 1.96                     | 0.46              |
| 8:1H:47:GLN:NE2    | 8:1H:51:ASP:OD1    | 2.48                     | 0.46              |
| 8:1H:179:TRP:N     | 8:1H:180:PRO:HD2   | 2.31                     | 0.46              |
| 9:1I:121:PHE:HA    | 9:1I:124:GLU:HG2   | 1.98                     | 0.46              |
| 10:1J:23:LYS:HE2   | 11:1K:23:ARG:HG3   | 1.96                     | 0.46              |
| 12:1L:207:GLU:C    | 12:1L:209:PRO:HD3  | 2.40                     | 0.46              |
| 14:1N:172:GLN:HB2  | 14:1N:178:ILE:HG13 | 1.97                     | 0.46              |
| 14:1N:266:ILE:O    | 14:1N:270:MET:HG3  | 2.16                     | 0.46              |
| 14:1N:270:MET:CE   | 14:1N:282:MET:CE   | 2.90                     | 0.46              |
| 15:1O:53:GLU:HG2   | 15:1O:104:ARG:HH12 | 1.80                     | 0.46              |
| 20:1U:4:PRO:O      | 20:1U:4:PRO:CD     | 2.63                     | 0.46              |
| 31:1f:1:MET:SD     | 31:1f:2:ASN:HB2    | 2.56                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:1g:63:PHE:O     | 32:1g:67:SER:HB2   | 2.15                     | 0.46              |
| 41:1p:78:GLU:HG2   | 41:1p:79:LYS:HG2   | 1.96                     | 0.46              |
| 47:3C:278:TYR:CZ   | 47:3C:282:ARG:HD3  | 2.50                     | 0.46              |
| 49:3E:226:ALA:HA   | 49:3E:234:TYR:HD1  | 1.80                     | 0.46              |
| 47:3P:24:PRO:HB2   | 47:3P:27:ILE:HG23  | 1.98                     | 0.46              |
| 55:4A:251:PHE:HB3  | 55:4A:319:LYS:NZ   | 2.30                     | 0.46              |
| 64:4J:52:TRP:O     | 64:4J:57:HIS:ND1   | 2.48                     | 0.46              |
| 55:8A:62:ALA:O     | 55:8A:66:ILE:HG22  | 2.16                     | 0.46              |
| 57:8C:6:HIS:CD2    | 57:8C:8:TYR:CD2    | 3.02                     | 0.46              |
| 57:8C:121:ILE:HG21 | 57:8C:193:TYR:CD2  | 2.50                     | 0.46              |
| 59:8E:24:ILE:CG2   | 59:8E:57:ARG:HH12  | 2.29                     | 0.46              |
| 64:8J:29:ASN:O     | 64:8J:33:ARG:HG2   | 2.16                     | 0.46              |
| 67:8M:32:TRP:CE3   | 67:8M:36:HIS:CE1   | 3.03                     | 0.46              |
| 68:8N:17:PRO:HA    | 68:8N:20:VAL:HG23  | 1.96                     | 0.46              |
| 1:1A:85:LYS:HG3    | 1:1A:86:THR:N      | 2.31                     | 0.46              |
| 4:1D:141:PHE:O     | 4:1D:145:THR:OG1   | 2.34                     | 0.46              |
| 6:1F:301:GLY:H     | 6:1F:333:ALA:HB3   | 1.80                     | 0.46              |
| 7:1G:281:GLN:HG2   | 7:1G:592:LEU:HD12  | 1.98                     | 0.46              |
| 8:1H:312:ALA:HA    | 27:1b:41:ALA:HB2   | 1.96                     | 0.46              |
| 9:1I:81:LYS:HE2    | 9:1I:94:ILE:HG22   | 1.98                     | 0.46              |
| 12:1L:136:ASN:OD1  | 12:1L:139:GLN:HB2  | 2.15                     | 0.46              |
| 13:1M:91:ARG:HH22  | 15:1O:290:ASP:CG   | 2.24                     | 0.46              |
| 13:1M:186:LEU:HD23 | 13:1M:253:LEU:HD22 | 1.96                     | 0.46              |
| 69:1M:502:3PE:H3E2 | 75:1X:201:CDL:H442 | 1.98                     | 0.46              |
| 69:1M:504:3PE:H3B1 | 14:1N:245:MET:HE1  | 1.97                     | 0.46              |
| 14:1N:187:MET:HA   | 14:1N:190:MET:HE3  | 1.98                     | 0.46              |
| 14:1N:270:MET:CE   | 14:1N:282:MET:HE2  | 2.39                     | 0.46              |
| 20:1U:73:PRO:O     | 20:1U:77:VAL:HG13  | 2.16                     | 0.46              |
| 22:1W:70:ASN:N     | 22:1W:70:ASN:ND2   | 2.63                     | 0.46              |
| 40:1o:2:ALA:O      | 40:1o:6:ARG:HG3    | 2.14                     | 0.46              |
| 49:3E:159:ILE:HD11 | 49:3E:167:PHE:HE2  | 1.80                     | 0.46              |
| 49:3R:265:PHE:O    | 49:3R:265:PHE:CG   | 2.69                     | 0.46              |
| 55:4A:275:TRP:HE3  | 87:4A:603:PGV:H12  | 1.80                     | 0.46              |
| 87:8A:602:PGV:H301 | 67:8M:19:LEU:HD12  | 1.98                     | 0.46              |
| 57:8C:148:HIS:CE1  | 57:8C:152:MET:HE2  | 2.47                     | 0.46              |
| 58:8D:59:LEU:HA    | 58:8D:59:LEU:HD23  | 1.64                     | 0.46              |
| 5:1E:151:ALA:HB3   | 5:1E:163:ASP:HA    | 1.98                     | 0.46              |
| 7:1G:469:ALA:O     | 7:1G:473:ILE:HG13  | 2.15                     | 0.46              |
| 12:1L:144:TRP:CE2  | 12:1L:223:LYS:HG3  | 2.51                     | 0.46              |
| 13:1M:243:MET:HB3  | 13:1M:301:ILE:HG21 | 1.98                     | 0.46              |
| 14:1N:26:TRP:CH2   | 14:1N:86:ILE:HD12  | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:1O:49:ARG:HB3   | 15:1O:122:VAL:HG12 | 1.96                     | 0.46              |
| 15:1O:134:PHE:O    | 15:1O:138:MET:HG3  | 2.15                     | 0.46              |
| 15:1O:287:HIS:HB2  | 32:1g:28:GLU:OE1   | 2.15                     | 0.46              |
| 17:1Q:70:MET:SD    | 42:1q:126:PRO:HB2  | 2.56                     | 0.46              |
| 25:1Z:122:GLY:C    | 30:1e:75:LEU:HD11  | 2.41                     | 0.46              |
| 29:1d:108:THR:HA   | 41:1p:77:GLU:HA    | 1.97                     | 0.46              |
| 33:1h:108:LEU:HD23 | 33:1h:108:LEU:HA   | 1.81                     | 0.46              |
| 40:1o:83:GLN:NE2   | 40:1o:87:ASP:OD1   | 2.49                     | 0.46              |
| 41:1p:35:ILE:O     | 41:1p:39:LEU:HG    | 2.16                     | 0.46              |
| 47:3C:377:LEU:HG   | 50:3F:32:TYR:HE2   | 1.81                     | 0.46              |
| 51:3G:40:LEU:O     | 51:3G:44:ARG:HG3   | 2.16                     | 0.46              |
| 50:3S:75:LEU:O     | 50:3S:80:TRP:NE1   | 2.39                     | 0.46              |
| 55:4A:211:THR:HG22 | 55:4A:215:LEU:HD22 | 1.98                     | 0.46              |
| 56:4B:82:ARG:HA    | 56:4B:82:ARG:HD3   | 1.82                     | 0.46              |
| 56:8B:100:MET:HE1  | 56:8B:156:SER:C    | 2.41                     | 0.46              |
| 64:8J:28:ASP:HA    | 64:8J:31:LEU:HD12  | 1.97                     | 0.46              |
| 4:1D:78:PRO:HG3    | 4:1D:402:LEU:HD23  | 1.98                     | 0.46              |
| 4:1D:116:GLN:NE2   | 4:1D:276:ASP:OD2   | 2.42                     | 0.46              |
| 7:1G:611:LEU:HD13  | 7:1G:613:TYR:OH    | 2.15                     | 0.46              |
| 11:1K:8:ILE:HG21   | 11:1K:43:MET:HB2   | 1.97                     | 0.46              |
| 15:1O:18:LEU:HD21  | 15:1O:256:PHE:CE2  | 2.50                     | 0.46              |
| 20:1U:17:TYR:O     | 20:1U:20:LYS:HG2   | 2.15                     | 0.46              |
| 32:1g:55:LEU:HD21  | 32:1g:59:ARG:NH1   | 2.31                     | 0.46              |
| 34:1i:13:GLN:HE22  | 39:1n:156:ALA:HB3  | 1.81                     | 0.46              |
| 34:1i:78:VAL:HG22  | 41:1p:40:VAL:HG11  | 1.98                     | 0.46              |
| 36:1k:61:SER:OG    | 36:1k:62:PHE:N     | 2.49                     | 0.46              |
| 38:1m:82:THR:HG23  | 38:1m:84:LYS:H     | 1.81                     | 0.46              |
| 39:1n:30:CYS:O     | 39:1n:32:HIS:N     | 2.48                     | 0.46              |
| 47:3C:29:SER:HA    | 47:3C:32:ASN:HD22  | 1.81                     | 0.46              |
| 47:3C:361:ILE:HG12 | 47:3C:365:LEU:HD12 | 1.97                     | 0.46              |
| 48:3D:102:HIS:O    | 48:3D:291:LYS:NZ   | 2.49                     | 0.46              |
| 49:3E:174:LEU:HD13 | 49:3E:214:ILE:HD13 | 1.96                     | 0.46              |
| 45:3N:356:ARG:O    | 45:3N:360:ILE:HG13 | 2.15                     | 0.46              |
| 69:3N:501:3PE:H31  | 75:3N:502:CDL:H512 | 1.98                     | 0.46              |
| 48:3Q:33:TYR:CD1   | 48:3Q:37:CYS:HB2   | 2.51                     | 0.46              |
| 49:3R:145:ASP:O    | 49:3R:149:MET:HB2  | 2.16                     | 0.46              |
| 52:3U:22:GLU:O     | 52:3U:26:GLN:HG2   | 2.16                     | 0.46              |
| 55:4A:35:LEU:HG    | 55:4A:462:LEU:HD22 | 1.98                     | 0.46              |
| 55:4A:239:GLY:O    | 55:4A:243:VAL:HG23 | 2.16                     | 0.46              |
| 55:4A:469:ILE:CD1  | 67:4M:26:PHE:CE1   | 2.98                     | 0.46              |
| 57:4C:122:HIS:CE1  | 61:4G:45:PRO:HB3   | 2.50                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:4C:305:CDL:H512 | 75:4C:305:CDL:HB4  | 1.41                     | 0.46              |
| 59:4E:78:HIS:CD2   | 59:4E:78:HIS:N     | 2.83                     | 0.46              |
| 87:4M:101:PGV:H81  | 87:4M:101:PGV:H242 | 1.97                     | 0.46              |
| 55:8A:155:VAL:O    | 55:8A:159:LEU:CD1  | 2.54                     | 0.46              |
| 56:8B:11:ASP:HB2   | 58:8D:129:ALA:HA   | 1.97                     | 0.46              |
| 56:8B:37:LEU:O     | 56:8B:41:ILE:HG13  | 2.15                     | 0.46              |
| 57:8C:72:THR:O     | 57:8C:76:GLN:HG3   | 2.16                     | 0.46              |
| 57:8C:221:ARG:HB3  | 57:8C:226:HIS:HB2  | 1.97                     | 0.46              |
| 1:1A:37:TYR:HB2    | 2:1B:81:ARG:NH1    | 2.30                     | 0.46              |
| 4:1D:352:TYR:HD1   | 9:1I:86:VAL:HG21   | 1.81                     | 0.46              |
| 6:1F:208:PRO:HG2   | 6:1F:213:VAL:HG22  | 1.98                     | 0.46              |
| 7:1G:237:ASN:HB3   | 7:1G:253:ARG:HE    | 1.79                     | 0.46              |
| 8:1H:257:ILE:HG13  | 26:1a:17:PHE:HE2   | 1.81                     | 0.46              |
| 10:1J:170:GLU:OE2  | 10:1J:173:ARG:NH2  | 2.49                     | 0.46              |
| 13:1M:367:LEU:HD12 | 13:1M:407:SER:HB2  | 1.96                     | 0.46              |
| 21:1V:54:LYS:O     | 21:1V:58:VAL:HG23  | 2.16                     | 0.46              |
| 32:1g:80:LEU:HA    | 32:1g:80:LEU:HD23  | 1.79                     | 0.46              |
| 75:1h:202:CDL:H712 | 75:1h:202:CDL:HB62 | 1.52                     | 0.46              |
| 69:3A:502:3PE:H32  | 69:3A:502:3PE:H322 | 1.66                     | 0.46              |
| 48:3D:314:HIS:NE2  | 51:3G:22:PRO:HB2   | 2.31                     | 0.46              |
| 49:3E:195:LEU:HD22 | 49:3E:250:ARG:HA   | 1.97                     | 0.46              |
| 49:3E:207:LYS:HB3  | 49:3E:209:GLU:OE2  | 2.16                     | 0.46              |
| 45:3N:284:TYR:CD2  | 49:3V:71:ASN:HA    | 2.50                     | 0.46              |
| 75:4B:303:CDL:C32  | 63:4I:34:PHE:HE1   | 2.29                     | 0.46              |
| 58:4D:112:GLU:O    | 58:4D:116:VAL:HG23 | 2.16                     | 0.46              |
| 55:8A:128:VAL:O    | 55:8A:128:VAL:HG12 | 2.15                     | 0.46              |
| 56:8B:165:VAL:HG11 | 56:8B:168:LEU:HD12 | 1.98                     | 0.46              |
| 60:8F:62:CYS:HB3   | 60:8F:85:CYS:HB3   | 1.98                     | 0.46              |
| 62:8H:41:LYS:HE3   | 62:8H:85:ILE:OXT   | 2.15                     | 0.46              |
| 1:1A:1:FME:HA      | 1:1A:1:FME:HE3     | 1.97                     | 0.46              |
| 6:1F:96:ASN:O      | 6:1F:225:VAL:HG23  | 2.16                     | 0.46              |
| 7:1G:596:ASP:OD1   | 7:1G:596:ASP:N     | 2.48                     | 0.46              |
| 8:1H:296:LEU:HD13  | 70:1H:402:PC1:H351 | 1.98                     | 0.46              |
| 10:1J:99:MET:SD    | 10:1J:103:MET:HG2  | 2.56                     | 0.46              |
| 12:1L:137:LEU:HD12 | 12:1L:137:LEU:HA   | 1.75                     | 0.46              |
| 13:1M:59:ASP:OD2   | 13:1M:245:ARG:NH1  | 2.42                     | 0.46              |
| 13:1M:203:PHE:HB2  | 13:1M:243:MET:HG3  | 1.98                     | 0.46              |
| 15:1O:129:TYR:CE2  | 15:1O:166:PRO:HD3  | 2.51                     | 0.46              |
| 17:1Q:16:LYS:HA    | 17:1Q:16:LYS:HD2   | 1.80                     | 0.46              |
| 20:1T:25:ILE:HD11  | 20:1T:42:LEU:HD11  | 1.98                     | 0.46              |
| 24:1Y:13:GLU:HA    | 24:1Y:20:LYS:NZ    | 2.30                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:1m:82:THR:HG23  | 38:1m:84:LYS:N     | 2.30                     | 0.46              |
| 44:1s:40:ASN:O     | 44:1s:43:HIS:ND1   | 2.39                     | 0.46              |
| 45:3A:117:VAL:HG23 | 45:3A:118:GLN:HG3  | 1.98                     | 0.46              |
| 46:3B:163:LEU:HD11 | 46:3B:258:VAL:HG22 | 1.97                     | 0.46              |
| 45:3N:87:ASN:ND2   | 45:3N:98:TYR:OH    | 2.34                     | 0.46              |
| 45:3N:145:MET:SD   | 45:3N:248:LEU:HD13 | 2.56                     | 0.46              |
| 75:3P:504:CDL:H312 | 75:3T:101:CDL:H731 | 1.98                     | 0.46              |
| 48:3Q:230:LEU:O    | 48:3Q:233:ARG:HG2  | 2.16                     | 0.46              |
| 49:3R:179:ARG:HB2  | 49:3R:183:GLU:HB2  | 1.98                     | 0.46              |
| 54:3X:48:ILE:O     | 54:3X:51:LYS:HG2   | 2.16                     | 0.46              |
| 55:4A:71:MET:HB2   | 55:4A:72:PRO:HD3   | 1.97                     | 0.46              |
| 55:4A:361:SER:HB3  | 56:4B:84:LEU:HD22  | 1.98                     | 0.46              |
| 55:4A:478:SER:OG   | 55:4A:480:ARG:NH2  | 2.49                     | 0.46              |
| 64:4J:40:LEU:HD12  | 87:4J:101:PGV:H142 | 1.98                     | 0.46              |
| 55:8A:3:VAL:HG11   | 87:8A:601:PGV:H02  | 1.98                     | 0.46              |
| 55:8A:346:PHE:HD2  | 55:8A:347:LEU:HD13 | 1.80                     | 0.46              |
| 57:8C:182:TYR:HD2  | 87:8C:305:PGV:O11  | 1.99                     | 0.46              |
| 57:8C:217:VAL:O    | 57:8C:221:ARG:HG3  | 2.15                     | 0.46              |
| 60:8F:76:LYS:HG3   | 60:8F:91:LEU:HD23  | 1.97                     | 0.46              |
| 2:1B:48:MET:CE     | 2:1B:80:PRO:HB3    | 2.46                     | 0.45              |
| 3:1C:204:GLU:OE2   | 3:1C:210:ARG:NE    | 2.49                     | 0.45              |
| 4:1D:143:GLU:HG3   | 4:1D:310:ILE:HB    | 1.98                     | 0.45              |
| 4:1D:171:PHE:HA    | 4:1D:174:ARG:HB2   | 1.98                     | 0.45              |
| 12:1L:419:THR:HA   | 12:1L:422:TYR:CZ   | 2.51                     | 0.45              |
| 19:1S:24:GLN:NE2   | 19:1S:56:GLU:HG3   | 2.29                     | 0.45              |
| 22:1W:64:ARG:O     | 22:1W:68:MET:HG2   | 2.16                     | 0.45              |
| 30:1e:31:ARG:NH2   | 30:1e:66:LEU:O     | 2.49                     | 0.45              |
| 75:1h:202:CDL:H511 | 75:1h:202:CDL:HB4  | 1.56                     | 0.45              |
| 34:1i:9:LEU:O      | 34:1i:13:GLN:HG3   | 2.16                     | 0.45              |
| 34:1i:31:GLU:HG2   | 39:1n:115:PRO:HD2  | 1.97                     | 0.45              |
| 37:1l:7:ASP:OD1    | 37:1l:8:MET:N      | 2.49                     | 0.45              |
| 37:1l:34:TYR:OH    | 37:1l:46:ASP:O     | 2.24                     | 0.45              |
| 37:1l:136:ASN:ND2  | 37:1l:150:PRO:HG2  | 2.30                     | 0.45              |
| 46:3B:46:ARG:HG2   | 46:3B:379:LEU:HD22 | 1.99                     | 0.45              |
| 48:3D:121:TYR:CD1  | 48:3D:125:CYS:HB2  | 2.51                     | 0.45              |
| 46:3O:257:LEU:HD11 | 46:3O:422:LYS:HB3  | 1.99                     | 0.45              |
| 48:3Q:3:LEU:HD23   | 48:3Q:3:LEU:H      | 1.81                     | 0.45              |
| 56:4B:100:MET:HE1  | 56:4B:155:SER:OG   | 2.16                     | 0.45              |
| 56:4B:145:PRO:HA   | 56:4B:214:VAL:O    | 2.17                     | 0.45              |
| 66:4L:42:HIS:NE2   | 66:4L:46:LYS:HD3   | 2.31                     | 0.45              |
| 55:8A:462:LEU:O    | 55:8A:465:VAL:HG12 | 2.15                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:8B:28:LEU:HG    | 63:8I:35:TYR:CE2   | 2.45                     | 0.45              |
| 75:8C:306:CDL:H371 | 75:8C:306:CDL:H251 | 1.98                     | 0.45              |
| 58:8D:78:TRP:CE2   | 58:8D:79:LYS:HG2   | 2.51                     | 0.45              |
| 5:1E:6:LEU:HD21    | 18:1R:76:ASP:OD2   | 2.16                     | 0.45              |
| 6:1F:121:GLY:HA2   | 6:1F:124:VAL:HG22  | 1.98                     | 0.45              |
| 9:1I:175:TYR:CZ    | 43:1r:38:PRO:HG3   | 2.50                     | 0.45              |
| 12:1L:36:VAL:HG21  | 12:1L:118:PHE:HB3  | 1.97                     | 0.45              |
| 13:1M:453:MET:HE1  | 32:1g:80:LEU:CD1   | 2.36                     | 0.45              |
| 14:1N:95:MET:CE    | 14:1N:149:ILE:HG23 | 2.46                     | 0.45              |
| 19:1S:34:ASP:O     | 19:1S:38:LYS:HG2   | 2.16                     | 0.45              |
| 20:1T:69:LYS:O     | 20:1T:71:MET:HG2   | 2.17                     | 0.45              |
| 20:1U:68:GLU:C     | 20:1U:68:GLU:OE1   | 2.59                     | 0.45              |
| 23:1X:131:LYS:HD2  | 23:1X:131:LYS:HA   | 1.76                     | 0.45              |
| 37:1l:134:PRO:HD3  | 40:1o:56:ASP:HA    | 1.97                     | 0.45              |
| 46:3B:56:ARG:NH1   | 46:3B:103:GLU:OE2  | 2.48                     | 0.45              |
| 46:3B:227:ARG:HG3  | 46:3B:229:GLY:N    | 2.29                     | 0.45              |
| 48:3D:226:PRO:HG3  | 52:3H:84:LEU:HD22  | 1.97                     | 0.45              |
| 49:3E:130:LYS:NZ   | 54:3Y:34:TRP:O     | 2.46                     | 0.45              |
| 45:3N:224:VAL:HG13 | 45:3N:225:GLU:CD   | 2.40                     | 0.45              |
| 49:3R:172:LYS:HB2  | 49:3R:214:ILE:HD12 | 1.99                     | 0.45              |
| 55:4A:266:GLU:HB3  | 60:4F:68:THR:HG21  | 1.98                     | 0.45              |
| 56:4B:110:TYR:CE2  | 56:4B:222:TRP:HH2  | 2.34                     | 0.45              |
| 55:8A:165:ILE:HG23 | 55:8A:169:ILE:HD11 | 1.97                     | 0.45              |
| 56:8B:188:ARG:HG3  | 56:8B:188:ARG:HH11 | 1.81                     | 0.45              |
| 58:8D:48:TRP:CZ3   | 59:8E:61:PHE:CG    | 2.99                     | 0.45              |
| 58:8D:82:VAL:O     | 58:8D:86:LEU:HG    | 2.16                     | 0.45              |
| 58:8D:89:ILE:HD12  | 58:8D:89:ILE:H     | 1.81                     | 0.45              |
| 58:8D:144:GLU:HG2  | 58:8D:145:TRP:O    | 2.16                     | 0.45              |
| 68:8N:50:ASN:OD1   | 68:8N:50:ASN:C     | 2.59                     | 0.45              |
| 12:1L:13:ILE:N     | 12:1L:13:ILE:HD13  | 2.32                     | 0.45              |
| 12:1L:362:LEU:HA   | 12:1L:365:ALA:HB3  | 1.98                     | 0.45              |
| 12:1L:435:PRO:HB3  | 12:1L:437:PHE:CZ   | 2.51                     | 0.45              |
| 69:1M:502:3PE:H111 | 15:1O:304:TYR:HE1  | 1.81                     | 0.45              |
| 69:1M:502:3PE:H2G2 | 69:1M:504:3PE:H3G2 | 1.98                     | 0.45              |
| 14:1N:122:ILE:HD12 | 14:1N:126:ALA:CB   | 2.46                     | 0.45              |
| 21:1V:75:GLN:O     | 21:1V:79:VAL:HG23  | 2.17                     | 0.45              |
| 39:1n:97:LYS:HD2   | 39:1n:173:PRO:HB2  | 1.98                     | 0.45              |
| 40:1o:62:LEU:HD23  | 40:1o:66:LEU:HD13  | 1.97                     | 0.45              |
| 45:3N:244:ARG:NH1  | 51:3T:10:MET:HE3   | 2.31                     | 0.45              |
| 55:4A:119:GLU:CD   | 55:4A:141:ALA:H    | 2.24                     | 0.45              |
| 56:4B:105:TYR:HE2  | 56:4B:119:ASP:OD1  | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:4B:303:CDL:H861 | 75:4B:303:CDL:H202 | 1.97                     | 0.45              |
| 58:4D:122:ARG:HG3  | 65:4K:53:TRP:CE2   | 2.52                     | 0.45              |
| 56:8B:98:LYS:HB2   | 56:8B:98:LYS:HE3   | 1.67                     | 0.45              |
| 57:8C:130:PRO:HB2  | 57:8C:253:TYR:CE1  | 2.51                     | 0.45              |
| 1:1A:49:LEU:H      | 8:1H:126:LYS:HE2   | 1.81                     | 0.45              |
| 5:1E:51:LEU:HD22   | 5:1E:61:LEU:HD11   | 1.98                     | 0.45              |
| 5:1E:168:ASP:HB3   | 5:1E:187:ARG:HG2   | 1.98                     | 0.45              |
| 6:1F:92:TYR:HB2    | 6:1F:220:THR:HG22  | 1.97                     | 0.45              |
| 8:1H:31:MET:HG3    | 9:1I:41:LEU:HB2    | 1.97                     | 0.45              |
| 12:1L:97:THR:O     | 12:1L:101:MET:HG3  | 2.15                     | 0.45              |
| 13:1M:30:HIS:CD2   | 31:1f:16:VAL:HB    | 2.52                     | 0.45              |
| 13:1M:126:LEU:HD21 | 13:1M:153:THR:OG1  | 2.16                     | 0.45              |
| 13:1M:187:SER:O    | 13:1M:192:ASN:ND2  | 2.44                     | 0.45              |
| 15:1O:308:TYR:CE1  | 15:1O:320:LYS:HG2  | 2.51                     | 0.45              |
| 16:1P:244:TYR:O    | 16:1P:248:VAL:HG23 | 2.15                     | 0.45              |
| 20:1T:37:MET:HE1   | 20:1T:71:MET:CE    | 2.47                     | 0.45              |
| 25:1Z:59:ARG:CA    | 25:1Z:62:ILE:HG22  | 2.47                     | 0.45              |
| 44:1s:46:TYR:CD2   | 44:1s:50:THR:HG21  | 2.51                     | 0.45              |
| 46:3B:97:SER:HA    | 49:3I:69:GLY:HA2   | 1.99                     | 0.45              |
| 49:3R:173:PRO:O    | 49:3R:215:GLY:N    | 2.40                     | 0.45              |
| 55:4A:229:ILE:HD11 | 56:4B:175:ILE:HD12 | 1.98                     | 0.45              |
| 75:4D:201:CDL:H171 | 75:4D:201:CDL:H721 | 1.97                     | 0.45              |
| 63:4I:21:ILE:CG2   | 63:4I:25:PHE:CE2   | 3.00                     | 0.45              |
| 55:8A:279:SER:HB3  | 68:8N:22:ILE:HG12  | 1.99                     | 0.45              |
| 62:8H:6:THR:HA     | 62:8H:9:LYS:HZ2    | 1.78                     | 0.45              |
| 62:8H:17:ASP:OD1   | 62:8H:18:SER:N     | 2.50                     | 0.45              |
| 62:8H:75:ARG:HG3   | 62:8H:75:ARG:NH1   | 2.32                     | 0.45              |
| 7:1G:215:PHE:HD1   | 9:1I:104:ARG:HH11  | 1.63                     | 0.45              |
| 7:1G:427:LYS:HA    | 7:1G:427:LYS:HD2   | 1.81                     | 0.45              |
| 8:1H:173:TRP:HB3   | 8:1H:175:ILE:HG22  | 1.98                     | 0.45              |
| 13:1M:76:MET:SD    | 13:1M:230:VAL:HB   | 2.57                     | 0.45              |
| 17:1Q:27:GLU:CD    | 17:1Q:28:GLU:OE1   | 2.60                     | 0.45              |
| 19:1S:43:LEU:HD12  | 19:1S:43:LEU:C     | 2.42                     | 0.45              |
| 19:1S:44:LYS:HE2   | 19:1S:52:ILE:HD13  | 1.97                     | 0.45              |
| 20:1T:35:HIS:ND1   | 20:1T:38:LYS:HE3   | 2.32                     | 0.45              |
| 20:1U:18:VAL:O     | 20:1U:21:LEU:HB2   | 2.16                     | 0.45              |
| 75:1X:201:CDL:H612 | 75:1X:201:CDL:H241 | 1.97                     | 0.45              |
| 24:1Y:105:ARG:NE   | 24:1Y:105:ARG:HA   | 2.31                     | 0.45              |
| 24:1Y:124:VAL:HA   | 69:1Y:204:3PE:H222 | 1.98                     | 0.45              |
| 27:1b:68:HIS:CD2   | 27:1b:70:GLN:HB2   | 2.52                     | 0.45              |
| 32:1g:73:GLY:O     | 32:1g:77:VAL:HG23  | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:1j:38:TRP:CZ3   | 35:1j:42:HIS:CE1   | 3.04                     | 0.45              |
| 43:1r:24:GLN:H     | 43:1r:24:GLN:HG2   | 1.62                     | 0.45              |
| 45:3A:155:ALA:HA   | 45:3A:164:ALA:HB1  | 1.99                     | 0.45              |
| 49:3E:155:LYS:HZ1  | 49:3E:176:VAL:HG21 | 1.80                     | 0.45              |
| 49:3R:149:MET:HA   | 49:3R:149:MET:HE2  | 1.99                     | 0.45              |
| 55:4A:25:TRP:HB2   | 87:4L:101:PGV:H281 | 1.97                     | 0.45              |
| 57:4C:91:VAL:O     | 57:4C:95:THR:HG23  | 2.16                     | 0.45              |
| 58:4D:84:THR:HG21  | 87:4M:101:PGV:H71  | 1.98                     | 0.45              |
| 58:4D:134:PHE:HE1  | 65:4K:44:PRO:HD2   | 1.82                     | 0.45              |
| 61:4G:47:PHE:CE1   | 61:4G:81:GLY:HA2   | 2.50                     | 0.45              |
| 55:8A:118:VAL:HA   | 64:8J:54:SER:HA    | 1.99                     | 0.45              |
| 75:8B:303:CDL:HA61 | 75:8B:303:CDL:H311 | 1.74                     | 0.45              |
| 58:8D:111:PHE:HE2  | 65:8K:41:ASN:HB2   | 1.82                     | 0.45              |
| 87:8K:101:PGV:H62  | 87:8K:101:PGV:H21  | 1.99                     | 0.45              |
| 68:8N:81:ASP:N     | 68:8N:81:ASP:OD1   | 2.50                     | 0.45              |
| 70:1A:202:PC1:H222 | 70:1A:202:PC1:H261 | 1.97                     | 0.45              |
| 70:1B:203:PC1:H321 | 8:1H:46:LEU:HD13   | 1.98                     | 0.45              |
| 4:1D:334:LYS:HB2   | 4:1D:337:GLU:CD    | 2.41                     | 0.45              |
| 4:1D:343:GLU:O     | 4:1D:347:HIS:ND1   | 2.37                     | 0.45              |
| 6:1F:21:ILE:CG2    | 6:1F:117:LYS:NZ    | 2.80                     | 0.45              |
| 6:1F:257:ASN:OD1   | 6:1F:267:THR:OG1   | 2.16                     | 0.45              |
| 7:1G:108:CYS:SG    | 7:1G:206:GLY:HA3   | 2.57                     | 0.45              |
| 8:1H:55:LEU:HD13   | 8:1H:221:ALA:HB2   | 1.98                     | 0.45              |
| 12:1L:19:ILE:HD12  | 12:1L:123:LEU:HG   | 1.98                     | 0.45              |
| 13:1M:159:PRO:HB3  | 69:1M:501:3PE:H2A1 | 1.99                     | 0.45              |
| 69:1M:501:3PE:O12  | 69:1M:501:3PE:N    | 2.35                     | 0.45              |
| 14:1N:230:LEU:HD21 | 14:1N:244:MET:SD   | 2.56                     | 0.45              |
| 16:1P:275:PHE:HE2  | 70:1P:401:PC1:C21  | 2.29                     | 0.45              |
| 17:1Q:23:THR:HG23  | 17:1Q:25:VAL:HG13  | 1.99                     | 0.45              |
| 28:1c:6:GLU:OE1    | 28:1c:7:PRO:HD2    | 2.16                     | 0.45              |
| 36:1k:33:GLU:OE1   | 36:1k:33:GLU:HA    | 2.17                     | 0.45              |
| 39:1n:12:GLN:NE2   | 39:1n:13:GLN:HG3   | 2.30                     | 0.45              |
| 39:1n:58:LYS:O     | 39:1n:62:LEU:HG    | 2.17                     | 0.45              |
| 48:3D:185:ASN:HD21 | 48:3Q:78:GLY:HA2   | 1.81                     | 0.45              |
| 49:3E:199:GLN:O    | 49:3E:248:ARG:HD3  | 2.17                     | 0.45              |
| 49:3V:65:VAL:HG22  | 49:3V:77:ARG:C     | 2.41                     | 0.45              |
| 54:3Y:14:ALA:O     | 54:3Y:18:ILE:HG12  | 2.17                     | 0.45              |
| 55:4A:131:PRO:HD3  | 56:4B:160:LEU:HD13 | 1.98                     | 0.45              |
| 55:4A:440:TYR:OH   | 56:4B:195:GLN:HB3  | 2.15                     | 0.45              |
| 56:4B:49:LYS:HE3   | 59:4E:76:GLY:HA2   | 1.98                     | 0.45              |
| 57:4C:33:MET:HE1   | 64:4J:49:CYS:O     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:4E:96:LEU:HB3   | 59:4E:98:ILE:HG13  | 1.99                     | 0.45              |
| 60:4F:50:PRO:O     | 60:4F:56:ARG:NH1   | 2.40                     | 0.45              |
| 67:4M:37:LEU:HA    | 67:4M:40:TYR:HB2   | 1.98                     | 0.45              |
| 55:8A:1:FME:SD     | 87:8A:601:PGV:H211 | 2.57                     | 0.45              |
| 55:8A:221:ASP:C    | 55:8A:221:ASP:OD1  | 2.59                     | 0.45              |
| 55:8A:282:PHE:HA   | 87:8A:603:PGV:H292 | 1.98                     | 0.45              |
| 56:8B:23:PHE:CZ    | 56:8B:80:SER:HB2   | 2.51                     | 0.45              |
| 56:8B:28:LEU:HD12  | 56:8B:28:LEU:O     | 2.16                     | 0.45              |
| 57:8C:31:LEU:HD12  | 87:8C:301:PGV:H181 | 1.98                     | 0.45              |
| 57:8C:182:TYR:CD2  | 87:8C:305:PGV:O11  | 2.69                     | 0.45              |
| 58:8D:77:GLU:C     | 58:8D:81:ILE:CD1   | 2.88                     | 0.45              |
| 58:8D:77:GLU:CG    | 58:8D:81:ILE:HD11  | 2.44                     | 0.45              |
| 62:8H:33:TYR:HD1   | 62:8H:60:TYR:CD2   | 2.35                     | 0.45              |
| 3:1C:45:PHE:HD1    | 3:1C:47:GLU:HG3    | 1.81                     | 0.45              |
| 3:1C:51:PHE:HB3    | 21:1V:111:TRP:CE2  | 2.52                     | 0.45              |
| 4:1D:62:LEU:HB2    | 4:1D:425:PHE:CZ    | 2.51                     | 0.45              |
| 10:1J:7:PHE:CD1    | 11:1K:3:LEU:HD13   | 2.51                     | 0.45              |
| 12:1L:49:VAL:HB    | 12:1L:50:PRO:HD3   | 1.99                     | 0.45              |
| 13:1M:71:TRP:CH2   | 13:1M:439:LEU:HD22 | 2.51                     | 0.45              |
| 69:1M:504:3PE:H2H2 | 14:1N:256:PRO:HG2  | 1.97                     | 0.45              |
| 16:1P:192:PRO:HB3  | 16:1P:256:TYR:CZ   | 2.52                     | 0.45              |
| 19:1S:33:ARG:O     | 19:1S:37:GLU:OE2   | 2.35                     | 0.45              |
| 23:1X:20:SER:HB3   | 26:1a:51:ASP:OD1   | 2.17                     | 0.45              |
| 23:1X:21:SER:OG    | 26:1a:51:ASP:OD2   | 2.28                     | 0.45              |
| 38:1m:82:THR:CG2   | 38:1m:85:THR:H     | 2.29                     | 0.45              |
| 39:1n:142:GLU:OE2  | 39:1n:157:ARG:NH1  | 2.49                     | 0.45              |
| 41:1p:73:ILE:HG23  | 41:1p:155:LEU:HD22 | 1.99                     | 0.45              |
| 46:3B:51:ILE:HG23  | 46:3B:204:MET:HG2  | 1.99                     | 0.45              |
| 51:3G:73:ARG:HA    | 52:3H:82:GLU:OE1   | 2.16                     | 0.45              |
| 45:3N:106:LEU:HD22 | 45:3N:203:VAL:HG12 | 1.98                     | 0.45              |
| 46:3O:223:PHE:O    | 46:3O:226:MET:HE2  | 2.17                     | 0.45              |
| 48:3Q:11:PRO:HG2   | 52:3U:74:PHE:HB2   | 1.97                     | 0.45              |
| 55:4A:192:ALA:HA   | 55:4A:195:LEU:HD12 | 1.99                     | 0.45              |
| 57:4C:221:ARG:NH1  | 87:4C:306:PGV:O13  | 2.49                     | 0.45              |
| 55:8A:151:HIS:CD2  | 55:8A:206:ILE:CD1  | 3.00                     | 0.45              |
| 55:8A:462:LEU:O    | 55:8A:462:LEU:HD12 | 2.17                     | 0.45              |
| 56:8B:26:HIS:HA    | 56:8B:29:MET:SD    | 2.56                     | 0.45              |
| 68:8N:32:TYR:CZ    | 68:8N:36:LEU:HD21  | 2.51                     | 0.45              |
| 3:1C:148:LEU:O     | 22:1W:88:MET:HE2   | 2.17                     | 0.45              |
| 4:1D:326:ASP:HB2   | 43:1r:44:PRO:HD2   | 1.97                     | 0.45              |
| 4:1D:350:LYS:HD2   | 7:1G:117:GLN:HB3   | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:338:VAL:HG13  | 7:1G:609:MET:HE3   | 1.98                     | 0.45              |
| 12:1L:66:TRP:HB2   | 69:1L:703:3PE:H351 | 1.97                     | 0.45              |
| 14:1N:315:TRP:HZ3  | 15:1O:292:VAL:HG12 | 1.82                     | 0.45              |
| 24:1Y:14:GLY:O     | 24:1Y:78:GLN:HG2   | 2.17                     | 0.45              |
| 46:3B:276:GLN:HB2  | 46:3B:322:PHE:HE1  | 1.82                     | 0.45              |
| 48:3D:314:HIS:CD2  | 51:3G:22:PRO:HB2   | 2.51                     | 0.45              |
| 46:3O:51:ILE:HG23  | 46:3O:204:MET:HG3  | 1.99                     | 0.45              |
| 49:3R:149:MET:O    | 49:3R:151:LYS:N    | 2.50                     | 0.45              |
| 53:3W:52:TRP:O     | 53:3W:56:LYS:HB2   | 2.16                     | 0.45              |
| 55:4A:283:LEU:HD11 | 68:4N:22:ILE:HD12  | 1.99                     | 0.45              |
| 56:4B:161:HIS:CE1  | 56:4B:200:CYS:HB2  | 2.52                     | 0.45              |
| 57:4C:45:LEU:CD1   | 64:4J:38:LEU:HD22  | 2.39                     | 0.45              |
| 87:4C:301:PGV:H132 | 87:4C:301:PGV:H322 | 1.99                     | 0.45              |
| 62:4H:30:TRP:CE2   | 62:4H:34:LEU:HD11  | 2.52                     | 0.45              |
| 55:8A:276:ALA:O    | 55:8A:280:ILE:HG12 | 2.17                     | 0.45              |
| 55:8A:316:THR:HG21 | 88:8A:605:HEA:H131 | 1.98                     | 0.45              |
| 55:8A:512:ASN:HD21 | 60:8F:38:ALA:HA    | 1.81                     | 0.45              |
| 57:8C:50:ASN:OD1   | 57:8C:50:ASN:C     | 2.60                     | 0.45              |
| 57:8C:86:PHE:O     | 57:8C:89:SER:OG    | 2.28                     | 0.45              |
| 75:8C:306:CDL:HB4  | 75:8C:306:CDL:H512 | 1.42                     | 0.45              |
| 58:8D:53:MET:N     | 58:8D:53:MET:SD    | 2.89                     | 0.45              |
| 60:8F:42:THR:OG1   | 60:8F:43:LYS:N     | 2.49                     | 0.45              |
| 4:1D:147:LEU:HD22  | 4:1D:218:PHE:HE2   | 1.82                     | 0.45              |
| 9:1I:17:VAL:HG21   | 27:1b:9:LYS:HE3    | 1.98                     | 0.45              |
| 10:1J:86:ASN:HD21  | 10:1J:88:THR:HB    | 1.82                     | 0.45              |
| 12:1L:207:GLU:HG2  | 12:1L:269:THR:HG21 | 1.98                     | 0.45              |
| 13:1M:311:GLY:HA2  | 13:1M:377:GLY:HA2  | 1.99                     | 0.45              |
| 15:1O:140:ARG:HB2  | 15:1O:201:ASP:OD2  | 2.16                     | 0.45              |
| 40:1o:61:TYR:HA    | 40:1o:64:GLN:HG2   | 1.98                     | 0.45              |
| 41:1p:7:ASP:OD1    | 41:1p:7:ASP:N      | 2.50                     | 0.45              |
| 45:3A:140:GLU:HG2  | 49:3I:48:SER:O     | 2.17                     | 0.45              |
| 45:3A:172:GLU:C    | 45:3A:172:GLU:CD   | 2.85                     | 0.45              |
| 47:3C:111:GLU:H    | 47:3C:111:GLU:CD   | 2.25                     | 0.45              |
| 49:3E:110:ARG:HD2  | 51:3G:23:PHE:O     | 2.17                     | 0.45              |
| 52:3H:52:ILE:O     | 52:3H:56:ILE:HG12  | 2.17                     | 0.45              |
| 49:3V:55:LEU:O     | 49:3V:58:GLN:HB2   | 2.17                     | 0.45              |
| 55:4A:32:ALA:HB3   | 66:4L:36:PRO:HG2   | 1.99                     | 0.45              |
| 55:4A:354:THR:HG22 | 55:4A:376:HIS:HB2  | 1.99                     | 0.45              |
| 55:8A:229:ILE:HD11 | 56:8B:175:ILE:HD12 | 1.98                     | 0.45              |
| 55:8A:283:LEU:O    | 55:8A:287:VAL:HG22 | 2.16                     | 0.45              |
| 55:8A:367:LEU:HD23 | 55:8A:367:LEU:HA   | 1.76                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:8C:91:VAL:O     | 57:8C:95:THR:HG23  | 2.17                     | 0.45              |
| 57:8C:240:TRP:CZ2  | 75:8C:306:CDL:H721 | 2.52                     | 0.45              |
| 58:8D:33:LEU:HB3   | 58:8D:38:LYS:HG3   | 1.98                     | 0.45              |
| 58:8D:86:LEU:HA    | 58:8D:89:ILE:HD13  | 1.97                     | 0.45              |
| 67:8M:39:HIS:HA    | 67:8M:42:ARG:HE    | 1.82                     | 0.45              |
| 2:1B:77:ARG:HG3    | 2:1B:78:ALA:H      | 1.82                     | 0.45              |
| 3:1C:51:PHE:CE2    | 3:1C:108:LYS:HD3   | 2.52                     | 0.45              |
| 4:1D:335:ARG:NH2   | 9:1I:129:ASP:OD1   | 2.50                     | 0.45              |
| 5:1E:67:ASN:OD1    | 5:1E:81:TYR:OH     | 2.25                     | 0.45              |
| 5:1E:206:PRO:HB3   | 6:1F:23:THR:HB     | 1.99                     | 0.45              |
| 6:1F:68:ARG:HD2    | 6:1F:254:LYS:HG3   | 1.99                     | 0.45              |
| 7:1G:13:VAL:HB     | 7:1G:33:VAL:HG21   | 1.98                     | 0.45              |
| 12:1L:400:ASN:HB3  | 12:1L:486:MET:HE3  | 1.99                     | 0.45              |
| 13:1M:207:MET:O    | 13:1M:294:MET:HG3  | 2.16                     | 0.45              |
| 13:1M:227:GLY:O    | 13:1M:231:LEU:HD12 | 2.17                     | 0.45              |
| 16:1P:157:ARG:HD3  | 16:1P:157:ARG:HA   | 1.80                     | 0.45              |
| 20:1T:6:LEU:O      | 20:1T:86:VAL:HG11  | 2.17                     | 0.45              |
| 22:1W:22:SER:N     | 22:1W:80:ASP:OD2   | 2.50                     | 0.45              |
| 23:1X:129:LYS:HD3  | 27:1b:65:VAL:HG13  | 1.98                     | 0.45              |
| 33:1h:56:PRO:HD3   | 41:1p:63:TYR:CE2   | 2.51                     | 0.45              |
| 38:1m:43:LYS:HD3   | 38:1m:47:LEU:HG    | 1.98                     | 0.45              |
| 45:3N:41:ILE:HG12  | 45:3N:195:MET:HG2  | 1.98                     | 0.45              |
| 46:3O:370:MET:HA   | 46:3O:373:GLU:HG3  | 1.99                     | 0.45              |
| 49:3R:136:PHE:O    | 49:3R:139:SER:OG   | 2.27                     | 0.45              |
| 55:4A:22:PHE:HE1   | 55:4A:109:PHE:HD2  | 1.65                     | 0.45              |
| 56:4B:123:ILE:HD11 | 56:4B:139:ASP:HB3  | 1.98                     | 0.45              |
| 57:4C:27:MET:CE    | 57:4C:50:ASN:ND2   | 2.80                     | 0.45              |
| 58:4D:63:LYS:CG    | 58:4D:64:PHE:CE1   | 2.98                     | 0.45              |
| 59:4E:41:LEU:C     | 59:4E:41:LEU:CD1   | 2.90                     | 0.45              |
| 62:4H:27:ARG:NH1   | 68:4N:54:TRP:CZ3   | 2.85                     | 0.45              |
| 65:4K:9:PHE:HA     | 65:4K:12:LYS:HE3   | 1.97                     | 0.45              |
| 87:8C:304:PGV:H171 | 75:8C:306:CDL:H872 | 1.99                     | 0.45              |
| 58:8D:80:THR:HG21  | 65:8K:10:HIS:ND1   | 2.32                     | 0.45              |
| 58:8D:97:ILE:HG22  | 65:8K:36:ILE:CD1   | 2.38                     | 0.45              |
| 59:8E:43:PRO:CB    | 59:8E:48:ILE:HD11  | 2.46                     | 0.45              |
| 66:8L:36:PRO:HA    | 66:8L:39:ILE:CD1   | 2.47                     | 0.45              |
| 1:1A:30:TYR:OH     | 2:1B:111:ARG:NH2   | 2.49                     | 0.44              |
| 8:1H:287:HIS:O     | 8:1H:291:LYS:HB2   | 2.17                     | 0.44              |
| 11:1K:70:GLU:HG2   | 14:1N:60:PHE:HE1   | 1.82                     | 0.44              |
| 13:1M:197:LEU:HB3  | 69:1M:501:3PE:H2D1 | 1.97                     | 0.44              |
| 14:1N:287:LEU:HB3  | 69:1N:901:3PE:H291 | 1.97                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:1O:135:LEU:HD13 | 15:1O:152:TYR:CG   | 2.52                     | 0.44              |
| 18:1R:19:ASP:OD1   | 18:1R:19:ASP:N     | 2.50                     | 0.44              |
| 28:1c:41:GLU:HA    | 28:1c:41:GLU:OE1   | 2.16                     | 0.44              |
| 34:1i:79:TRP:HE1   | 41:1p:40:VAL:HA    | 1.81                     | 0.44              |
| 42:1q:17:HIS:CD2   | 42:1q:26:VAL:HG21  | 2.53                     | 0.44              |
| 45:3A:244:ARG:NH2  | 45:3A:429:GLU:OE1  | 2.50                     | 0.44              |
| 46:3B:340:ALA:O    | 46:3B:344:VAL:HG23 | 2.17                     | 0.44              |
| 51:3G:38:ASN:O     | 51:3G:42:ARG:HG3   | 2.17                     | 0.44              |
| 47:3P:30:TRP:HB3   | 47:3P:100:ARG:HG3  | 1.99                     | 0.44              |
| 49:3R:179:ARG:NH1  | 49:3R:246:SER:OG   | 2.50                     | 0.44              |
| 53:3W:51:LEU:HB2   | 53:3W:54:HIS:ND1   | 2.32                     | 0.44              |
| 58:4D:24:LEU:HD11  | 59:4E:67:ILE:HG22  | 1.99                     | 0.44              |
| 61:4G:72:ASN:OD1   | 61:4G:75:VAL:HG12  | 2.17                     | 0.44              |
| 57:8C:59:ARG:O     | 57:8C:63:ARG:HG2   | 2.17                     | 0.44              |
| 2:1B:90:GLY:HA2    | 71:1B:201:SF4:S2   | 2.57                     | 0.44              |
| 3:1C:32:ILE:HG23   | 21:1V:43:TYR:HB2   | 1.99                     | 0.44              |
| 4:1D:406:SER:HB2   | 4:1D:414:VAL:HG22  | 1.98                     | 0.44              |
| 7:1G:43:HIS:NE2    | 7:1G:261:GLU:OE2   | 2.42                     | 0.44              |
| 7:1G:575:ASN:ND2   | 7:1G:577:GLU:OE2   | 2.51                     | 0.44              |
| 10:1J:99:MET:HE3   | 10:1J:100:GLU:H    | 1.81                     | 0.44              |
| 11:1K:59:MET:HE2   | 14:1N:84:TRP:HH2   | 1.81                     | 0.44              |
| 12:1L:375:ILE:HG12 | 35:1j:32:MET:SD    | 2.57                     | 0.44              |
| 69:1M:504:3PE:H241 | 69:1M:504:3PE:H3C1 | 2.00                     | 0.44              |
| 14:1N:197:ASN:OD1  | 14:1N:200:MET:HG2  | 2.17                     | 0.44              |
| 16:1P:188:PHE:CG   | 69:1P:403:3PE:H3B2 | 2.52                     | 0.44              |
| 21:1V:105:GLU:OE1  | 21:1V:106:PRO:HD2  | 2.17                     | 0.44              |
| 25:1Z:98:MET:HE3   | 25:1Z:104:TRP:CZ2  | 2.52                     | 0.44              |
| 26:1a:59:ARG:HE    | 26:1a:61:HIS:HE1   | 1.59                     | 0.44              |
| 31:1f:53:GLU:HG2   | 31:1f:54:VAL:HG22  | 1.99                     | 0.44              |
| 45:3A:431:LEU:HD12 | 45:3A:432:PRO:HD2  | 2.00                     | 0.44              |
| 47:3C:181:PHE:HA   | 47:3C:184:ILE:HG22 | 1.99                     | 0.44              |
| 50:3F:119:TRP:CZ2  | 46:3O:87:ARG:HB3   | 2.53                     | 0.44              |
| 49:3R:164:ASN:HB3  | 49:3R:227:ASN:ND2  | 2.32                     | 0.44              |
| 55:4A:5:ARG:NH2    | 66:4L:10:ASN:OD1   | 2.47                     | 0.44              |
| 55:4A:22:PHE:CE1   | 55:4A:109:PHE:HD2  | 2.35                     | 0.44              |
| 56:4B:218:TYR:HA   | 56:4B:221:LYS:HG2  | 1.98                     | 0.44              |
| 57:4C:240:TRP:CZ2  | 75:4C:305:CDL:H721 | 2.52                     | 0.44              |
| 58:4D:20:ARG:HD2   | 59:4E:73:ASP:OD2   | 2.16                     | 0.44              |
| 58:4D:64:PHE:CD1   | 58:4D:64:PHE:N     | 2.85                     | 0.44              |
| 59:4E:52:LEU:CD1   | 59:4E:98:ILE:CD1   | 2.94                     | 0.44              |
| 68:4N:9:ALA:HB1    | 68:4N:16:ILE:HD13  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:8A:251:PHE:HB3  | 55:8A:319:LYS:HZ3  | 1.81                     | 0.44              |
| 55:8A:345:ILE:O    | 55:8A:349:THR:OG1  | 2.26                     | 0.44              |
| 55:8A:466:MET:HE2  | 67:8M:23:PHE:CD1   | 2.52                     | 0.44              |
| 57:8C:171:VAL:O    | 57:8C:175:LEU:HG   | 2.17                     | 0.44              |
| 59:8E:43:PRO:HB3   | 59:8E:47:ILE:HD11  | 1.98                     | 0.44              |
| 66:8L:20:ARG:CZ    | 66:8L:24:MET:CE    | 2.93                     | 0.44              |
| 9:1I:50:TYR:OH     | 9:1I:138:GLU:OE2   | 2.24                     | 0.44              |
| 11:1K:94:ASN:ND2   | 12:1L:581:LYS:O    | 2.42                     | 0.44              |
| 12:1L:264:TYR:CD2  | 12:1L:265:PRO:HD3  | 2.53                     | 0.44              |
| 12:1L:331:MET:SD   | 12:1L:465:GLY:HA2  | 2.58                     | 0.44              |
| 12:1L:600:THR:HB   | 12:1L:601:LEU:H    | 1.65                     | 0.44              |
| 13:1M:30:HIS:HB3   | 31:1f:16:VAL:HG21  | 2.00                     | 0.44              |
| 14:1N:281:LEU:O    | 14:1N:285:THR:OG1  | 2.28                     | 0.44              |
| 42:1q:10:GLY:O     | 42:1q:14:VAL:HG23  | 2.18                     | 0.44              |
| 42:1q:78:ASP:C     | 42:1q:78:ASP:OD1   | 2.60                     | 0.44              |
| 48:3D:115:ARG:O    | 48:3D:119:GLN:HG3  | 2.16                     | 0.44              |
| 48:3D:306:PRO:HB3  | 69:3G:101:3PE:H362 | 1.98                     | 0.44              |
| 45:3N:371:GLY:C    | 45:3N:374:PRO:HD2  | 2.43                     | 0.44              |
| 47:3P:234:PHE:CE2  | 75:3P:504:CDL:H141 | 2.53                     | 0.44              |
| 48:3Q:143:LEU:HD23 | 48:3Q:147:LEU:HB3  | 2.00                     | 0.44              |
| 49:3R:230:ASP:OD1  | 49:3R:231:PHE:N    | 2.48                     | 0.44              |
| 60:4F:25:ARG:HG2   | 60:4F:25:ARG:NH1   | 2.31                     | 0.44              |
| 64:4J:33:ARG:HH11  | 87:4J:101:PGV:H171 | 1.82                     | 0.44              |
| 64:4J:36:MET:CB    | 87:4J:101:PGV:H182 | 2.47                     | 0.44              |
| 68:4N:58:GLY:HA3   | 68:4N:61:ASP:OD1   | 2.17                     | 0.44              |
| 55:8A:21:LEU:HD22  | 87:8L:101:PGV:H242 | 1.98                     | 0.44              |
| 55:8A:168:ILE:HD13 | 55:8A:189:LEU:HB2  | 1.99                     | 0.44              |
| 55:8A:229:ILE:HD13 | 56:8B:178:ARG:NH1  | 2.32                     | 0.44              |
| 55:8A:343:GLY:O    | 55:8A:347:LEU:HD23 | 2.18                     | 0.44              |
| 87:8A:602:PGV:H271 | 87:8A:602:PGV:H132 | 1.99                     | 0.44              |
| 57:8C:248:VAL:O    | 57:8C:252:LEU:HG   | 2.17                     | 0.44              |
| 61:8G:32:THR:OG1   | 87:8G:101:PGV:H302 | 2.17                     | 0.44              |
| 64:8J:28:ASP:OD1   | 64:8J:28:ASP:C     | 2.60                     | 0.44              |
| 4:1D:242:ILE:HD12  | 4:1D:413:ASP:OD2   | 2.18                     | 0.44              |
| 6:1F:299:PRO:HG3   | 6:1F:327:THR:HG21  | 1.98                     | 0.44              |
| 7:1G:7:ASN:OD1     | 7:1G:7:ASN:N       | 2.46                     | 0.44              |
| 8:1H:228:TYR:HA    | 8:1H:231:ILE:HD12  | 1.99                     | 0.44              |
| 11:1K:10:MET:HE2   | 11:1K:10:MET:HB2   | 1.90                     | 0.44              |
| 12:1L:203:MET:HB2  | 41:1p:113:GLN:HG3  | 1.98                     | 0.44              |
| 12:1L:575:ILE:HD13 | 14:1N:171:ASN:ND2  | 2.32                     | 0.44              |
| 13:1M:74:PRO:HA    | 13:1M:77:LEU:HD12  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:1M:502:3PE:H362 | 29:1d:44:ILE:HG12  | 1.99                     | 0.44              |
| 35:1j:43:ASP:OD1   | 35:1j:43:ASP:C     | 2.60                     | 0.44              |
| 35:1j:64:LEU:HD23  | 35:1j:64:LEU:HA    | 1.81                     | 0.44              |
| 37:1l:12:PRO:O     | 37:1l:46:ASP:HB3   | 2.17                     | 0.44              |
| 45:3A:248:LEU:HD12 | 45:3A:426:GLY:HA2  | 1.99                     | 0.44              |
| 46:3B:179:PRO:O    | 46:3B:183:ILE:HG13 | 2.17                     | 0.44              |
| 47:3C:168:PHE:HZ   | 49:3R:147:LEU:HD23 | 1.81                     | 0.44              |
| 49:3I:53:GLU:HA    | 49:3I:56:ARG:NH1   | 2.32                     | 0.44              |
| 47:3P:197:LEU:HD11 | 85:3P:502:HEM:HMA3 | 1.98                     | 0.44              |
| 48:3Q:158:ILE:HG12 | 48:3Q:160:MET:HB2  | 1.99                     | 0.44              |
| 49:3R:160:PRO:HD2  | 49:3R:163:LYS:HB3  | 1.99                     | 0.44              |
| 57:4C:144:ILE:HD13 | 57:4C:239:ALA:HA   | 1.99                     | 0.44              |
| 62:4H:4:ILE:HD11   | 68:4N:79:GLY:HA2   | 2.00                     | 0.44              |
| 56:8B:32:PHE:CZ    | 75:8B:303:CDL:H132 | 2.52                     | 0.44              |
| 58:8D:143:ASN:HB2  | 58:8D:144:GLU:OE1  | 2.17                     | 0.44              |
| 61:8G:68:THR:HG22  | 61:8G:69:LEU:N     | 2.29                     | 0.44              |
| 9:1I:44:GLU:OE1    | 81:1q:202:AYA:CT   | 2.66                     | 0.44              |
| 9:1I:50:TYR:CD1    | 9:1I:51:PRO:HA     | 2.53                     | 0.44              |
| 17:1Q:88:THR:OG1   | 17:1Q:91:ASP:OD2   | 2.30                     | 0.44              |
| 31:1f:1:MET:SD     | 31:1f:1:MET:C      | 3.00                     | 0.44              |
| 31:1f:29:ARG:HD3   | 31:1f:29:ARG:HA    | 1.60                     | 0.44              |
| 34:1i:92:LYS:HG2   | 34:1i:93:PRO:HD2   | 2.00                     | 0.44              |
| 45:3A:301:ARG:HB2  | 45:3A:303:LEU:HG   | 2.00                     | 0.44              |
| 47:3C:318:ARG:O    | 47:3C:322:GLN:HG3  | 2.16                     | 0.44              |
| 50:3F:79:ASP:OD1   | 50:3F:82:MET:HE1   | 2.18                     | 0.44              |
| 52:3H:63:GLU:O     | 52:3H:67:GLN:HG3   | 2.18                     | 0.44              |
| 52:3H:76:GLU:HA    | 52:3H:76:GLU:OE2   | 2.17                     | 0.44              |
| 45:3N:270:LEU:HD22 | 45:3N:320:LEU:HD21 | 1.99                     | 0.44              |
| 46:3O:28:ARG:NH2   | 46:3O:390:GLY:CA   | 2.79                     | 0.44              |
| 92:4B:305:PSC:H21  | 92:4B:305:PSC:H02  | 1.58                     | 0.44              |
| 57:4C:79:LEU:HB3   | 57:4C:233:PHE:CE2  | 2.52                     | 0.44              |
| 59:4E:33:MET:CE    | 59:4E:67:ILE:HD12  | 2.47                     | 0.44              |
| 57:8C:57:TRP:NE1   | 87:8C:301:PGV:O14  | 2.45                     | 0.44              |
| 59:8E:61:PHE:HE1   | 59:8E:65:VAL:HG21  | 1.82                     | 0.44              |
| 68:8N:40:ASN:OD1   | 68:8N:40:ASN:N     | 2.50                     | 0.44              |
| 1:1A:55:PHE:HE1    | 8:1H:134:ARG:HD3   | 1.82                     | 0.44              |
| 6:1F:423:ARG:N     | 6:1F:424:PRO:HD2   | 2.33                     | 0.44              |
| 7:1G:366:THR:HB    | 7:1G:450:MET:HE2   | 1.99                     | 0.44              |
| 12:1L:83:ASP:OD1   | 12:1L:83:ASP:C     | 2.59                     | 0.44              |
| 13:1M:425:ASN:HB2  | 38:1m:57:GLY:HA2   | 2.00                     | 0.44              |
| 14:1N:36:ASN:OD1   | 14:1N:134:GLN:NE2  | 2.50                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:179:MET:HE3  | 14:1N:179:MET:HB3  | 1.83                     | 0.44              |
| 14:1N:193:VAL:HB   | 14:1N:266:ILE:HG23 | 2.00                     | 0.44              |
| 16:1P:147:ARG:HH12 | 59:8E:9:GLU:N      | 2.02                     | 0.44              |
| 24:1Y:91:ILE:HD13  | 24:1Y:91:ILE:HA    | 1.89                     | 0.44              |
| 25:1Z:36:PHE:O     | 25:1Z:40:ILE:HG12  | 2.17                     | 0.44              |
| 49:3E:155:LYS:O    | 49:3E:270:LEU:HA   | 2.18                     | 0.44              |
| 49:3E:263:TYR:CD1  | 49:3E:271:VAL:HG12 | 2.52                     | 0.44              |
| 51:3G:38:ASN:ND2   | 75:3G:103:CDL:OA3  | 2.36                     | 0.44              |
| 45:3N:50:GLU:HG2   | 45:3N:51:LYS:HD3   | 2.00                     | 0.44              |
| 48:3Q:8:PRO:HG3    | 52:3U:66:ASP:HB3   | 2.00                     | 0.44              |
| 49:3R:222:CYS:HB3  | 49:3R:238:CYS:HB3  | 1.49                     | 0.44              |
| 49:3R:234:TYR:HB2  | 49:3R:243:TYR:HB2  | 2.00                     | 0.44              |
| 50:3S:18:LYS:HB2   | 50:3S:18:LYS:HE3   | 1.69                     | 0.44              |
| 56:4B:45:MET:CE    | 92:4B:305:PSC:H62  | 2.47                     | 0.44              |
| 56:4B:148:MET:C    | 56:4B:185:MET:HE1  | 2.43                     | 0.44              |
| 87:4J:101:PGV:H302 | 87:4J:101:PGV:H343 | 2.00                     | 0.44              |
| 67:4M:24:LEU:HD23  | 67:4M:24:LEU:HA    | 1.85                     | 0.44              |
| 55:8A:308:ALA:C    | 55:8A:311:ILE:HD12 | 2.42                     | 0.44              |
| 55:8A:427:PRO:HB3  | 55:8A:450:TRP:HE3  | 1.83                     | 0.44              |
| 55:8A:452:THR:O    | 55:8A:456:MET:HG3  | 2.16                     | 0.44              |
| 57:8C:62:ILE:HG13  | 87:8C:307:PGV:H21  | 2.00                     | 0.44              |
| 57:8C:141:GLY:O    | 57:8C:145:THR:HG23 | 2.17                     | 0.44              |
| 58:8D:48:TRP:HH2   | 59:8E:61:PHE:CA    | 2.30                     | 0.44              |
| 58:8D:99:GLU:OE1   | 58:8D:103:VAL:CG2  | 2.65                     | 0.44              |
| 59:8E:25:ASP:C     | 59:8E:28:GLU:OE2   | 2.60                     | 0.44              |
| 59:8E:33:MET:CE    | 59:8E:67:ILE:CG2   | 2.87                     | 0.44              |
| 62:8H:37:HIS:HB2   | 62:8H:85:ILE:HB    | 1.99                     | 0.44              |
| 63:8I:54:TYR:CD1   | 63:8I:54:TYR:C     | 2.94                     | 0.44              |
| 2:1B:46:TRP:HB3    | 2:1B:77:ARG:HG2    | 1.99                     | 0.44              |
| 5:1E:63:ILE:HD12   | 5:1E:63:ILE:HA     | 1.82                     | 0.44              |
| 7:1G:105:CYS:N     | 71:1G:801:SF4:S4   | 2.91                     | 0.44              |
| 7:1G:376:VAL:HG12  | 7:1G:405:LYS:HB3   | 2.00                     | 0.44              |
| 8:1H:277:TYR:CZ    | 9:1I:30:LEU:HB3    | 2.53                     | 0.44              |
| 10:1J:25:SER:HB2   | 10:1J:81:GLU:C     | 2.43                     | 0.44              |
| 19:1S:17:GLU:HG2   | 19:1S:67:ARG:HH21  | 1.83                     | 0.44              |
| 23:1X:168:PHE:CE1  | 75:1X:201:CDL:H172 | 2.53                     | 0.44              |
| 34:1i:92:LYS:HB3   | 34:1i:95:THR:HG21  | 1.98                     | 0.44              |
| 39:1n:122:GLU:O    | 39:1n:126:ARG:HG3  | 2.17                     | 0.44              |
| 41:1p:5:ASP:HB3    | 41:1p:8:VAL:CG1    | 2.47                     | 0.44              |
| 48:3D:268:MET:N    | 52:3H:40:ASP:OD2   | 2.51                     | 0.44              |
| 45:3N:248:LEU:HD12 | 45:3N:426:GLY:HA2  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:3R:170:ARG:C    | 49:3R:172:LYS:H    | 2.26                     | 0.44              |
| 52:3U:49:GLN:OE1   | 52:3U:49:GLN:C     | 2.61                     | 0.44              |
| 56:4B:1:FME:HE3    | 58:4D:128:VAL:HG22 | 1.99                     | 0.44              |
| 55:8A:305:PHE:O    | 55:8A:309:THR:HG22 | 2.18                     | 0.44              |
| 57:8C:33:MET:HE2   | 64:8J:49:CYS:SG    | 2.58                     | 0.44              |
| 8:1H:84:THR:O      | 8:1H:87:VAL:HG22   | 2.18                     | 0.44              |
| 8:1H:186:PHE:CD2   | 70:1H:402:PC1:H2D2 | 2.52                     | 0.44              |
| 9:1I:13:ASP:O      | 9:1I:17:VAL:HG22   | 2.18                     | 0.44              |
| 11:1K:40:LEU:HD23  | 14:1N:72:MET:HE2   | 1.99                     | 0.44              |
| 13:1M:19:LYS:HE2   | 13:1M:19:LYS:HB3   | 1.81                     | 0.44              |
| 13:1M:206:LYS:HE3  | 13:1M:206:LYS:HB3  | 1.75                     | 0.44              |
| 75:1N:902:CDL:H392 | 75:1N:902:CDL:H232 | 2.00                     | 0.44              |
| 16:1P:187:TRP:CE2  | 69:1P:403:3PE:H262 | 2.53                     | 0.44              |
| 21:1V:49:GLN:HA    | 21:1V:52:ASN:HD21  | 1.83                     | 0.44              |
| 24:1Y:109:ILE:HG23 | 70:1Y:207:PC1:H342 | 2.00                     | 0.44              |
| 25:1Z:20:ASP:N     | 25:1Z:20:ASP:OD1   | 2.49                     | 0.44              |
| 39:1n:166:TRP:CE3  | 39:1n:170:VAL:HG11 | 2.53                     | 0.44              |
| 42:1q:66:THR:HG23  | 42:1q:74:PHE:HD1   | 1.83                     | 0.44              |
| 47:3C:376:LEU:O    | 50:3F:29:ARG:HD3   | 2.17                     | 0.44              |
| 45:3N:268:VAL:HB   | 45:3N:269:PRO:HD3  | 2.00                     | 0.44              |
| 52:3U:28:GLU:OE1   | 52:3U:29:LYS:N     | 2.50                     | 0.44              |
| 53:3W:51:LEU:HD12  | 53:3W:54:HIS:HE1   | 1.82                     | 0.44              |
| 55:4A:187:SER:HB3  | 55:4A:277:MET:HE3  | 1.99                     | 0.44              |
| 58:4D:129:ALA:HB1  | 58:4D:133:GLY:HA3  | 1.98                     | 0.44              |
| 66:4L:28:TYR:HE2   | 87:4L:101:PGV:H302 | 1.80                     | 0.44              |
| 55:8A:46:THR:O     | 55:8A:46:THR:OG1   | 2.35                     | 0.44              |
| 55:8A:88:GLY:HA2   | 55:8A:505:PHE:CZ   | 2.53                     | 0.44              |
| 58:8D:122:ARG:HG3  | 65:8K:53:TRP:CD1   | 2.52                     | 0.44              |
| 59:8E:18:TYR:CE2   | 59:8E:32:GLY:HA3   | 2.53                     | 0.44              |
| 69:1A:201:3PE:H362 | 27:1b:11:ALA:HB1   | 1.99                     | 0.44              |
| 8:1H:58:LYS:HG2    | 8:1H:217:ALA:HB2   | 1.99                     | 0.44              |
| 69:1L:703:3PE:H2A1 | 34:1i:80:ILE:HG12  | 1.99                     | 0.44              |
| 13:1M:95:TYR:CE1   | 13:1M:132:ILE:HD12 | 2.53                     | 0.44              |
| 69:1M:502:3PE:H271 | 69:1M:502:3PE:H222 | 2.00                     | 0.44              |
| 20:1T:6:LEU:HD23   | 20:1T:6:LEU:H      | 1.82                     | 0.44              |
| 21:1V:43:TYR:CE2   | 21:1V:93:MET:HG3   | 2.53                     | 0.44              |
| 22:1W:49:LEU:HD23  | 22:1W:49:LEU:C     | 2.42                     | 0.44              |
| 22:1W:70:ASN:N     | 22:1W:70:ASN:HD22  | 2.14                     | 0.44              |
| 23:1X:165:ARG:HH12 | 29:1d:87:ASP:CG    | 2.26                     | 0.44              |
| 69:1Y:203:3PE:H2   | 69:1Y:203:3PE:H221 | 1.43                     | 0.44              |
| 47:3C:8:HIS:O      | 47:3C:12:LYS:N     | 2.45                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:3D:120:VAL:HG21 | 48:3D:271:VAL:HG13 | 1.98                     | 0.44              |
| 49:3E:234:TYR:HB2  | 49:3E:243:TYR:HB3  | 1.99                     | 0.44              |
| 45:3N:4:TYR:CZ     | 45:3N:8:LEU:HD11   | 2.52                     | 0.44              |
| 69:3N:501:3PE:H351 | 47:3P:11:MET:SD    | 2.57                     | 0.44              |
| 47:3P:28:SER:HB2   | 75:3P:504:CDL:HA22 | 2.00                     | 0.44              |
| 49:3R:217:CYS:HB2  | 49:3R:224:PRO:HD3  | 2.00                     | 0.44              |
| 55:4A:129:TYR:CZ   | 55:4A:232:GLN:HG2  | 2.53                     | 0.44              |
| 56:4B:11:ASP:OD1   | 58:4D:129:ALA:HA   | 2.18                     | 0.44              |
| 56:4B:62:GLU:HG3   | 68:4N:14:SER:CB    | 2.48                     | 0.44              |
| 56:4B:115:ASP:OD1  | 56:4B:115:ASP:C    | 2.61                     | 0.44              |
| 56:4B:161:HIS:HB2  | 56:4B:174:ALA:HB3  | 2.00                     | 0.44              |
| 87:4B:301:PGV:H281 | 75:4D:201:CDL:H261 | 2.00                     | 0.44              |
| 57:4C:109:THR:CG2  | 57:4C:111:GLU:OE2  | 2.66                     | 0.44              |
| 58:4D:77:GLU:O     | 58:4D:81:ILE:HD12  | 2.18                     | 0.44              |
| 87:4G:101:PGV:H202 | 87:4G:101:PGV:H012 | 1.23                     | 0.44              |
| 66:4L:37:PHE:O     | 66:4L:40:VAL:HG22  | 2.17                     | 0.44              |
| 55:8A:275:TRP:O    | 55:8A:279:SER:OG   | 2.29                     | 0.44              |
| 57:8C:90:GLU:HB2   | 57:8C:244:PHE:HE2  | 1.81                     | 0.44              |
| 58:8D:78:TRP:CA    | 58:8D:81:ILE:CD1   | 2.90                     | 0.44              |
| 75:8D:201:CDL:HB61 | 75:8D:201:CDL:H711 | 1.49                     | 0.44              |
| 59:8E:72:LYS:HD2   | 59:8E:82:TYR:CE2   | 2.52                     | 0.44              |
| 62:8H:49:ASP:O     | 62:8H:52:VAL:HG12  | 2.18                     | 0.44              |
| 2:1B:175:ILE:O     | 2:1B:179:ARG:HG3   | 2.18                     | 0.43              |
| 4:1D:165:THR:HG22  | 4:1D:169:TRP:CE2   | 2.53                     | 0.43              |
| 4:1D:373:GLU:OE1   | 4:1D:392:LYS:NZ    | 2.51                     | 0.43              |
| 8:1H:98:MET:HE2    | 70:1H:403:PC1:H2   | 2.01                     | 0.43              |
| 10:1J:115:ILE:O    | 10:1J:117:PHE:N    | 2.49                     | 0.43              |
| 16:1P:206:TYR:O    | 16:1P:210:VAL:HG23 | 2.18                     | 0.43              |
| 16:1P:215:ILE:O    | 16:1P:218:ILE:HB   | 2.18                     | 0.43              |
| 20:1U:17:TYR:C     | 20:1U:21:LEU:HD23  | 2.40                     | 0.43              |
| 28:1c:19:LEU:C     | 75:1d:203:CDL:H122 | 2.43                     | 0.43              |
| 51:3G:73:ARG:CZ    | 52:3H:82:GLU:HG2   | 2.48                     | 0.43              |
| 49:3I:65:VAL:HG22  | 49:3I:77:ARG:HB3   | 2.00                     | 0.43              |
| 55:4A:383:MET:CE   | 55:4A:421:VAL:HG13 | 2.45                     | 0.43              |
| 59:4E:61:PHE:O     | 59:4E:65:VAL:HG13  | 2.18                     | 0.43              |
| 55:8A:104:LEU:HD12 | 55:8A:152:LEU:HD13 | 1.99                     | 0.43              |
| 57:8C:160:ILE:HG23 | 57:8C:219:LEU:HD11 | 2.00                     | 0.43              |
| 62:8H:4:ILE:HB     | 62:8H:52:VAL:HG23  | 1.99                     | 0.43              |
| 63:8I:45:LYS:HD2   | 63:8I:45:LYS:O     | 2.17                     | 0.43              |
| 68:8N:8:GLN:CA     | 68:8N:11:LYS:HZ1   | 2.24                     | 0.43              |
| 2:1B:162:GLN:NE2   | 9:1I:142:GLU:HG2   | 2.33                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:71:GLU:OE2    | 4:1D:410:MET:HE1   | 2.18                     | 0.43              |
| 5:1E:68:LYS:HE3    | 5:1E:68:LYS:HB2    | 1.84                     | 0.43              |
| 6:1F:263:ASN:HB2   | 6:1F:264:HIS:CD2   | 2.53                     | 0.43              |
| 7:1G:433:ALA:HB2   | 7:1G:473:ILE:HG12  | 2.01                     | 0.43              |
| 8:1H:124:ASN:C     | 8:1H:126:LYS:H     | 2.25                     | 0.43              |
| 8:1H:264:LEU:HD22  | 26:1a:12:MET:HE2   | 1.99                     | 0.43              |
| 12:1L:233:LEU:HB3  | 12:1L:234:PRO:HD3  | 1.99                     | 0.43              |
| 15:1O:37:ARG:NH2   | 15:1O:40:ARG:HH11  | 2.15                     | 0.43              |
| 16:1P:279:THR:OG1  | 69:1P:403:3PE:H352 | 2.18                     | 0.43              |
| 21:1V:6:LYS:HE3    | 21:1V:6:LYS:HB2    | 1.83                     | 0.43              |
| 23:1X:17:VAL:HG22  | 23:1X:19:VAL:HG22  | 1.99                     | 0.43              |
| 29:1d:120:ARG:O    | 38:1m:108:ARG:NH2  | 2.34                     | 0.43              |
| 47:3P:183:PHE:CZ   | 85:3P:501:HEM:HBC1 | 2.53                     | 0.43              |
| 55:4A:21:LEU:HB3   | 87:4L:101:PGV:H271 | 1.99                     | 0.43              |
| 55:4A:508:PRO:HG3  | 57:4C:6:HIS:HB3    | 2.00                     | 0.43              |
| 56:4B:214:VAL:HG12 | 63:4I:60:PHE:HE1   | 1.83                     | 0.43              |
| 58:4D:145:TRP:CZ3  | 65:4K:45:VAL:HA    | 2.53                     | 0.43              |
| 55:8A:66:ILE:HG23  | 55:8A:67:PHE:CD2   | 2.53                     | 0.43              |
| 57:8C:222:GLN:HE21 | 57:8C:222:GLN:C    | 2.24                     | 0.43              |
| 75:8D:201:CDL:HB4  | 75:8D:201:CDL:H512 | 1.39                     | 0.43              |
| 59:8E:27:TRP:CH2   | 59:8E:31:LYS:HD3   | 2.54                     | 0.43              |
| 59:8E:69:GLU:O     | 59:8E:72:LYS:HB3   | 2.18                     | 0.43              |
| 61:8G:15:THR:HG22  | 61:8G:19:LEU:HD11  | 2.00                     | 0.43              |
| 3:1C:78:LEU:HB3    | 3:1C:130:TYR:HB3   | 2.01                     | 0.43              |
| 4:1D:291:GLY:O     | 4:1D:296:ARG:NH2   | 2.52                     | 0.43              |
| 6:1F:97:ALA:HB3    | 6:1F:138:ILE:HA    | 1.99                     | 0.43              |
| 6:1F:277:LYS:HE2   | 6:1F:277:LYS:HB2   | 1.69                     | 0.43              |
| 7:1G:343:LEU:HB3   | 7:1G:507:TYR:CE2   | 2.52                     | 0.43              |
| 7:1G:444:LYS:HA    | 7:1G:444:LYS:HD2   | 1.85                     | 0.43              |
| 8:1H:102:VAL:HG21  | 8:1H:154:LEU:CD1   | 2.48                     | 0.43              |
| 75:1H:401:CDL:H511 | 75:1H:401:CDL:HB4  | 1.41                     | 0.43              |
| 12:1L:213:LEU:HD21 | 12:1L:266:LEU:HG   | 2.00                     | 0.43              |
| 13:1M:150:LEU:HG   | 13:1M:154:LEU:HD12 | 2.00                     | 0.43              |
| 14:1N:55:ALA:HB1   | 14:1N:118:VAL:HA   | 1.99                     | 0.43              |
| 14:1N:158:ALA:HB1  | 14:1N:188:GLY:O    | 2.18                     | 0.43              |
| 15:1O:73:LEU:HD23  | 15:1O:292:VAL:HG13 | 2.00                     | 0.43              |
| 15:1O:174:VAL:HG22 | 15:1O:225:ALA:HB2  | 2.00                     | 0.43              |
| 16:1P:145:TYR:CE1  | 16:1P:149:LYS:HD2  | 2.53                     | 0.43              |
| 22:1W:23:ARG:N     | 22:1W:27:GLU:OE2   | 2.45                     | 0.43              |
| 32:1g:95:ARG:HH21  | 41:1p:64:HIS:CE1   | 2.36                     | 0.43              |
| 33:1h:134:ASP:C    | 33:1h:134:ASP:OD1  | 2.61                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:1o:30:PHE:HB2   | 40:1o:33:ARG:HD3   | 2.00                     | 0.43              |
| 45:3A:388:ARG:HH22 | 45:3A:394:GLU:CD   | 2.25                     | 0.43              |
| 46:3B:54:GLY:O     | 46:3B:194:TYR:OH   | 2.37                     | 0.43              |
| 49:3E:112:GLY:CA   | 53:3J:14:TYR:HB2   | 2.48                     | 0.43              |
| 46:3O:276:GLN:HG2  | 46:3O:281:ALA:HB2  | 1.98                     | 0.43              |
| 55:4A:471:ILE:HG13 | 55:4A:472:ILE:N    | 2.33                     | 0.43              |
| 56:4B:62:GLU:CA    | 56:4B:65:TRP:CZ2   | 3.00                     | 0.43              |
| 65:4K:44:PRO:HB3   | 65:4K:48:VAL:CG2   | 2.47                     | 0.43              |
| 55:8A:440:TYR:CZ   | 56:8B:205:SER:HA   | 2.54                     | 0.43              |
| 87:8B:301:PGV:O14  | 87:8B:301:PGV:O05  | 2.27                     | 0.43              |
| 57:8C:90:GLU:HB2   | 57:8C:244:PHE:CZ   | 2.53                     | 0.43              |
| 58:8D:40:LEU:HD21  | 58:8D:59:LEU:CD2   | 2.48                     | 0.43              |
| 58:8D:42:GLU:O     | 58:8D:45:LYS:HG2   | 2.17                     | 0.43              |
| 58:8D:64:PHE:CE2   | 59:8E:66:ARG:HD3   | 2.53                     | 0.43              |
| 66:8L:39:ILE:HD12  | 66:8L:39:ILE:H     | 1.83                     | 0.43              |
| 1:1A:70:ALA:HB2    | 10:1J:59:ILE:HG13  | 1.99                     | 0.43              |
| 2:1B:34:ASP:OD2    | 2:1B:171:LYS:HA    | 2.18                     | 0.43              |
| 70:1B:202:PC1:H3D1 | 8:1H:53:LEU:HG     | 2.00                     | 0.43              |
| 6:1F:147:SER:O     | 6:1F:151:VAL:HG12  | 2.19                     | 0.43              |
| 7:1G:190:MET:HE1   | 7:1G:690:ALA:O     | 2.19                     | 0.43              |
| 7:1G:314:ASP:O     | 7:1G:520:LYS:N     | 2.49                     | 0.43              |
| 8:1H:103:LEU:HD23  | 8:1H:103:LEU:HA    | 1.88                     | 0.43              |
| 10:1J:21:SER:O     | 10:1J:23:LYS:NZ    | 2.51                     | 0.43              |
| 12:1L:152:PHE:CD1  | 12:1L:168:ALA:HB1  | 2.53                     | 0.43              |
| 12:1L:558:LEU:HB3  | 13:1M:214:LEU:HD21 | 2.00                     | 0.43              |
| 13:1M:269:MET:SD   | 13:1M:399:ASN:ND2  | 2.91                     | 0.43              |
| 13:1M:318:ALA:HB2  | 13:1M:373:ILE:HG13 | 2.00                     | 0.43              |
| 14:1N:143:CYS:HB3  | 14:1N:198:THR:CG2  | 2.48                     | 0.43              |
| 14:1N:170:LEU:O    | 14:1N:295:ARG:NH2  | 2.49                     | 0.43              |
| 20:1T:30:LEU:HA    | 20:1T:40:LEU:HD21  | 2.00                     | 0.43              |
| 22:1W:29:LYS:HB3   | 22:1W:29:LYS:NZ    | 2.27                     | 0.43              |
| 29:1d:11:LEU:HA    | 70:1d:202:PC1:H12  | 1.99                     | 0.43              |
| 32:1g:26:LEU:HD12  | 32:1g:26:LEU:HA    | 1.75                     | 0.43              |
| 35:1j:35:TRP:CH2   | 35:1j:39:ARG:HD3   | 2.54                     | 0.43              |
| 46:3B:137:VAL:HG12 | 46:3B:141:GLN:HE21 | 1.84                     | 0.43              |
| 47:3C:152:ALA:HB2  | 47:3C:287:LYS:HE3  | 2.00                     | 0.43              |
| 49:3E:150:SER:HB3  | 49:3E:170:ARG:HG3  | 1.99                     | 0.43              |
| 49:3E:181:LYS:HA   | 49:3E:184:ILE:HB   | 1.99                     | 0.43              |
| 49:3E:263:TYR:HB3  | 49:3E:273:VAL:HG22 | 1.99                     | 0.43              |
| 47:3P:215:MET:O    | 51:3T:10:MET:HE1   | 2.19                     | 0.43              |
| 47:3P:223:TYR:HB3  | 48:3Q:227:TRP:CZ2  | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:86:MET:HE3   | 55:4A:185:VAL:HG23 | 2.01                     | 0.43              |
| 55:4A:219:PHE:HE2  | 57:4C:199:VAL:HG21 | 1.83                     | 0.43              |
| 56:4B:28:LEU:HG    | 56:4B:32:PHE:CE2   | 2.52                     | 0.43              |
| 58:4D:23:PRO:HG3   | 59:4E:37:VAL:HG21  | 2.00                     | 0.43              |
| 64:4J:36:MET:HG2   | 87:4J:101:PGV:C18  | 2.49                     | 0.43              |
| 55:8A:100:MET:N    | 57:8C:17:PRO:HB3   | 2.34                     | 0.43              |
| 56:8B:146:MET:HE1  | 56:8B:189:PRO:HD3  | 1.99                     | 0.43              |
| 92:8B:305:PSC:H02  | 92:8B:305:PSC:H21  | 1.45                     | 0.43              |
| 75:8D:201:CDL:H562 | 75:8D:201:CDL:H191 | 2.00                     | 0.43              |
| 68:8N:57:LEU:HD23  | 68:8N:57:LEU:HA    | 1.85                     | 0.43              |
| 4:1D:379:VAL:HB    | 4:1D:388:ARG:HB3   | 1.99                     | 0.43              |
| 6:1F:56:ILE:HG23   | 6:1F:235:CYS:SG    | 2.58                     | 0.43              |
| 6:1F:133:ALA:HA    | 6:1F:174:ASP:O     | 2.17                     | 0.43              |
| 7:1G:174:THR:HG22  | 7:1G:183:VAL:HG22  | 1.99                     | 0.43              |
| 7:1G:668:ILE:HD12  | 7:1G:668:ILE:HA    | 1.89                     | 0.43              |
| 12:1L:51:LEU:HD22  | 12:1L:91:PRO:HG2   | 2.00                     | 0.43              |
| 12:1L:510:TYR:HE2  | 64:4J:29:ASN:HD21  | 1.66                     | 0.43              |
| 12:1L:548:SER:HA   | 12:1L:552:LEU:HB3  | 1.99                     | 0.43              |
| 14:1N:1:FME:CN     | 15:1O:258:ARG:NH1  | 2.76                     | 0.43              |
| 15:1O:83:TYR:HB2   | 15:1O:190:HIS:HB3  | 1.99                     | 0.43              |
| 15:1O:145:ARG:O    | 15:1O:149:VAL:HG13 | 2.19                     | 0.43              |
| 20:1T:64:ASP:CG    | 22:1W:37:ARG:HH22  | 2.26                     | 0.43              |
| 28:1c:43:LYS:NZ    | 28:1c:49:GLU:OE2   | 2.52                     | 0.43              |
| 30:1e:4:ASP:OD1    | 30:1e:4:ASP:O      | 2.37                     | 0.43              |
| 34:1i:83:TYR:CD1   | 34:1i:87:TYR:HD2   | 2.36                     | 0.43              |
| 35:1j:35:TRP:O     | 35:1j:39:ARG:HG2   | 2.17                     | 0.43              |
| 39:1n:54:LYS:HD3   | 39:1n:54:LYS:HA    | 1.63                     | 0.43              |
| 46:3B:33:LEU:HD12  | 46:3B:204:MET:O    | 2.18                     | 0.43              |
| 50:3F:84:GLN:HB2   | 75:3G:103:CDL:HA22 | 2.00                     | 0.43              |
| 45:3N:283:THR:HA   | 46:3O:143:GLN:NE2  | 2.32                     | 0.43              |
| 46:3O:163:LEU:HD11 | 46:3O:258:VAL:HG22 | 1.99                     | 0.43              |
| 48:3Q:27:ARG:NH2   | 48:3Q:60:GLU:OE1   | 2.48                     | 0.43              |
| 49:3R:143:SER:OG   | 49:3R:145:ASP:OD1  | 2.35                     | 0.43              |
| 49:3R:207:LYS:NZ   | 49:3R:209:GLU:OE1  | 2.50                     | 0.43              |
| 55:4A:53:ILE:O     | 55:4A:56:VAL:HG22  | 2.18                     | 0.43              |
| 55:4A:319:LYS:HE2  | 55:4A:319:LYS:HB3  | 1.81                     | 0.43              |
| 56:4B:62:GLU:CB    | 56:4B:65:TRP:CE2   | 3.02                     | 0.43              |
| 75:4B:303:CDL:H811 | 75:4B:303:CDL:H262 | 2.01                     | 0.43              |
| 59:4E:31:LYS:CE    | 60:4F:83:PRO:O     | 2.65                     | 0.43              |
| 55:8A:115:SER:HB2  | 55:8A:145:LEU:HB2  | 2.00                     | 0.43              |
| 55:8A:354:THR:HG22 | 55:8A:376:HIS:HB2  | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:8A:602:PGV:H31  | 65:8K:9:PHE:HE2    | 1.82                     | 0.43              |
| 56:8B:105:TYR:HB2  | 56:8B:120:SER:O    | 2.18                     | 0.43              |
| 57:8C:15:PRO:O     | 57:8C:19:THR:OG1   | 2.32                     | 0.43              |
| 59:8E:104:LEU:HB3  | 59:8E:106:LEU:CD2  | 2.48                     | 0.43              |
| 63:8I:35:TYR:O     | 63:8I:35:TYR:HD1   | 2.02                     | 0.43              |
| 3:1C:114:LEU:HD12  | 22:1W:77:ARG:HB2   | 1.99                     | 0.43              |
| 5:1E:104:THR:O     | 5:1E:104:THR:OG1   | 2.37                     | 0.43              |
| 7:1G:324:ASP:CB    | 7:1G:571:ALA:HB1   | 2.48                     | 0.43              |
| 8:1H:96:ILE:CG2    | 8:1H:98:MET:HE3    | 2.49                     | 0.43              |
| 8:1H:169:GLN:CG    | 8:1H:174:MET:HG3   | 2.46                     | 0.43              |
| 16:1P:145:TYR:O    | 16:1P:149:LYS:HG3  | 2.19                     | 0.43              |
| 20:1T:52:MET:CE    | 22:1W:40:TYR:CD2   | 3.01                     | 0.43              |
| 20:1U:49:GLU:HB3   | 36:1k:44:TRP:HE1   | 1.83                     | 0.43              |
| 41:1p:76:CYS:SG    | 41:1p:84:MET:HG2   | 2.58                     | 0.43              |
| 42:1q:32:ASP:OD1   | 42:1q:32:ASP:C     | 2.62                     | 0.43              |
| 45:3A:411:CYS:O    | 45:3A:415:PHE:HB2  | 2.18                     | 0.43              |
| 45:3N:436:ARG:HD3  | 47:3P:222:PRO:HD3  | 2.01                     | 0.43              |
| 69:3N:503:3PE:H2   | 69:3N:503:3PE:H221 | 1.37                     | 0.43              |
| 55:4A:279:SER:HB3  | 68:4N:22:ILE:HG13  | 1.99                     | 0.43              |
| 55:4A:356:ILE:HD12 | 56:4B:73:LEU:HD11  | 1.99                     | 0.43              |
| 55:4A:377:PHE:O    | 55:4A:381:LEU:HB2  | 2.18                     | 0.43              |
| 55:4A:425:PHE:HA   | 55:4A:428:GLN:HG3  | 2.01                     | 0.43              |
| 57:4C:62:ILE:HG13  | 87:4C:306:PGV:H21  | 2.00                     | 0.43              |
| 59:4E:29:LEU:HD23  | 59:4E:29:LEU:C     | 2.44                     | 0.43              |
| 62:4H:14:ALA:HB3   | 62:4H:63:PHE:CE1   | 2.53                     | 0.43              |
| 63:4I:59:ASP:OD1   | 63:4I:59:ASP:C     | 2.61                     | 0.43              |
| 64:4J:21:HIS:O     | 64:4J:22:LEU:HD12  | 2.18                     | 0.43              |
| 55:8A:66:ILE:HD13  | 55:8A:126:TRP:CZ2  | 2.54                     | 0.43              |
| 55:8A:254:ILE:HD11 | 55:8A:388:ALA:CB   | 2.48                     | 0.43              |
| 56:8B:61:VAL:HG12  | 56:8B:65:TRP:CZ3   | 2.54                     | 0.43              |
| 56:8B:110:TYR:HB2  | 56:8B:116:LEU:HB3  | 2.00                     | 0.43              |
| 59:8E:33:MET:HE1   | 59:8E:67:ILE:CB    | 2.48                     | 0.43              |
| 60:8F:55:LYS:HG3   | 60:8F:73:TRP:CZ3   | 2.53                     | 0.43              |
| 4:1D:50:ASN:HB2    | 4:1D:65:VAL:HG22   | 2.00                     | 0.43              |
| 4:1D:247:ALA:HA    | 4:1D:265:ILE:HD11  | 2.01                     | 0.43              |
| 7:1G:196:SER:OG    | 7:1G:265:ASP:OD2   | 2.29                     | 0.43              |
| 8:1H:230:ASN:O     | 8:1H:234:MET:HG2   | 2.18                     | 0.43              |
| 10:1J:20:PHE:CE1   | 11:1K:32:CYS:HA    | 2.45                     | 0.43              |
| 10:1J:173:ARG:NH1  | 15:1O:254:ARG:NH1  | 2.66                     | 0.43              |
| 11:1K:3:LEU:CD2    | 11:1K:6:MET:SD     | 3.06                     | 0.43              |
| 12:1L:161:ARG:NH1  | 12:1L:238:GLU:OE1  | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:1M:401:MET:O    | 13:1M:405:LEU:HG   | 2.19                     | 0.43              |
| 14:1N:226:THR:HG23 | 14:1N:229:SER:H    | 1.83                     | 0.43              |
| 20:1T:22:TYR:CE2   | 20:1T:24:LYS:HB2   | 2.53                     | 0.43              |
| 25:1Z:141:ILE:H    | 25:1Z:141:ILE:HG12 | 1.63                     | 0.43              |
| 30:1e:29:PRO:HB3   | 33:1h:138:LYS:HG3  | 2.00                     | 0.43              |
| 32:1g:93:ALA:O     | 32:1g:97:VAL:HG22  | 2.18                     | 0.43              |
| 37:1l:32:GLU:OE1   | 37:1l:32:GLU:N     | 2.51                     | 0.43              |
| 45:3N:50:GLU:H     | 45:3N:50:GLU:CD    | 2.26                     | 0.43              |
| 46:3O:350:GLY:HA2  | 46:3O:411:ILE:HD13 | 2.00                     | 0.43              |
| 57:4C:206:LEU:HD23 | 57:4C:206:LEU:HA   | 1.85                     | 0.43              |
| 60:4F:29:ASP:OD1   | 60:4F:32:ASN:N     | 2.52                     | 0.43              |
| 66:4L:21:LEU:HD12  | 66:4L:21:LEU:O     | 2.18                     | 0.43              |
| 66:4L:36:PRO:O     | 66:4L:40:VAL:HG13  | 2.19                     | 0.43              |
| 55:8A:340:TRP:HH2  | 55:8A:417:MET:HG2  | 1.84                     | 0.43              |
| 57:8C:156:ARG:HB3  | 60:8F:5:GLY:HA3    | 1.99                     | 0.43              |
| 57:8C:187:THR:HA   | 93:8C:308:PEK:O12  | 2.19                     | 0.43              |
| 58:8D:37:GLN:HG3   | 58:8D:37:GLN:H     | 1.61                     | 0.43              |
| 64:8J:38:LEU:HD12  | 64:8J:38:LEU:HA    | 1.90                     | 0.43              |
| 65:8K:24:PHE:CD1   | 65:8K:24:PHE:C     | 2.96                     | 0.43              |
| 1:1A:41:PHE:CZ     | 2:1B:99:ALA:HB2    | 2.54                     | 0.43              |
| 6:1F:112:ARG:HB3   | 6:1F:145:GLU:HG3   | 2.01                     | 0.43              |
| 7:1G:40:PHE:HB2    | 7:1G:52:CYS:SG     | 2.58                     | 0.43              |
| 7:1G:299:ALA:O     | 7:1G:303:VAL:HG23  | 2.18                     | 0.43              |
| 10:1J:61:LEU:HA    | 10:1J:61:LEU:HD12  | 1.80                     | 0.43              |
| 12:1L:15:LEU:HB3   | 12:1L:126:ILE:HG12 | 2.01                     | 0.43              |
| 12:1L:361:GLY:HA2  | 36:1k:59:ASN:HD21  | 1.84                     | 0.43              |
| 15:1O:52:PRO:O     | 15:1O:107:GLN:NE2  | 2.43                     | 0.43              |
| 16:1P:315:ILE:HG13 | 16:1P:322:ARG:HH12 | 1.84                     | 0.43              |
| 70:1P:401:PC1:H222 | 70:1P:401:PC1:H152 | 2.01                     | 0.43              |
| 20:1U:18:VAL:HG21  | 20:1U:57:GLU:OE1   | 2.18                     | 0.43              |
| 21:1V:25:ILE:HG13  | 21:1V:26:LEU:N     | 2.33                     | 0.43              |
| 24:1Y:34:ILE:HD12  | 69:1Y:205:3PE:H372 | 2.01                     | 0.43              |
| 70:1d:202:PC1:H2   | 70:1d:202:PC1:H222 | 1.50                     | 0.43              |
| 30:1e:68:ARG:O     | 30:1e:72:MET:HG2   | 2.18                     | 0.43              |
| 35:1j:69:ASP:HB3   | 40:1o:117:ARG:NH2  | 2.33                     | 0.43              |
| 38:1m:3:PRO:HD2    | 39:1n:72:TYR:CE1   | 2.54                     | 0.43              |
| 39:1n:156:ALA:HB1  | 39:1n:161:ASP:OD1  | 2.18                     | 0.43              |
| 46:3B:309:VAL:HG23 | 46:3B:326:THR:HG22 | 2.01                     | 0.43              |
| 50:3F:114:LYS:O    | 50:3F:118:GLU:HG2  | 2.18                     | 0.43              |
| 87:4G:101:PGV:H21  | 87:4G:101:PGV:H02  | 1.52                     | 0.43              |
| 55:8A:233:HIS:HB3  | 57:8C:99:TRP:CZ2   | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:8A:347:LEU:HD21 | 55:8A:418:PHE:HE2  | 1.84                     | 0.43              |
| 55:8A:406:ASN:HB3  | 55:8A:471:ILE:HD11 | 2.01                     | 0.43              |
| 57:8C:98:PHE:CE2   | 87:8C:304:PGV:H182 | 2.54                     | 0.43              |
| 57:8C:165:ILE:HD12 | 93:8G:102:PEK:H11  | 1.99                     | 0.43              |
| 65:8K:8:ASP:O      | 65:8K:12:LYS:HD2   | 2.19                     | 0.43              |
| 4:1D:111:MET:SD    | 4:1D:111:MET:N     | 2.92                     | 0.43              |
| 7:1G:150:MET:HE2   | 7:1G:183:VAL:O     | 2.19                     | 0.43              |
| 10:1J:124:ASP:OD1  | 11:1K:4:VAL:HG22   | 2.19                     | 0.43              |
| 12:1L:73:THR:HG22  | 12:1L:194:ASN:ND2  | 2.13                     | 0.43              |
| 12:1L:140:LEU:HD23 | 12:1L:140:LEU:C    | 2.43                     | 0.43              |
| 12:1L:172:ILE:HG21 | 13:1M:408:LEU:HD12 | 1.99                     | 0.43              |
| 12:1L:331:MET:HG3  | 12:1L:391:SER:HB3  | 2.01                     | 0.43              |
| 13:1M:167:ILE:HG12 | 13:1M:195:MET:HE3  | 2.01                     | 0.43              |
| 14:1N:249:LEU:HD23 | 14:1N:294:MET:HE1  | 2.00                     | 0.43              |
| 17:1Q:60:ASP:OD2   | 17:1Q:62:ARG:NH1   | 2.51                     | 0.43              |
| 19:1S:91:GLU:O     | 19:1S:95:SER:HB3   | 2.18                     | 0.43              |
| 22:1W:54:ILE:HD13  | 22:1W:107:PHE:CE2  | 2.54                     | 0.43              |
| 25:1Z:98:MET:HE3   | 25:1Z:104:TRP:CH2  | 2.54                     | 0.43              |
| 25:1Z:113:THR:HG21 | 30:1e:35:PHE:HE1   | 1.84                     | 0.43              |
| 40:1o:47:ASP:OD1   | 40:1o:47:ASP:C     | 2.62                     | 0.43              |
| 40:1o:55:ARG:NH2   | 41:1p:119:SER:HB3  | 2.30                     | 0.43              |
| 41:1p:158:GLN:C    | 41:1p:162:MET:HE3  | 2.44                     | 0.43              |
| 44:1s:33:PHE:O     | 44:1s:33:PHE:CD1   | 2.72                     | 0.43              |
| 45:3A:328:ASN:HB3  | 45:3A:427:PRO:HB2  | 2.00                     | 0.43              |
| 48:3D:222:TYR:HH   | 48:3D:249:MET:HB3  | 1.84                     | 0.43              |
| 45:3N:142:ASP:OD2  | 49:3R:79:SER:N     | 2.52                     | 0.43              |
| 47:3P:229:ILE:CG2  | 70:3R:303:PC1:H371 | 2.49                     | 0.43              |
| 50:3S:35:ASP:OD2   | 50:3S:61:ARG:NH1   | 2.51                     | 0.43              |
| 56:4B:28:LEU:HD11  | 75:4B:303:CDL:H592 | 2.01                     | 0.43              |
| 56:4B:68:LEU:HG    | 92:4B:305:PSC:H183 | 2.00                     | 0.43              |
| 65:4K:41:ASN:OD1   | 65:4K:41:ASN:O     | 2.37                     | 0.43              |
| 56:8B:83:ILE:O     | 56:8B:87:MET:HG3   | 2.19                     | 0.43              |
| 57:8C:157:LYS:NZ   | 87:8C:302:PGV:H02  | 2.34                     | 0.43              |
| 64:8J:31:LEU:O     | 64:8J:35:THR:OG1   | 2.37                     | 0.43              |
| 64:8J:36:MET:O     | 64:8J:39:CYS:SG    | 2.68                     | 0.43              |
| 1:1A:39:CYS:O      | 4:1D:53:PRO:HD2    | 2.19                     | 0.43              |
| 1:1A:53:MET:HE3    | 10:1J:172:THR:HG23 | 2.01                     | 0.43              |
| 4:1D:208:LEU:HD22  | 4:1D:315:LEU:HD23  | 1.99                     | 0.43              |
| 6:1F:16:LYS:HB2    | 6:1F:16:LYS:HE2    | 1.79                     | 0.43              |
| 6:1F:110:ILE:CD1   | 6:1F:114:ASP:HB2   | 2.48                     | 0.43              |
| 6:1F:137:TYR:HB3   | 6:1F:192:LEU:HD11  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:9:ILE:HG13    | 7:1G:75:LYS:HD2    | 2.00                     | 0.43              |
| 7:1G:394:ARG:HD3   | 7:1G:394:ARG:HA    | 1.89                     | 0.43              |
| 12:1L:90:ILE:HB    | 12:1L:91:PRO:HD3   | 2.01                     | 0.43              |
| 13:1M:318:ALA:HB1  | 13:1M:374:ASN:CG   | 2.43                     | 0.43              |
| 33:1h:110:VAL:HG12 | 33:1h:114:MET:HE2  | 1.99                     | 0.43              |
| 35:1j:61:ASP:N     | 35:1j:61:ASP:OD1   | 2.52                     | 0.43              |
| 36:1k:27:PRO:HG2   | 36:1k:52:TYR:CE2   | 2.54                     | 0.43              |
| 47:3P:63:PHE:O     | 47:3P:67:THR:HG23  | 2.19                     | 0.43              |
| 48:3Q:203:ARG:NH2  | 53:3W:53:LYS:HZ2   | 2.16                     | 0.43              |
| 55:4A:3:VAL:HG22   | 55:4A:7:LEU:HD22   | 2.00                     | 0.43              |
| 55:4A:69:MET:HG2   | 55:4A:70:VAL:N     | 2.34                     | 0.43              |
| 57:4C:148:HIS:HA   | 57:4C:235:PHE:HE2  | 1.84                     | 0.43              |
| 57:4C:151:LEU:CG   | 57:4C:159:MET:SD   | 3.06                     | 0.43              |
| 93:4C:307:PEK:H42  | 93:4C:307:PEK:H72  | 1.89                     | 0.43              |
| 58:4D:141:ASP:OD1  | 58:4D:141:ASP:C    | 2.61                     | 0.43              |
| 55:8A:96:ARG:NH2   | 57:8C:61:ILE:HG13  | 2.34                     | 0.43              |
| 55:8A:309:THR:HG23 | 55:8A:359:ALA:HB1  | 2.01                     | 0.43              |
| 75:8B:303:CDL:H141 | 75:8B:303:CDL:H631 | 2.00                     | 0.43              |
| 57:8C:150:SER:HB3  | 57:8C:155:ASP:HB3  | 2.01                     | 0.43              |
| 57:8C:172:TYR:CE2  | 93:8G:102:PEK:H181 | 2.53                     | 0.43              |
| 59:8E:52:LEU:HD21  | 59:8E:68:LEU:CD1   | 2.48                     | 0.43              |
| 60:8F:13:ALA:O     | 60:8F:18:ARG:CZ    | 2.67                     | 0.43              |
| 64:8J:36:MET:HE2   | 64:8J:39:CYS:SG    | 2.59                     | 0.43              |
| 1:1A:90:MET:HA     | 1:1A:90:MET:CE     | 2.41                     | 0.42              |
| 4:1D:170:MET:HE2   | 4:1D:225:LEU:HD22  | 2.00                     | 0.42              |
| 6:1F:194:GLU:OE2   | 17:1Q:133:LYS:HD3  | 2.19                     | 0.42              |
| 6:1F:394:GLU:OE2   | 43:1r:50:ASN:N     | 2.39                     | 0.42              |
| 8:1H:66:SER:HA     | 8:1H:122:ALA:O     | 2.19                     | 0.42              |
| 8:1H:96:ILE:HG23   | 25:1Z:144:THR:HB   | 2.01                     | 0.42              |
| 10:1J:126:VAL:O    | 25:1Z:120:MET:HE3  | 2.19                     | 0.42              |
| 13:1M:122:PHE:HE1  | 13:1M:206:LYS:HD3  | 1.84                     | 0.42              |
| 13:1M:270:ILE:HD11 | 13:1M:395:LEU:O    | 2.19                     | 0.42              |
| 30:1e:85:LEU:HB3   | 30:1e:91:TYR:HB2   | 2.01                     | 0.42              |
| 32:1g:83:TYR:CE2   | 32:1g:84:ARG:HG3   | 2.54                     | 0.42              |
| 34:1i:83:TYR:CE1   | 41:1p:48:ARG:HD3   | 2.54                     | 0.42              |
| 48:3D:115:ARG:HB2  | 48:3D:143:CYS:HB2  | 2.01                     | 0.42              |
| 46:3O:307:PHE:CD2  | 49:3V:52:ARG:HD2   | 2.53                     | 0.42              |
| 54:3Y:23:MET:O     | 54:3Y:27:VAL:HG23  | 2.18                     | 0.42              |
| 55:4A:110:LEU:HB2  | 87:4A:601:PGV:H181 | 2.01                     | 0.42              |
| 55:4A:168:ILE:HD13 | 55:4A:189:LEU:HB2  | 2.01                     | 0.42              |
| 55:4A:278:MET:HB3  | 87:4A:603:PGV:H11  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:40:TYR:O     | 56:4B:40:TYR:CD1   | 2.72                     | 0.42              |
| 56:4B:102:HIS:O    | 56:4B:207:MET:CE   | 2.67                     | 0.42              |
| 59:4E:18:TYR:HD1   | 59:4E:19:PHE:CD1   | 2.36                     | 0.42              |
| 62:4H:4:ILE:HD13   | 62:4H:7:LYS:HE2    | 2.00                     | 0.42              |
| 55:8A:124:THR:OG1  | 55:8A:132:LEU:HD23 | 2.19                     | 0.42              |
| 55:8A:246:LEU:HD13 | 55:8A:381:LEU:HD21 | 2.01                     | 0.42              |
| 56:8B:103:GLN:HA   | 56:8B:104:TRP:HA   | 1.80                     | 0.42              |
| 56:8B:162:SER:HB2  | 56:8B:198:GLU:HB2  | 2.00                     | 0.42              |
| 58:8D:52:SER:O     | 58:8D:56:LYS:HG3   | 2.18                     | 0.42              |
| 58:8D:99:GLU:OE2   | 58:8D:104:TYR:CZ   | 2.68                     | 0.42              |
| 59:8E:37:VAL:HG11  | 59:8E:70:VAL:HG21  | 2.00                     | 0.42              |
| 1:1A:38:GLU:O      | 4:1D:51:PHE:HD2    | 2.02                     | 0.42              |
| 2:1B:94:ASN:HB3    | 3:1C:174:LEU:HD22  | 2.01                     | 0.42              |
| 6:1F:96:ASN:HD22   | 73:1F:501:FMN:C2   | 2.31                     | 0.42              |
| 6:1F:418:LEU:HD12  | 6:1F:422:PHE:HB2   | 2.01                     | 0.42              |
| 7:1G:328:LEU:O     | 7:1G:507:TYR:OH    | 2.35                     | 0.42              |
| 7:1G:364:LEU:HB3   | 7:1G:577:GLU:HA    | 2.02                     | 0.42              |
| 7:1G:377:ILE:HG12  | 7:1G:450:MET:HB3   | 2.01                     | 0.42              |
| 7:1G:510:GLY:HA3   | 7:1G:512:GLU:OE2   | 2.18                     | 0.42              |
| 10:1J:33:LEU:HD23  | 10:1J:65:LEU:HD21  | 2.00                     | 0.42              |
| 10:1J:60:TYR:CD1   | 11:1K:64:LEU:HD11  | 2.54                     | 0.42              |
| 12:1L:243:VAL:HG13 | 12:1L:247:LEU:HD13 | 2.01                     | 0.42              |
| 15:1O:37:ARG:NE    | 15:1O:37:ARG:HA    | 2.34                     | 0.42              |
| 16:1P:172:PHE:HB2  | 16:1P:179:LEU:HD21 | 2.00                     | 0.42              |
| 23:1X:36:ASP:OD1   | 23:1X:36:ASP:C     | 2.62                     | 0.42              |
| 35:1j:61:ASP:HB3   | 35:1j:66:ILE:HB    | 2.01                     | 0.42              |
| 38:1m:29:ARG:HB3   | 39:1n:8:TYR:OH     | 2.19                     | 0.42              |
| 39:1n:43:MET:HE2   | 39:1n:43:MET:HB2   | 1.93                     | 0.42              |
| 46:3B:74:SER:O     | 46:3B:74:SER:OG    | 2.32                     | 0.42              |
| 47:3C:10:LEU:O     | 47:3C:14:ILE:HG12  | 2.19                     | 0.42              |
| 48:3D:297:MET:HA   | 69:3D:502:3PE:H321 | 2.00                     | 0.42              |
| 47:3P:124:MET:HE1  | 47:3P:298:ILE:HD11 | 2.01                     | 0.42              |
| 55:4A:485:VAL:HG12 | 67:4M:1:ILE:HD12   | 2.01                     | 0.42              |
| 56:4B:16:ILE:HG12  | 56:4B:87:MET:HG2   | 1.99                     | 0.42              |
| 55:8A:69:MET:HE1   | 88:8A:604:HEA:C18  | 2.49                     | 0.42              |
| 55:8A:271:MET:HA   | 55:8A:274:VAL:HG22 | 2.01                     | 0.42              |
| 60:8F:93:SER:O     | 60:8F:94:HIS:HB3   | 2.19                     | 0.42              |
| 3:1C:168:LEU:HD21  | 4:1D:90:LEU:HD23   | 2.00                     | 0.42              |
| 5:1E:22:ASP:OD1    | 5:1E:68:LYS:NZ     | 2.42                     | 0.42              |
| 5:1E:76:PRO:HA     | 5:1E:77:PRO:HD3    | 1.93                     | 0.42              |
| 6:1F:184:TYR:CE1   | 73:1F:501:FMN:H6   | 2.53                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:180:PRO:HB3   | 70:1H:402:PC1:H381 | 2.01                     | 0.42              |
| 9:1I:29:GLU:HG2    | 9:1I:30:LEU:N      | 2.33                     | 0.42              |
| 12:1L:291:CYS:SG   | 12:1L:526:LEU:HA   | 2.59                     | 0.42              |
| 12:1L:555:LEU:HD13 | 38:1m:75:ILE:HD13  | 2.01                     | 0.42              |
| 13:1M:54:LEU:HD11  | 33:1h:96:ILE:HD11  | 2.01                     | 0.42              |
| 13:1M:71:TRP:CD1   | 70:1M:505:PC1:H2C2 | 2.54                     | 0.42              |
| 69:1M:506:3PE:H271 | 69:1M:506:3PE:H2B2 | 2.00                     | 0.42              |
| 14:1N:78:LEU:HD12  | 14:1N:82:GLY:HA2   | 2.01                     | 0.42              |
| 16:1P:196:LEU:O    | 16:1P:239:PHE:HB2  | 2.20                     | 0.42              |
| 19:1S:52:ILE:HD12  | 19:1S:52:ILE:N     | 2.32                     | 0.42              |
| 29:1d:12:GLN:HG2   | 69:1d:201:3PE:H111 | 2.01                     | 0.42              |
| 30:1e:68:ARG:HB3   | 30:1e:71:THR:HB    | 2.00                     | 0.42              |
| 32:1g:55:LEU:HD12  | 32:1g:58:MET:HE3   | 2.01                     | 0.42              |
| 43:1r:100:ILE:HD12 | 43:1r:100:ILE:HA   | 1.92                     | 0.42              |
| 45:3A:30:SER:HB2   | 45:3A:32:GLN:HG3   | 2.00                     | 0.42              |
| 45:3A:78:GLU:OE1   | 45:3A:108:LYS:NZ   | 2.53                     | 0.42              |
| 49:3E:225:ILE:HG12 | 49:3E:237:PRO:HD3  | 2.00                     | 0.42              |
| 53:3J:8:THR:HG23   | 53:3J:11:ALA:H     | 1.85                     | 0.42              |
| 45:3N:270:LEU:HD13 | 45:3N:320:LEU:HD22 | 2.00                     | 0.42              |
| 69:3N:503:3PE:H322 | 70:3R:303:PC1:H31  | 2.02                     | 0.42              |
| 46:3O:109:VAL:HG22 | 46:3O:123:LEU:HD22 | 2.02                     | 0.42              |
| 49:3R:150:SER:CB   | 49:3R:170:ARG:H    | 2.27                     | 0.42              |
| 55:4A:271:MET:HG3  | 68:4N:12:HIS:CD2   | 2.53                     | 0.42              |
| 56:4B:61:VAL:HG13  | 92:4B:305:PSC:H271 | 2.01                     | 0.42              |
| 92:4B:305:PSC:H252 | 92:4B:305:PSC:H302 | 2.00                     | 0.42              |
| 87:4C:302:PGV:H011 | 87:4C:302:PGV:H202 | 1.24                     | 0.42              |
| 60:4F:10:GLU:OE1   | 60:4F:11:GLU:OE2   | 2.37                     | 0.42              |
| 55:8A:5:ARG:HD2    | 66:8L:3:TYR:CE2    | 2.54                     | 0.42              |
| 55:8A:65:MET:HB3   | 88:8A:604:HEA:HBC1 | 2.01                     | 0.42              |
| 55:8A:509:THR:HG22 | 60:8F:57:ILE:HB    | 2.02                     | 0.42              |
| 87:8C:305:PGV:H21  | 87:8C:305:PGV:H222 | 2.00                     | 0.42              |
| 58:8D:103:VAL:HG13 | 67:8M:34:LEU:O     | 2.19                     | 0.42              |
| 75:8D:201:CDL:H402 | 75:8D:201:CDL:H592 | 2.02                     | 0.42              |
| 61:8G:32:THR:OG1   | 87:8G:101:PGV:H301 | 2.19                     | 0.42              |
| 2:1B:77:ARG:HA     | 2:1B:77:ARG:HD2    | 1.66                     | 0.42              |
| 70:1B:203:PC1:O14  | 70:1B:203:PC1:H121 | 2.20                     | 0.42              |
| 4:1D:100:LEU:HD13  | 4:1D:196:PRO:HD3   | 2.00                     | 0.42              |
| 4:1D:342:MET:HB2   | 7:1G:134:LYS:NZ    | 2.34                     | 0.42              |
| 7:1G:186:TYR:CD2   | 7:1G:187:ILE:HG23  | 2.54                     | 0.42              |
| 7:1G:643:GLN:O     | 7:1G:647:GLU:HG2   | 2.19                     | 0.42              |
| 8:1H:19:PHE:CZ     | 70:1q:201:PC1:H2D1 | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:87:VAL:HG12   | 8:1H:95:LEU:HD23   | 2.02                     | 0.42              |
| 9:1I:74:GLU:HG2    | 18:1R:87:CYS:O     | 2.19                     | 0.42              |
| 12:1L:294:THR:O    | 12:1L:294:THR:OG1  | 2.36                     | 0.42              |
| 12:1L:575:ILE:HD13 | 14:1N:171:ASN:HD21 | 1.83                     | 0.42              |
| 13:1M:42:LEU:CB    | 13:1M:453:MET:HE3  | 2.49                     | 0.42              |
| 13:1M:71:TRP:HH2   | 13:1M:439:LEU:HD22 | 1.85                     | 0.42              |
| 14:1N:3:PRO:O      | 14:1N:7:THR:HG23   | 2.19                     | 0.42              |
| 15:1O:27:VAL:HG21  | 15:1O:39:ALA:HB2   | 2.02                     | 0.42              |
| 15:1O:138:MET:CE   | 76:1O:401:GTP:HN21 | 2.32                     | 0.42              |
| 16:1P:151:VAL:HG23 | 59:8E:9:GLU:OE1    | 2.18                     | 0.42              |
| 16:1P:315:ILE:HD12 | 16:1P:331:MET:HB3  | 2.01                     | 0.42              |
| 20:1U:40:LEU:HB3   | 20:1U:42:LEU:HD13  | 2.00                     | 0.42              |
| 22:1W:68:MET:HA    | 22:1W:68:MET:HE3   | 2.01                     | 0.42              |
| 27:1b:78:GLU:OE2   | 27:1b:82:ASN:OD1   | 2.38                     | 0.42              |
| 37:1l:134:PRO:HD2  | 37:1l:138:LEU:HD21 | 2.02                     | 0.42              |
| 38:1m:17:LEU:HD11  | 39:1n:71:TRP:HB2   | 2.01                     | 0.42              |
| 38:1m:82:THR:HG22  | 38:1m:85:THR:H     | 1.84                     | 0.42              |
| 45:3N:191:LYS:HE3  | 45:3N:191:LYS:HB3  | 1.87                     | 0.42              |
| 46:3O:54:GLY:O     | 46:3O:194:TYR:OH   | 2.37                     | 0.42              |
| 47:3P:185:LEU:HA   | 47:3P:185:LEU:HD23 | 1.82                     | 0.42              |
| 49:3R:152:ILE:O    | 49:3R:153:GLU:HG2  | 2.20                     | 0.42              |
| 55:4A:467:LEU:O    | 55:4A:471:ILE:HG23 | 2.19                     | 0.42              |
| 56:4B:56:MET:HE3   | 56:4B:56:MET:HB2   | 1.92                     | 0.42              |
| 57:4C:189:SER:O    | 61:4G:55:ILE:HD12  | 2.19                     | 0.42              |
| 55:8A:93:ALA:HA    | 55:8A:171:MET:SD   | 2.60                     | 0.42              |
| 55:8A:129:TYR:OH   | 55:8A:236:TRP:NE1  | 2.46                     | 0.42              |
| 55:8A:377:PHE:CD1  | 55:8A:377:PHE:C    | 2.98                     | 0.42              |
| 55:8A:415:VAL:HG22 | 75:8D:201:CDL:HB32 | 2.01                     | 0.42              |
| 55:8A:473:TRP:CG   | 66:8L:22:LEU:HD13  | 2.54                     | 0.42              |
| 56:8B:30:ILE:HG21  | 56:8B:76:ILE:HD11  | 2.02                     | 0.42              |
| 57:8C:146:TRP:CE2  | 61:8G:17:ARG:HB3   | 2.54                     | 0.42              |
| 57:8C:206:LEU:HD11 | 93:8C:308:PEK:H11  | 2.00                     | 0.42              |
| 93:8C:308:PEK:H42  | 93:8C:308:PEK:H72  | 1.88                     | 0.42              |
| 1:1A:53:MET:HE1    | 11:1K:79:VAL:CG1   | 2.50                     | 0.42              |
| 2:1B:129:SER:HB2   | 4:1D:90:LEU:HD11   | 2.01                     | 0.42              |
| 4:1D:47:LEU:O      | 4:1D:67:GLU:HA     | 2.20                     | 0.42              |
| 4:1D:112:MET:HG3   | 4:1D:181:TYR:CZ    | 2.54                     | 0.42              |
| 8:1H:107:ALA:HB1   | 10:1J:57:PHE:HB3   | 2.01                     | 0.42              |
| 11:1K:11:ALA:O     | 11:1K:14:ILE:HG13  | 2.18                     | 0.42              |
| 12:1L:295:GLN:O    | 12:1L:425:ARG:NH1  | 2.51                     | 0.42              |
| 12:1L:315:VAL:HG11 | 12:1L:412:THR:HG21 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:425:ARG:HA   | 12:1L:505:ASN:HD21 | 1.84                     | 0.42              |
| 12:1L:572:LYS:NZ   | 69:1Y:203:3PE:H351 | 2.34                     | 0.42              |
| 13:1M:164:LEU:O    | 13:1M:174:LEU:HD11 | 2.19                     | 0.42              |
| 13:1M:341:THR:HG22 | 13:1M:343:ILE:H    | 1.84                     | 0.42              |
| 20:1T:24:LYS:HA    | 20:1T:24:LYS:HD3   | 1.81                     | 0.42              |
| 70:1Y:207:PC1:H231 | 70:1Y:207:PC1:H122 | 2.02                     | 0.42              |
| 37:1l:117:TRP:O    | 37:1l:121:ILE:HG23 | 2.20                     | 0.42              |
| 48:3D:198:PRO:HA   | 48:3D:199:PRO:HD3  | 1.94                     | 0.42              |
| 46:3O:195:VAL:O    | 46:3O:199:PHE:HB2  | 2.19                     | 0.42              |
| 57:4C:121:ILE:HD11 | 61:4G:53:LEU:HD21  | 2.00                     | 0.42              |
| 57:4C:128:GLU:OE1  | 57:4C:128:GLU:N    | 2.53                     | 0.42              |
| 87:4C:303:PGV:H171 | 75:4C:305:CDL:H872 | 2.01                     | 0.42              |
| 59:4E:72:LYS:HA    | 59:4E:82:TYR:HD2   | 1.85                     | 0.42              |
| 59:4E:85:VAL:HG13  | 59:4E:86:ILE:HD13  | 2.00                     | 0.42              |
| 59:4E:91:PRO:O     | 59:4E:95:GLU:HG2   | 2.19                     | 0.42              |
| 55:8A:399:LEU:HB2  | 55:8A:494:TRP:CZ3  | 2.55                     | 0.42              |
| 56:8B:116:LEU:CD2  | 56:8B:226:MET:HE2  | 2.49                     | 0.42              |
| 87:8B:302:PGV:C20  | 87:8C:304:PGV:H62  | 2.49                     | 0.42              |
| 92:8B:305:PSC:H302 | 92:8B:305:PSC:H252 | 2.01                     | 0.42              |
| 87:8C:302:PGV:H012 | 87:8C:302:PGV:H21  | 2.01                     | 0.42              |
| 60:8F:21:MET:HB3   | 60:8F:22:MET:HE2   | 2.00                     | 0.42              |
| 62:8H:56:TYR:O     | 62:8H:60:TYR:HD1   | 2.02                     | 0.42              |
| 64:8J:34:VAL:O     | 64:8J:38:LEU:HB2   | 2.19                     | 0.42              |
| 6:1F:193:ILE:HG23  | 6:1F:215:VAL:HA    | 2.02                     | 0.42              |
| 10:1J:33:LEU:HD23  | 10:1J:65:LEU:HD11  | 2.01                     | 0.42              |
| 12:1L:142:ILE:HA   | 13:1M:370:PRO:HG2  | 2.01                     | 0.42              |
| 12:1L:197:ASP:OD2  | 41:1p:110:LYS:HD3  | 2.19                     | 0.42              |
| 12:1L:565:THR:HG23 | 70:1Y:207:PC1:H32  | 2.02                     | 0.42              |
| 13:1M:24:TRP:CE3   | 13:1M:81:GLN:HB3   | 2.54                     | 0.42              |
| 17:1Q:57:MET:HE3   | 17:1Q:86:PHE:CE1   | 2.54                     | 0.42              |
| 18:1R:39:PHE:O     | 18:1R:43:LEU:HG    | 2.20                     | 0.42              |
| 23:1X:53:ARG:HG3   | 23:1X:54:ARG:HG2   | 2.01                     | 0.42              |
| 24:1Y:103:ARG:HD2  | 24:1Y:103:ARG:HA   | 1.84                     | 0.42              |
| 29:1d:94:VAL:HG21  | 33:1h:106:LYS:HD2  | 2.02                     | 0.42              |
| 32:1g:114:ASP:OD1  | 32:1g:114:ASP:C    | 2.61                     | 0.42              |
| 35:1j:60:THR:C     | 35:1j:62:GLU:H     | 2.28                     | 0.42              |
| 45:3A:41:ILE:HG23  | 45:3A:195:MET:HG2  | 2.01                     | 0.42              |
| 45:3A:41:ILE:HG12  | 45:3A:195:MET:HG2  | 2.01                     | 0.42              |
| 49:3E:159:ILE:HD11 | 49:3E:165:MET:HB2  | 2.01                     | 0.42              |
| 49:3E:195:LEU:HD13 | 49:3E:249:ILE:O    | 2.20                     | 0.42              |
| 45:3N:303:LEU:HD23 | 45:3N:303:LEU:HA   | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:3P:128:PHE:CE1  | 47:3P:146:ILE:HD11 | 2.54                     | 0.42              |
| 47:3P:307:LEU:HD11 | 47:3P:363:LEU:HD23 | 2.01                     | 0.42              |
| 51:3T:51:PRO:O     | 51:3T:54:VAL:HG22  | 2.20                     | 0.42              |
| 55:4A:73:ILE:HD13  | 88:4A:604:HEA:H242 | 2.01                     | 0.42              |
| 55:4A:243:VAL:HG13 | 88:4A:605:HEA:C4C  | 2.50                     | 0.42              |
| 55:4A:462:LEU:O    | 55:4A:465:VAL:HG12 | 2.20                     | 0.42              |
| 57:4C:60:ASP:OD1   | 57:4C:60:ASP:N     | 2.53                     | 0.42              |
| 58:4D:68:PHE:CD1   | 59:4E:69:GLU:HB3   | 2.54                     | 0.42              |
| 62:4H:28:ASN:ND2   | 62:4H:63:PHE:HE2   | 2.18                     | 0.42              |
| 68:4N:35:ARG:NH2   | 68:4N:63:TYR:CE1   | 2.88                     | 0.42              |
| 55:8A:273:MET:HE3  | 55:8A:322:SER:HB2  | 2.00                     | 0.42              |
| 56:8B:59:GLN:HG2   | 68:8N:13:PRO:HD2   | 2.01                     | 0.42              |
| 56:8B:122:MET:SD   | 56:8B:135:LEU:HA   | 2.59                     | 0.42              |
| 57:8C:58:TRP:CD1   | 57:8C:61:ILE:HD12  | 2.54                     | 0.42              |
| 75:8D:201:CDL:HA4  | 75:8D:201:CDL:OB4  | 2.20                     | 0.42              |
| 59:8E:26:ALA:O     | 59:8E:30:ARG:HD3   | 2.19                     | 0.42              |
| 64:8J:33:ARG:HD2   | 87:8J:101:PGV:H181 | 2.02                     | 0.42              |
| 1:1A:54:LYS:HE3    | 1:1A:113:TRP:HB3   | 2.01                     | 0.42              |
| 2:1B:86:MET:HE1    | 2:1B:104:TYR:HB2   | 2.01                     | 0.42              |
| 70:1B:203:PC1:O14  | 42:1q:75:TRP:HB3   | 2.20                     | 0.42              |
| 6:1F:92:TYR:CE1    | 6:1F:133:ALA:HB3   | 2.54                     | 0.42              |
| 6:1F:197:GLU:OE2   | 17:1Q:129:ARG:NH2  | 2.47                     | 0.42              |
| 6:1F:292:ASP:OD1   | 6:1F:292:ASP:N     | 2.52                     | 0.42              |
| 7:1G:53:ARG:N      | 72:1G:803:FES:S1   | 2.81                     | 0.42              |
| 8:1H:2:PHE:CE2     | 8:1H:6:ILE:HD11    | 2.55                     | 0.42              |
| 8:1H:24:GLU:OE1    | 8:1H:228:TYR:OH    | 2.23                     | 0.42              |
| 8:1H:65:THR:HA     | 16:1P:324:TYR:HB2  | 2.01                     | 0.42              |
| 11:1K:4:VAL:O      | 11:1K:8:ILE:HG12   | 2.20                     | 0.42              |
| 12:1L:175:ASN:C    | 12:1L:179:ASP:OD2  | 2.63                     | 0.42              |
| 16:1P:115:HIS:CE1  | 16:1P:119:GLN:OE1  | 2.70                     | 0.42              |
| 16:1P:169:SER:HB3  | 16:1P:231:VAL:HG23 | 2.01                     | 0.42              |
| 20:1T:64:ASP:HA    | 20:1T:67:ALA:HB3   | 2.02                     | 0.42              |
| 25:1Z:108:GLU:O    | 30:1e:74:ARG:NH1   | 2.53                     | 0.42              |
| 29:1d:11:LEU:HD21  | 30:1e:3:PHE:HB3    | 2.01                     | 0.42              |
| 30:1e:75:LEU:HA    | 30:1e:78:ILE:HG22  | 2.02                     | 0.42              |
| 45:3A:195:MET:HE1  | 45:3A:219:LEU:HD12 | 2.01                     | 0.42              |
| 46:3B:86:THR:O     | 46:3B:90:GLU:HG3   | 2.19                     | 0.42              |
| 48:3D:320:LYS:HA   | 48:3D:320:LYS:HD2  | 1.95                     | 0.42              |
| 49:3E:112:GLY:HA2  | 53:3J:14:TYR:HB2   | 2.01                     | 0.42              |
| 49:3E:143:SER:OG   | 49:3E:145:ASP:OD1  | 2.36                     | 0.42              |
| 46:3O:369:LEU:HD11 | 46:3O:399:LEU:HD11 | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 57:4C:132:LEU:HD22 | 57:4C:176:LEU:HD23 | 2.02                     | 0.42              |
| 87:4C:303:PGV:H032 | 87:4C:303:PGV:H042 | 2.02                     | 0.42              |
| 55:8A:403:TYR:CZ   | 55:8A:479:LYS:HG2  | 2.54                     | 0.42              |
| 55:8A:409:TRP:HB2  | 55:8A:471:ILE:HD11 | 1.98                     | 0.42              |
| 56:8B:7:LEU:O      | 75:8B:303:CDL:H552 | 2.19                     | 0.42              |
| 56:8B:43:SER:OG    | 87:8B:301:PGV:O02  | 2.33                     | 0.42              |
| 58:8D:78:TRP:HB3   | 75:8D:201:CDL:H182 | 2.01                     | 0.42              |
| 61:8G:72:ASN:HB3   | 61:8G:75:VAL:HG12  | 2.02                     | 0.42              |
| 1:1A:92:LEU:HD13   | 27:1b:29:ILE:HG12  | 2.01                     | 0.42              |
| 2:1B:65:PRO:HD3    | 4:1D:168:PHE:HB3   | 2.02                     | 0.42              |
| 2:1B:114:VAL:HG22  | 2:1B:144:ILE:HB    | 2.00                     | 0.42              |
| 4:1D:126:LEU:HD23  | 4:1D:359:PRO:HD3   | 2.02                     | 0.42              |
| 4:1D:193:TYR:OH    | 4:1D:201:GLN:O     | 2.34                     | 0.42              |
| 5:1E:12:THR:O      | 5:1E:16:ASN:ND2    | 2.52                     | 0.42              |
| 5:1E:55:GLN:NE2    | 5:1E:90:TYR:HD1    | 2.18                     | 0.42              |
| 6:1F:129:MET:CE    | 6:1F:221:THR:HB    | 2.49                     | 0.42              |
| 6:1F:150:GLN:HB3   | 44:1s:54:LEU:HD12  | 2.02                     | 0.42              |
| 7:1G:616:LEU:HA    | 7:1G:619:VAL:HG12  | 2.02                     | 0.42              |
| 10:1J:130:THR:HG22 | 25:1Z:121:MET:SD   | 2.60                     | 0.42              |
| 12:1L:73:THR:HG21  | 12:1L:194:ASN:HD21 | 1.77                     | 0.42              |
| 13:1M:61:LEU:HB2   | 13:1M:457:PRO:HD3  | 2.01                     | 0.42              |
| 15:1O:3:TYR:CZ     | 15:1O:260:ARG:HD3  | 2.55                     | 0.42              |
| 17:1Q:9:GLN:CB     | 22:1W:23:ARG:NH2   | 2.80                     | 0.42              |
| 32:1g:112:CYS:N    | 41:1p:158:GLN:OE1  | 2.53                     | 0.42              |
| 33:1h:94:LEU:HD23  | 33:1h:94:LEU:HA    | 1.92                     | 0.42              |
| 45:3A:146:ARG:HA   | 45:3A:149:VAL:HG12 | 2.02                     | 0.42              |
| 46:3B:31:ASN:OD1   | 46:3B:228:GLY:HA2  | 2.19                     | 0.42              |
| 46:3O:118:ILE:H    | 46:3O:118:ILE:HG13 | 1.60                     | 0.42              |
| 47:3P:105:GLY:O    | 47:3P:108:MET:HG2  | 2.20                     | 0.42              |
| 47:3P:141:TRP:HB3  | 47:3P:268:ILE:HD13 | 2.02                     | 0.42              |
| 75:3P:504:CDL:H721 | 51:3T:41:THR:OG1   | 2.19                     | 0.42              |
| 49:3R:225:ILE:HG22 | 49:3R:228:ALA:HB3  | 2.02                     | 0.42              |
| 54:3Y:39:ARG:O     | 54:3Y:43:ASP:OD1   | 2.36                     | 0.42              |
| 55:4A:65:MET:HE3   | 88:4A:604:HEA:H131 | 2.02                     | 0.42              |
| 87:4A:603:PGV:H141 | 87:4A:603:PGV:H182 | 2.01                     | 0.42              |
| 56:4B:1:FME:HG2    | 56:4B:10:GLN:OE1   | 2.20                     | 0.42              |
| 56:4B:122:MET:HE2  | 56:4B:122:MET:HB3  | 1.99                     | 0.42              |
| 57:4C:15:PRO:HB2   | 64:4J:36:MET:CE    | 2.49                     | 0.42              |
| 57:4C:112:LEU:HG   | 57:4C:118:PRO:HB3  | 2.00                     | 0.42              |
| 58:4D:96:LEU:C     | 58:4D:96:LEU:CD2   | 2.89                     | 0.42              |
| 60:4F:70:ILE:HG21  | 60:4F:83:PRO:HD2   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:4N:44:CYS:HB2   | 68:4N:53:PRO:HG3   | 2.02                     | 0.42              |
| 55:8A:8:TYR:O      | 57:8C:13:PRO:HB3   | 2.20                     | 0.42              |
| 55:8A:92:MET:HB3   | 55:8A:163:ASN:HD21 | 1.85                     | 0.42              |
| 55:8A:114:ALA:O    | 55:8A:118:VAL:HG13 | 2.20                     | 0.42              |
| 55:8A:232:GLN:HB3  | 55:8A:292:MET:HE1  | 1.99                     | 0.42              |
| 55:8A:239:GLY:O    | 55:8A:243:VAL:N    | 2.45                     | 0.42              |
| 55:8A:318:VAL:HG13 | 56:8B:65:TRP:HE1   | 1.85                     | 0.42              |
| 55:8A:364:ASP:O    | 55:8A:368:HIS:HB2  | 2.20                     | 0.42              |
| 55:8A:427:PRO:HB3  | 55:8A:450:TRP:CE3  | 2.55                     | 0.42              |
| 55:8A:439:ARG:NH2  | 88:8A:604:HEA:O1D  | 2.52                     | 0.42              |
| 64:8J:36:MET:CA    | 64:8J:39:CYS:SG    | 3.06                     | 0.42              |
| 2:1B:50:PHE:CZ     | 2:1B:103:VAL:HG21  | 2.55                     | 0.42              |
| 70:1B:202:PC1:H3D2 | 8:1H:56:VAL:HG21   | 2.02                     | 0.42              |
| 3:1C:72:PHE:O      | 3:1C:124:TYR:OH    | 2.27                     | 0.42              |
| 6:1F:36:ALA:HB1    | 6:1F:41:ASP:HB2    | 2.02                     | 0.42              |
| 6:1F:46:LYS:HB2    | 6:1F:46:LYS:HE2    | 1.77                     | 0.42              |
| 7:1G:216:THR:HG22  | 7:1G:248:MET:CE    | 2.49                     | 0.42              |
| 8:1H:183:MET:HB3   | 9:1I:27:TRP:CH2    | 2.54                     | 0.42              |
| 9:1I:153:LYS:HA    | 9:1I:153:LYS:HD2   | 1.73                     | 0.42              |
| 10:1J:7:PHE:CZ     | 11:1K:3:LEU:HD13   | 2.55                     | 0.42              |
| 70:1M:505:PC1:H332 | 75:1h:202:CDL:OA8  | 2.20                     | 0.42              |
| 14:1N:322:GLN:HE22 | 29:1d:49:ARG:HG2   | 1.84                     | 0.42              |
| 16:1P:46:ILE:HD12  | 18:1R:26:VAL:HG21  | 2.02                     | 0.42              |
| 16:1P:81:ILE:HD13  | 16:1P:117:ILE:HD13 | 2.00                     | 0.42              |
| 16:1P:136:ASN:HB3  | 16:1P:146:LEU:HD13 | 2.02                     | 0.42              |
| 16:1P:319:ARG:HA   | 16:1P:322:ARG:HD3  | 2.00                     | 0.42              |
| 19:1S:87:THR:O     | 19:1S:91:GLU:OE2   | 2.38                     | 0.42              |
| 20:1T:70:LEU:HD11  | 20:1T:79:TYR:CG    | 2.54                     | 0.42              |
| 27:1b:58:ASP:HA    | 27:1b:62:MET:SD    | 2.59                     | 0.42              |
| 28:1c:31:LEU:HD13  | 29:1d:70:PHE:HA    | 2.02                     | 0.42              |
| 31:1f:48:LEU:H     | 31:1f:48:LEU:HD12  | 1.85                     | 0.42              |
| 32:1g:68:ILE:O     | 32:1g:72:LEU:HB2   | 2.20                     | 0.42              |
| 33:1h:40:ILE:HG22  | 75:1h:202:CDL:OB9  | 2.19                     | 0.42              |
| 34:1i:74:VAL:C     | 34:1i:77:PRO:HD2   | 2.45                     | 0.42              |
| 40:1o:33:ARG:HA    | 40:1o:33:ARG:HD2   | 1.83                     | 0.42              |
| 41:1p:35:ILE:N     | 41:1p:35:ILE:HD13  | 2.35                     | 0.42              |
| 45:3A:356:ARG:HG3  | 46:3B:91:ALA:HA    | 2.02                     | 0.42              |
| 69:3A:503:3PE:H2   | 69:3A:503:3PE:O14  | 2.19                     | 0.42              |
| 47:3C:322:GLN:NE2  | 69:3C:503:3PE:H111 | 2.35                     | 0.42              |
| 48:3Q:126:TYR:OH   | 86:3Q:501:HEC:O2A  | 2.22                     | 0.42              |
| 52:3U:77:LEU:HD23  | 52:3U:77:LEU:HA    | 1.86                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:3Y:40:LEU:HB2   | 69:3Y:101:3PE:H122 | 2.02                     | 0.42              |
| 55:4A:142:SER:O    | 55:4A:146:THR:HG23 | 2.20                     | 0.42              |
| 55:4A:202:LEU:HB2  | 55:4A:238:PHE:CG   | 2.54                     | 0.42              |
| 56:4B:62:GLU:HA    | 56:4B:65:TRP:CE3   | 2.52                     | 0.42              |
| 56:4B:142:VAL:HG12 | 56:4B:144:LEU:HG   | 2.02                     | 0.42              |
| 75:4B:303:CDL:H442 | 75:4B:303:CDL:H182 | 2.01                     | 0.42              |
| 57:4C:158:HIS:HE2  | 93:4G:102:PEK:H041 | 1.85                     | 0.42              |
| 55:8A:200:PRO:HB2  | 57:8C:92:LEU:HB3   | 2.01                     | 0.42              |
| 87:8A:601:PGV:H92  | 87:8A:601:PGV:H241 | 2.01                     | 0.42              |
| 56:8B:1:FME:HE2    | 56:8B:192:TYR:HA   | 2.01                     | 0.42              |
| 56:8B:103:GLN:OE1  | 56:8B:104:TRP:CE2  | 2.73                     | 0.42              |
| 56:8B:108:TYR:HB2  | 56:8B:118:PHE:CE1  | 2.53                     | 0.42              |
| 56:8B:193:TYR:HD1  | 56:8B:210:VAL:HG22 | 1.84                     | 0.42              |
| 67:8M:42:ARG:H     | 67:8M:42:ARG:HG3   | 1.67                     | 0.42              |
| 1:1A:24:LEU:HD21   | 70:1B:202:PC1:H3C2 | 2.02                     | 0.42              |
| 4:1D:6:PRO:HB3     | 4:1D:10:TRP:CD1    | 2.55                     | 0.42              |
| 7:1G:528:ASP:OD1   | 7:1G:545:TYR:OH    | 2.36                     | 0.42              |
| 9:1I:155:LEU:HD23  | 9:1I:155:LEU:HA    | 1.88                     | 0.42              |
| 10:1J:64:MET:HE3   | 10:1J:64:MET:HB2   | 1.60                     | 0.42              |
| 11:1K:37:MET:HG3   | 11:1K:67:ALA:CB    | 2.50                     | 0.42              |
| 12:1L:538:THR:HB   | 69:1L:701:3PE:H271 | 2.01                     | 0.42              |
| 14:1N:137:ALA:HB3  | 14:1N:138:PRO:HD3  | 2.02                     | 0.42              |
| 16:1P:289:MET:HE3  | 16:1P:289:MET:HB2  | 1.82                     | 0.42              |
| 20:1T:76:ILE:O     | 20:1T:80:ILE:HG13  | 2.19                     | 0.42              |
| 20:1U:37:MET:HA    | 20:1U:42:LEU:O     | 2.20                     | 0.42              |
| 39:1n:132:TRP:O    | 39:1n:135:GLU:HG2  | 2.19                     | 0.42              |
| 45:3A:206:ARG:HG3  | 45:3A:207:GLN:N    | 2.35                     | 0.42              |
| 47:3C:111:GLU:OE2  | 47:3C:111:GLU:N    | 2.45                     | 0.42              |
| 47:3C:186:PRO:HA   | 47:3C:189:ILE:HD12 | 2.02                     | 0.42              |
| 48:3D:232:ARG:HG3  | 49:3R:235:TYR:HE1  | 1.84                     | 0.42              |
| 49:3E:145:ASP:OD1  | 49:3E:145:ASP:N    | 2.53                     | 0.42              |
| 53:3J:57:LYS:N     | 53:3J:60:LYS:HG3   | 2.35                     | 0.42              |
| 45:3N:155:ALA:HA   | 45:3N:164:ALA:HB1  | 2.02                     | 0.42              |
| 47:3P:5:ARG:HG2    | 47:3P:15:ASN:HB2   | 2.02                     | 0.42              |
| 49:3R:263:TYR:HB2  | 49:3R:271:VAL:HG22 | 2.01                     | 0.42              |
| 87:4B:302:PGV:H102 | 87:4B:302:PGV:H271 | 2.02                     | 0.42              |
| 57:4C:103:HIS:HA   | 87:4C:303:PGV:O02  | 2.19                     | 0.42              |
| 57:4C:137:LEU:HD23 | 57:4C:137:LEU:HA   | 1.72                     | 0.42              |
| 66:4L:45:LEU:CD2   | 67:4M:40:TYR:CD2   | 3.03                     | 0.42              |
| 55:8A:25:TRP:CD1   | 87:8L:101:PGV:H291 | 2.55                     | 0.42              |
| 59:8E:42:VAL:CG2   | 63:8I:9:MET:SD     | 3.08                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 59:8E:102:GLU:HA   | 59:8E:107:ASP:OD2  | 2.20                     | 0.42              |
| 61:8G:26:PRO:HB2   | 93:8G:102:PEK:H383 | 2.01                     | 0.42              |
| 68:8N:52:GLU:HG3   | 68:8N:55:ASN:OD1   | 2.19                     | 0.42              |
| 1:1A:84:LEU:HD23   | 1:1A:84:LEU:HA     | 1.90                     | 0.41              |
| 2:1B:99:ALA:O      | 2:1B:103:VAL:HG13  | 2.19                     | 0.41              |
| 2:1B:154:GLU:HB3   | 9:1I:137:PHE:HE2   | 1.84                     | 0.41              |
| 6:1F:189:GLU:HG2   | 6:1F:190:THR:N     | 2.34                     | 0.41              |
| 6:1F:319:PHE:CZ    | 6:1F:329:LEU:HD23  | 2.55                     | 0.41              |
| 7:1G:74:MET:HE2    | 7:1G:77:TRP:CZ2    | 2.54                     | 0.41              |
| 8:1H:30:TYR:HE1    | 9:1I:45:PRO:HG3    | 1.85                     | 0.41              |
| 12:1L:63:ILE:HG13  | 34:1i:96:VAL:HG22  | 2.02                     | 0.41              |
| 12:1L:386:LEU:HD23 | 12:1L:386:LEU:HA   | 1.89                     | 0.41              |
| 13:1M:196:TRP:HZ2  | 13:1M:254:THR:HG23 | 1.85                     | 0.41              |
| 14:1N:339:MET:HE3  | 14:1N:339:MET:HB3  | 1.88                     | 0.41              |
| 15:1O:211:LEU:HD13 | 15:1O:222:GLN:HE21 | 1.85                     | 0.41              |
| 16:1P:200:THR:OG1  | 16:1P:288:HIS:O    | 2.22                     | 0.41              |
| 25:1Z:105:LYS:HD3  | 25:1Z:105:LYS:N    | 2.35                     | 0.41              |
| 33:1h:111:ARG:NH1  | 82:1h:201:AME:O    | 2.49                     | 0.41              |
| 47:3C:326:TRP:NE1  | 51:3G:50:VAL:HG22  | 2.34                     | 0.41              |
| 48:3D:145:THR:HG22 | 53:3J:56:TRP:HZ2   | 1.85                     | 0.41              |
| 52:3H:53:GLU:HG3   | 52:3H:57:LYS:HE3   | 2.02                     | 0.41              |
| 56:4B:104:TRP:CG   | 56:4B:203:ASN:HB2  | 2.55                     | 0.41              |
| 62:4H:24:ASN:OD1   | 62:4H:26:THR:HG22  | 2.20                     | 0.41              |
| 63:4I:21:ILE:HG22  | 63:4I:25:PHE:CE2   | 2.55                     | 0.41              |
| 55:8A:157:SER:HB2  | 55:8A:199:LEU:CD1  | 2.49                     | 0.41              |
| 56:8B:105:TYR:CE2  | 56:8B:119:ASP:OD2  | 2.71                     | 0.41              |
| 57:8C:176:LEU:O    | 57:8C:180:GLU:HG2  | 2.19                     | 0.41              |
| 59:8E:10:GLU:O     | 59:8E:14:ARG:HG2   | 2.19                     | 0.41              |
| 59:8E:23:ASP:OD1   | 59:8E:23:ASP:C     | 2.63                     | 0.41              |
| 1:1A:46:SER:HB3    | 1:1A:49:LEU:HD11   | 2.02                     | 0.41              |
| 3:1C:192:GLN:HB2   | 17:1Q:72:TRP:CD1   | 2.55                     | 0.41              |
| 6:1F:94:VAL:HB     | 6:1F:222:VAL:HG22  | 2.01                     | 0.41              |
| 6:1F:355:LYS:HE3   | 6:1F:355:LYS:HB3   | 1.97                     | 0.41              |
| 7:1G:139:ASP:HB3   | 7:1G:148:THR:O     | 2.20                     | 0.41              |
| 7:1G:209:THR:HG22  | 7:1G:210:SER:H     | 1.85                     | 0.41              |
| 12:1L:203:MET:HE2  | 41:1p:113:GLN:HG2  | 2.02                     | 0.41              |
| 12:1L:257:VAL:HG23 | 12:1L:329:ILE:HD11 | 2.02                     | 0.41              |
| 12:1L:416:THR:O    | 12:1L:419:THR:OG1  | 2.37                     | 0.41              |
| 12:1L:499:MET:HE1  | 64:4J:37:THR:CG2   | 2.49                     | 0.41              |
| 13:1M:393:ILE:HD12 | 13:1M:393:ILE:HA   | 1.85                     | 0.41              |
| 15:1O:72:GLN:H     | 15:1O:72:GLN:HG3   | 1.63                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:1P:194:ILE:HG13 | 16:1P:263:TYR:CE2  | 2.55                     | 0.41              |
| 20:1T:87:TYR:C     | 20:1T:88:GLU:HG2   | 2.45                     | 0.41              |
| 24:1Y:51:GLY:HA3   | 69:1Y:206:3PE:H232 | 2.01                     | 0.41              |
| 34:1i:43:GLU:O     | 34:1i:47:ASN:ND2   | 2.53                     | 0.41              |
| 45:3A:50:GLU:O     | 45:3A:173:ASN:ND2  | 2.37                     | 0.41              |
| 47:3C:240:LEU:HD21 | 69:3D:502:3PE:H242 | 2.02                     | 0.41              |
| 47:3C:326:TRP:CH2  | 69:3C:503:3PE:H231 | 2.55                     | 0.41              |
| 46:3O:100:SER:OG   | 46:3O:105:MET:HG2  | 2.20                     | 0.41              |
| 47:3P:138:MET:HG2  | 47:3P:254:ASP:HB3  | 2.02                     | 0.41              |
| 48:3Q:225:HIS:CD2  | 51:3T:20:PRO:HB2   | 2.55                     | 0.41              |
| 49:3R:169:TRP:HD1  | 49:3R:174:LEU:HD22 | 1.84                     | 0.41              |
| 64:4J:55:PHE:HB2   | 64:4J:57:HIS:CE1   | 2.55                     | 0.41              |
| 55:8A:331:ASN:OD1  | 58:8D:20:ARG:NE    | 2.53                     | 0.41              |
| 55:8A:404:THR:HG21 | 67:8M:3:ALA:HB2    | 2.03                     | 0.41              |
| 56:8B:63:THR:HG22  | 56:8B:67:ILE:CD1   | 2.40                     | 0.41              |
| 58:8D:44:GLU:OE1   | 59:8E:59:ASN:C     | 2.63                     | 0.41              |
| 66:8L:18:LYS:NZ    | 66:8L:19:TRP:CE2   | 2.71                     | 0.41              |
| 67:8M:2:TYR:HD1    | 67:8M:2:TYR:H      | 1.68                     | 0.41              |
| 1:1A:3:ILE:HG21    | 70:1H:403:PC1:H252 | 2.01                     | 0.41              |
| 2:1B:60:MET:HG3    | 4:1D:171:PHE:HE2   | 1.84                     | 0.41              |
| 3:1C:138:PHE:O     | 3:1C:163:ARG:NE    | 2.53                     | 0.41              |
| 4:1D:107:ASP:OD2   | 4:1D:371:LYS:HE2   | 2.20                     | 0.41              |
| 4:1D:152:MET:HE2   | 4:1D:152:MET:HB2   | 1.98                     | 0.41              |
| 6:1F:250:ASN:HB2   | 6:1F:319:PHE:HD2   | 1.85                     | 0.41              |
| 7:1G:157:THR:HG22  | 7:1G:161:ARG:HG3   | 2.02                     | 0.41              |
| 7:1G:210:SER:HB2   | 7:1G:269:PHE:HE1   | 1.86                     | 0.41              |
| 7:1G:510:GLY:C     | 7:1G:512:GLU:OE2   | 2.64                     | 0.41              |
| 7:1G:625:GLU:O     | 19:1S:21:HIS:HE1   | 2.03                     | 0.41              |
| 8:1H:260:VAL:O     | 8:1H:264:LEU:HG    | 2.19                     | 0.41              |
| 12:1L:281:GLY:HA3  | 12:1L:314:MET:HB3  | 2.02                     | 0.41              |
| 13:1M:244:MET:HG3  | 13:1M:301:ILE:HD13 | 2.02                     | 0.41              |
| 14:1N:323:MET:HE3  | 14:1N:323:MET:HB3  | 1.94                     | 0.41              |
| 14:1N:337:LEU:O    | 14:1N:340:THR:OG1  | 2.24                     | 0.41              |
| 15:1O:154:GLU:O    | 15:1O:158:VAL:HG23 | 2.20                     | 0.41              |
| 17:1Q:116:LYS:HD3  | 17:1Q:116:LYS:HA   | 1.92                     | 0.41              |
| 28:1c:39:VAL:O     | 28:1c:43:LYS:HG3   | 2.20                     | 0.41              |
| 39:1n:144:PRO:HD3  | 39:1n:147:GLY:O    | 2.20                     | 0.41              |
| 46:3B:257:LEU:HD11 | 46:3B:422:LYS:HB3  | 2.02                     | 0.41              |
| 48:3D:160:ASP:HB3  | 48:3D:169:PHE:CZ   | 2.56                     | 0.41              |
| 50:3F:110:ILE:O    | 50:3F:114:LYS:HG2  | 2.21                     | 0.41              |
| 47:3P:291:VAL:O    | 47:3P:295:VAL:HG22 | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:3P:377:LEU:HD23 | 47:3P:377:LEU:HA   | 1.89                     | 0.41              |
| 49:3R:219:HIS:CE1  | 49:3R:239:HIS:ND1  | 2.89                     | 0.41              |
| 49:3R:226:ALA:HA   | 49:3R:234:TYR:HD1  | 1.86                     | 0.41              |
| 55:4A:489:SER:OG   | 60:4F:70:ILE:HG23  | 2.20                     | 0.41              |
| 62:4H:54:GLU:O     | 62:4H:54:GLU:HG3   | 2.20                     | 0.41              |
| 56:8B:29:MET:HE3   | 63:8I:36:LYS:HG3   | 2.02                     | 0.41              |
| 57:8C:61:ILE:HD11  | 87:8C:301:PGV:H031 | 2.02                     | 0.41              |
| 57:8C:247:VAL:CG1  | 57:8C:251:PHE:HE1  | 2.28                     | 0.41              |
| 59:8E:49:ASP:O     | 59:8E:53:ARG:HG3   | 2.20                     | 0.41              |
| 65:8K:52:GLU:OE2   | 65:8K:54:ARG:N     | 2.53                     | 0.41              |
| 4:1D:148:LEU:HG    | 4:1D:177:MET:SD    | 2.61                     | 0.41              |
| 4:1D:164:MET:O     | 4:1D:167:PHE:HB3   | 2.20                     | 0.41              |
| 5:1E:15:ASN:OD1    | 5:1E:60:TRP:CH2    | 2.73                     | 0.41              |
| 5:1E:159:ASN:OD1   | 5:1E:159:ASN:N     | 2.51                     | 0.41              |
| 5:1E:205:PRO:HA    | 5:1E:206:PRO:HD2   | 1.97                     | 0.41              |
| 6:1F:293:ASN:OD1   | 6:1F:339:ARG:HB2   | 2.20                     | 0.41              |
| 7:1G:441:GLN:OE1   | 7:1G:441:GLN:HA    | 2.21                     | 0.41              |
| 10:1J:17:PHE:HA    | 10:1J:20:PHE:CE2   | 2.56                     | 0.41              |
| 12:1L:558:LEU:HD23 | 12:1L:558:LEU:HA   | 1.83                     | 0.41              |
| 69:1N:901:3PE:H2   | 69:1N:901:3PE:H111 | 2.02                     | 0.41              |
| 15:1O:19:THR:HG22  | 15:1O:20:GLU:H     | 1.85                     | 0.41              |
| 16:1P:29:PHE:HZ    | 16:1P:173:GLY:HA3  | 1.86                     | 0.41              |
| 16:1P:110:PHE:HB2  | 16:1P:148:SER:OG   | 2.20                     | 0.41              |
| 19:1S:19:ARG:HG3   | 19:1S:53:LEU:HB2   | 2.03                     | 0.41              |
| 22:1W:82:LEU:HD12  | 22:1W:82:LEU:HA    | 1.95                     | 0.41              |
| 23:1X:47:TRP:CG    | 27:1b:54:VAL:HG21  | 2.54                     | 0.41              |
| 23:1X:84:TYR:CE1   | 23:1X:103:GLN:HB2  | 2.56                     | 0.41              |
| 69:1Y:203:3PE:H282 | 70:1Y:207:PC1:H3D1 | 2.03                     | 0.41              |
| 34:1i:44:GLN:O     | 34:1i:48:LYS:HG3   | 2.21                     | 0.41              |
| 45:3A:93:GLU:HG3   | 45:3A:94:HIS:CD2   | 2.56                     | 0.41              |
| 48:3D:225:PRO:HA   | 48:3D:226:PRO:HD3  | 1.91                     | 0.41              |
| 48:3D:326:TYR:HB2  | 50:3F:72:PHE:CE1   | 2.56                     | 0.41              |
| 49:3E:213:LEU:HD13 | 49:3E:247:GLY:HA3  | 2.01                     | 0.41              |
| 49:3E:231:PHE:CE1  | 49:3E:242:HIS:HB3  | 2.47                     | 0.41              |
| 46:3O:181:TYR:CZ   | 46:3O:182:ARG:HG2  | 2.55                     | 0.41              |
| 47:3P:138:MET:HE1  | 47:3P:268:ILE:HA   | 2.02                     | 0.41              |
| 48:3Q:124:GLU:HG2  | 48:3Q:191:ARG:HB2  | 2.02                     | 0.41              |
| 55:4A:291:HIS:CE1  | 88:4A:605:HEA:HBD1 | 2.55                     | 0.41              |
| 55:4A:420:GLY:O    | 55:4A:424:THR:OG1  | 2.33                     | 0.41              |
| 56:4B:152:MET:HA   | 56:4B:152:MET:HE3  | 2.02                     | 0.41              |
| 58:4D:63:LYS:HB3   | 58:4D:64:PHE:CE1   | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:4F:33:ILE:HG22  | 60:4F:34:LEU:HD13  | 2.02                     | 0.41              |
| 55:8A:155:VAL:CG1  | 55:8A:159:LEU:HD11 | 2.51                     | 0.41              |
| 75:8C:306:CDL:H111 | 75:8C:306:CDL:H152 | 2.01                     | 0.41              |
| 87:8J:101:PGV:H302 | 87:8J:101:PGV:H343 | 2.02                     | 0.41              |
| 1:1A:54:LYS:HZ3    | 4:1D:71:GLU:HB2    | 1.86                     | 0.41              |
| 3:1C:137:MET:HB3   | 3:1C:162:PHE:HB2   | 2.02                     | 0.41              |
| 7:1G:41:CYS:O      | 7:1G:161:ARG:NH2   | 2.51                     | 0.41              |
| 8:1H:161:THR:HG22  | 8:1H:163:SER:H     | 1.85                     | 0.41              |
| 9:1I:47:THR:O      | 42:1q:58:ARG:HD2   | 2.21                     | 0.41              |
| 9:1I:143:THR:OG1   | 9:1I:146:GLU:HG3   | 2.21                     | 0.41              |
| 12:1L:295:GLN:HB2  | 12:1L:301:ILE:HG12 | 2.02                     | 0.41              |
| 13:1M:343:ILE:HG13 | 13:1M:346:ARG:HD3  | 2.02                     | 0.41              |
| 15:1O:163:TYR:OH   | 15:1O:269:VAL:HG13 | 2.20                     | 0.41              |
| 16:1P:136:ASN:HA   | 16:1P:292:MET:HG3  | 2.01                     | 0.41              |
| 17:1Q:34:LYS:HE2   | 17:1Q:34:LYS:HB2   | 1.81                     | 0.41              |
| 18:1R:22:ASP:OD2   | 18:1R:24:ARG:NH1   | 2.53                     | 0.41              |
| 24:1Y:72:THR:HG22  | 24:1Y:91:ILE:HG22  | 2.02                     | 0.41              |
| 40:1o:93:ASP:O     | 40:1o:97:ARG:HG3   | 2.21                     | 0.41              |
| 44:1s:58:LEU:HA    | 44:1s:61:PHE:CE1   | 2.55                     | 0.41              |
| 46:3B:122:PHE:O    | 46:3B:126:VAL:HG13 | 2.20                     | 0.41              |
| 46:3B:160:LEU:HD12 | 49:3I:64:LEU:HD13  | 2.02                     | 0.41              |
| 47:3C:111:GLU:CD   | 47:3C:111:GLU:N    | 2.78                     | 0.41              |
| 47:3C:185:LEU:HD23 | 47:3C:188:ILE:HD12 | 2.01                     | 0.41              |
| 47:3C:326:TRP:CZ2  | 69:3C:503:3PE:H231 | 2.55                     | 0.41              |
| 49:3E:101:LYS:HE2  | 49:3E:101:LYS:HB2  | 1.88                     | 0.41              |
| 49:3E:196:ARG:HD2  | 49:3E:196:ARG:HA   | 1.78                     | 0.41              |
| 49:3I:62:ARG:HB3   | 49:3I:63:PRO:HD2   | 2.03                     | 0.41              |
| 45:3N:87:ASN:HB3   | 45:3N:98:TYR:CZ    | 2.56                     | 0.41              |
| 45:3N:344:ARG:HH12 | 45:3N:353:GLU:CD   | 2.27                     | 0.41              |
| 47:3P:309:THR:HG1  | 47:3P:370:SER:HG   | 1.59                     | 0.41              |
| 51:3T:71:ARG:HD2   | 52:3U:56:GLU:OE1   | 2.21                     | 0.41              |
| 56:4B:40:TYR:CD2   | 63:4I:27:VAL:HG11  | 2.55                     | 0.41              |
| 57:4C:27:MET:CE    | 57:4C:50:ASN:HD22  | 2.33                     | 0.41              |
| 57:4C:203:PHE:O    | 57:4C:207:HIS:ND1  | 2.38                     | 0.41              |
| 58:4D:76:ASN:HD22  | 58:4D:79:LYS:NZ    | 2.18                     | 0.41              |
| 58:4D:93:ALA:O     | 58:4D:97:ILE:HG13  | 2.20                     | 0.41              |
| 55:8A:51:ASP:HB2   | 56:8B:202:SER:O    | 2.20                     | 0.41              |
| 56:8B:129:LYS:N    | 56:8B:132:GLU:OE2  | 2.53                     | 0.41              |
| 87:8C:303:PGV:H202 | 87:8C:303:PGV:H011 | 1.24                     | 0.41              |
| 1:1A:18:VAL:HG21   | 8:1H:76:ILE:HG13   | 2.03                     | 0.41              |
| 2:1B:68:ASP:O      | 2:1B:71:ARG:HG2    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:100:LEU:HD12  | 4:1D:118:TYR:HD2   | 1.85                     | 0.41              |
| 4:1D:275:TYR:CZ    | 4:1D:367:ILE:HB    | 2.55                     | 0.41              |
| 4:1D:423:ILE:HG23  | 4:1D:428:VAL:HG21  | 2.01                     | 0.41              |
| 5:1E:55:GLN:NE2    | 5:1E:90:TYR:HA     | 2.30                     | 0.41              |
| 7:1G:237:ASN:H     | 7:1G:259:ASN:HD22  | 1.66                     | 0.41              |
| 8:1H:100:LEU:HB3   | 8:1H:103:LEU:HB2   | 2.03                     | 0.41              |
| 8:1H:310:MET:O     | 27:1b:37:TYR:HB2   | 2.21                     | 0.41              |
| 12:1L:161:ARG:NH2  | 39:1n:87:GLY:O     | 2.41                     | 0.41              |
| 12:1L:169:LEU:HD12 | 12:1L:169:LEU:HA   | 1.91                     | 0.41              |
| 12:1L:313:MET:HA   | 12:1L:316:THR:HG22 | 2.01                     | 0.41              |
| 12:1L:401:MET:HE3  | 12:1L:401:MET:HB3  | 1.88                     | 0.41              |
| 12:1L:560:THR:O    | 12:1L:565:THR:OG1  | 2.37                     | 0.41              |
| 13:1M:56:PHE:CZ    | 13:1M:108:MET:HG2  | 2.56                     | 0.41              |
| 13:1M:71:TRP:O     | 13:1M:74:PRO:HD2   | 2.20                     | 0.41              |
| 13:1M:88:THR:OG1   | 13:1M:91:ARG:HG3   | 2.20                     | 0.41              |
| 15:1O:6:LEU:HD12   | 15:1O:6:LEU:HA     | 1.81                     | 0.41              |
| 18:1R:27:ARG:HE    | 18:1R:27:ARG:HB3   | 1.67                     | 0.41              |
| 25:1Z:56:GLU:OE1   | 25:1Z:59:ARG:NH2   | 2.40                     | 0.41              |
| 37:1l:118:VAL:O    | 37:1l:121:ILE:HG12 | 2.21                     | 0.41              |
| 41:1p:42:ARG:O     | 41:1p:46:LEU:HG    | 2.20                     | 0.41              |
| 45:3A:156:THR:O    | 45:3A:239:SER:OG   | 2.39                     | 0.41              |
| 46:3B:35:ILE:HG22  | 46:3B:213:HIS:CE1  | 2.56                     | 0.41              |
| 47:3C:113:TRP:O    | 47:3C:117:VAL:HG23 | 2.21                     | 0.41              |
| 47:3C:223:TYR:O    | 47:3C:226:ILE:HG22 | 2.20                     | 0.41              |
| 69:3C:504:3PE:H281 | 54:3X:35:ALA:HB1   | 2.03                     | 0.41              |
| 49:3E:130:LYS:NZ   | 54:3Y:37:ASP:OD1   | 2.54                     | 0.41              |
| 49:3E:242:HIS:CG   | 49:3E:251:LYS:HB3  | 2.56                     | 0.41              |
| 46:3O:102:ARG:NH2  | 46:3O:161:GLU:OE1  | 2.46                     | 0.41              |
| 49:3R:152:ILE:HD12 | 49:3R:152:ILE:HA   | 1.66                     | 0.41              |
| 49:3R:207:LYS:HB2  | 49:3R:265:PHE:HD2  | 1.85                     | 0.41              |
| 51:3T:71:ARG:HD3   | 51:3T:71:ARG:HA    | 1.80                     | 0.41              |
| 55:4A:28:MET:HE2   | 67:4M:26:PHE:CZ    | 2.55                     | 0.41              |
| 88:4A:604:HEA:H171 | 88:4A:604:HEA:H202 | 1.80                     | 0.41              |
| 56:4B:134:ARG:HD3  | 58:4D:110:THR:OG1  | 2.21                     | 0.41              |
| 57:4C:15:PRO:O     | 57:4C:19:THR:OG1   | 2.36                     | 0.41              |
| 66:4L:41:ARG:HG3   | 67:4M:40:TYR:OH    | 2.21                     | 0.41              |
| 67:4M:11:SER:OG    | 67:4M:14:GLU:HG3   | 2.20                     | 0.41              |
| 68:4N:57:LEU:HD23  | 68:4N:57:LEU:HA    | 1.91                     | 0.41              |
| 55:8A:177:SER:HB3  | 55:8A:180:GLN:HG3  | 2.02                     | 0.41              |
| 55:8A:489:SER:OG   | 60:8F:70:ILE:HG23  | 2.21                     | 0.41              |
| 57:8C:140:SER:CB   | 57:8C:242:TRP:HE1  | 2.34                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:8D:48:TRP:NE1   | 59:8E:56:ARG:CD    | 2.77                     | 0.41              |
| 58:8D:57:VAL:O     | 58:8D:61:ARG:HG2   | 2.20                     | 0.41              |
| 68:8N:46:ASP:OD1   | 68:8N:48:LYS:HG3   | 2.20                     | 0.41              |
| 2:1B:71:ARG:HB2    | 8:1H:38:ASN:OD1    | 2.21                     | 0.41              |
| 4:1D:230:THR:HG23  | 4:1D:298:LEU:HD21  | 2.01                     | 0.41              |
| 5:1E:143:GLU:HB3   | 6:1F:353:PHE:HD1   | 1.86                     | 0.41              |
| 6:1F:45:THR:O      | 6:1F:49:LEU:HD23   | 2.20                     | 0.41              |
| 6:1F:256:PHE:CD1   | 6:1F:317:MET:HE2   | 2.56                     | 0.41              |
| 12:1L:161:ARG:HH21 | 39:1n:90:TYR:N     | 2.18                     | 0.41              |
| 69:1L:703:3PE:H282 | 75:1h:202:CDL:OA9  | 2.21                     | 0.41              |
| 13:1M:86:LYS:HB2   | 13:1M:86:LYS:HE2   | 1.71                     | 0.41              |
| 13:1M:281:ASP:HB3  | 13:1M:284:SER:HB3  | 2.02                     | 0.41              |
| 15:1O:318:TRP:CD2  | 15:1O:319:LEU:HD12 | 2.55                     | 0.41              |
| 16:1P:64:ASP:HB3   | 16:1P:67:GLN:HG2   | 2.02                     | 0.41              |
| 16:1P:113:ILE:HB   | 16:1P:114:PRO:HD3  | 2.03                     | 0.41              |
| 20:1U:60:PHE:CE1   | 20:1U:80:ILE:HG13  | 2.55                     | 0.41              |
| 21:1V:13:LEU:HD23  | 21:1V:13:LEU:HA    | 1.79                     | 0.41              |
| 26:1a:59:ARG:NE    | 26:1a:61:HIS:NE2   | 2.69                     | 0.41              |
| 32:1g:113:PHE:HB2  | 41:1p:158:GLN:HE22 | 1.86                     | 0.41              |
| 34:1i:89:VAL:O     | 34:1i:95:THR:OG1   | 2.37                     | 0.41              |
| 37:1l:72:ASN:HB3   | 37:1l:75:GLU:HG2   | 2.03                     | 0.41              |
| 40:1o:83:GLN:C     | 40:1o:83:GLN:OE1   | 2.63                     | 0.41              |
| 70:1q:201:PC1:H3B2 | 70:1q:201:PC1:H2E1 | 2.01                     | 0.41              |
| 45:3A:77:LYS:HE3   | 45:3A:77:LYS:HB2   | 1.77                     | 0.41              |
| 45:3A:316:GLU:OE1  | 45:3A:316:GLU:N    | 2.54                     | 0.41              |
| 45:3A:439:SER:HA   | 45:3A:442:PHE:CE2  | 2.55                     | 0.41              |
| 46:3B:70:ARG:HD3   | 46:3B:100:SER:OG   | 2.20                     | 0.41              |
| 47:3C:33:PHE:HA    | 47:3C:36:LEU:HB2   | 2.03                     | 0.41              |
| 69:3N:501:3PE:H262 | 75:3N:502:CDL:HB62 | 2.02                     | 0.41              |
| 47:3P:50:PHE:HZ    | 69:3R:302:3PE:H2I3 | 1.86                     | 0.41              |
| 47:3P:150:LEU:HD23 | 47:3P:150:LEU:HA   | 1.89                     | 0.41              |
| 55:4A:94:PHE:N     | 55:4A:163:ASN:OD1  | 2.49                     | 0.41              |
| 55:4A:113:LEU:HD22 | 66:4L:39:ILE:HD11  | 2.02                     | 0.41              |
| 55:4A:362:SER:O    | 56:4B:87:MET:HE1   | 2.20                     | 0.41              |
| 55:8A:467:LEU:HD13 | 58:8D:88:PHE:CE2   | 2.56                     | 0.41              |
| 55:8A:508:PRO:HD2  | 57:8C:5:THR:HG22   | 2.01                     | 0.41              |
| 2:1B:32:LYS:HA     | 2:1B:32:LYS:HD2    | 1.75                     | 0.41              |
| 4:1D:283:PHE:CG    | 4:1D:310:ILE:HD11  | 2.55                     | 0.41              |
| 5:1E:14:GLU:N      | 5:1E:14:GLU:CD     | 2.79                     | 0.41              |
| 5:1E:31:ILE:HG13   | 5:1E:53:LEU:HD23   | 2.03                     | 0.41              |
| 6:1F:95:VAL:HB     | 6:1F:136:ILE:HA    | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:210:SER:HB2   | 7:1G:269:PHE:CE1   | 2.56                     | 0.41              |
| 8:1H:153:VAL:O     | 8:1H:156:MET:HG2   | 2.21                     | 0.41              |
| 9:1I:64:GLU:OE2    | 9:1I:149:TYR:OH    | 2.35                     | 0.41              |
| 10:1J:125:TRP:HH2  | 25:1Z:126:GLY:HA2  | 1.84                     | 0.41              |
| 11:1K:44:SER:CB    | 11:1K:59:MET:HE1   | 2.51                     | 0.41              |
| 12:1L:316:THR:HG23 | 12:1L:325:ALA:HB2  | 2.02                     | 0.41              |
| 13:1M:88:THR:O     | 13:1M:92:LYS:HG3   | 2.20                     | 0.41              |
| 14:1N:74:ILE:HG13  | 14:1N:98:MET:HE1   | 2.03                     | 0.41              |
| 14:1N:231:SER:O    | 14:1N:234:TRP:HD1  | 2.04                     | 0.41              |
| 14:1N:276:ILE:C    | 14:1N:279:PRO:HD2  | 2.45                     | 0.41              |
| 15:1O:133:VAL:HG21 | 15:1O:206:TYR:CE2  | 2.56                     | 0.41              |
| 15:1O:135:LEU:HD21 | 15:1O:149:VAL:HB   | 2.02                     | 0.41              |
| 23:1X:73:ILE:HD13  | 23:1X:73:ILE:HA    | 1.97                     | 0.41              |
| 24:1Y:31:THR:O     | 24:1Y:35:VAL:HG12  | 2.21                     | 0.41              |
| 25:1Z:53:TRP:NE1   | 25:1Z:57:ARG:HD2   | 2.35                     | 0.41              |
| 41:1p:27:ASN:OD1   | 41:1p:29:VAL:HG22  | 2.20                     | 0.41              |
| 41:1p:140:ASP:O    | 41:1p:161:ARG:NH2  | 2.52                     | 0.41              |
| 42:1q:22:GLY:O     | 42:1q:26:VAL:HG22  | 2.21                     | 0.41              |
| 45:3A:27:SER:HA    | 45:3A:199:ALA:O    | 2.20                     | 0.41              |
| 45:3A:36:THR:HG21  | 45:3A:373:THR:HA   | 2.01                     | 0.41              |
| 45:3A:172:GLU:O    | 45:3A:176:LYS:HD3  | 2.21                     | 0.41              |
| 49:3E:236:CYS:HB2  | 49:3E:241:SER:O    | 2.20                     | 0.41              |
| 49:3E:249:ILE:H    | 49:3E:257:ASN:HB3  | 1.86                     | 0.41              |
| 45:3N:223:TYR:O    | 45:3N:224:VAL:C    | 2.63                     | 0.41              |
| 45:3N:242:ARG:NH2  | 45:3N:432:PRO:O    | 2.53                     | 0.41              |
| 55:4A:383:MET:HE1  | 55:4A:422:ASN:HA   | 2.03                     | 0.41              |
| 61:4G:73:PRO:CA    | 61:4G:83:GLU:OE2   | 2.66                     | 0.41              |
| 55:8A:53:ILE:HA    | 55:8A:56:VAL:HG22  | 2.03                     | 0.41              |
| 55:8A:282:PHE:CD1  | 55:8A:282:PHE:C    | 2.97                     | 0.41              |
| 55:8A:442:ASP:HB3  | 56:8B:135:LEU:HD21 | 2.02                     | 0.41              |
| 57:8C:51:THR:HA    | 57:8C:54:MET:HE3   | 2.03                     | 0.41              |
| 1:1A:49:LEU:N      | 1:1A:50:PRO:HD2    | 2.35                     | 0.41              |
| 4:1D:49:LEU:HD12   | 4:1D:49:LEU:HA     | 1.97                     | 0.41              |
| 6:1F:230:VAL:O     | 6:1F:234:ILE:HG12  | 2.21                     | 0.41              |
| 6:1F:405:CYS:HB2   | 71:1F:502:SF4:S1   | 2.59                     | 0.41              |
| 7:1G:24:THR:O      | 7:1G:73:VAL:HG22   | 2.21                     | 0.41              |
| 7:1G:118:ASP:O     | 7:1G:122:MET:HG2   | 2.20                     | 0.41              |
| 7:1G:190:MET:HG2   | 7:1G:192:MET:HE3   | 1.99                     | 0.41              |
| 7:1G:549:HIS:NE2   | 7:1G:677:ILE:HG22  | 2.35                     | 0.41              |
| 8:1H:26:LYS:NZ     | 8:1H:35:LYS:O      | 2.47                     | 0.41              |
| 8:1H:130:ILE:HD13  | 8:1H:130:ILE:HA    | 1.95                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:54:LYS:HZ2    | 9:1I:54:LYS:HG2    | 1.74                     | 0.41              |
| 70:1I:203:PC1:H362 | 70:1I:203:PC1:H3A1 | 2.02                     | 0.41              |
| 10:1J:86:ASN:ND2   | 11:1K:23:ARG:NH1   | 2.67                     | 0.41              |
| 11:1K:3:LEU:HD23   | 11:1K:6:MET:SD     | 2.60                     | 0.41              |
| 11:1K:26:LEU:HB3   | 11:1K:78:LEU:HD12  | 2.02                     | 0.41              |
| 12:1L:27:TYR:O     | 12:1L:115:ASN:ND2  | 2.49                     | 0.41              |
| 12:1L:371:THR:HG21 | 35:1j:25:ALA:HB1   | 2.02                     | 0.41              |
| 13:1M:207:MET:HE1  | 13:1M:240:GLY:HA2  | 2.03                     | 0.41              |
| 15:1O:180:GLN:OE1  | 15:1O:196:ALA:HB2  | 2.21                     | 0.41              |
| 16:1P:268:ARG:O    | 16:1P:272:VAL:HG23 | 2.21                     | 0.41              |
| 19:1S:13:LEU:HD22  | 19:1S:69:ALA:HB3   | 2.02                     | 0.41              |
| 25:1Z:59:ARG:HA    | 25:1Z:62:ILE:CG2   | 2.50                     | 0.41              |
| 25:1Z:97:ILE:HD13  | 30:1e:82:ARG:HB2   | 2.03                     | 0.41              |
| 27:1b:56:LEU:HD13  | 27:1b:62:MET:HE1   | 2.02                     | 0.41              |
| 28:1c:41:GLU:OE2   | 28:1c:45:ARG:NH2   | 2.48                     | 0.41              |
| 29:1d:30:ARG:O     | 29:1d:34:MET:HG2   | 2.21                     | 0.41              |
| 70:1d:202:PC1:H112 | 70:1d:202:PC1:H321 | 2.02                     | 0.41              |
| 30:1e:75:LEU:HA    | 30:1e:75:LEU:HD23  | 1.79                     | 0.41              |
| 31:1f:11:TRP:O     | 31:1f:14:ILE:HG12  | 2.20                     | 0.41              |
| 35:1j:65:GLY:HA3   | 40:1o:30:PHE:CD1   | 2.54                     | 0.41              |
| 37:1l:6:LYS:HA     | 37:1l:9:PHE:HD1    | 1.86                     | 0.41              |
| 37:1l:156:TYR:CD1  | 40:1o:33:ARG:HB3   | 2.56                     | 0.41              |
| 40:1o:16:PRO:HG2   | 40:1o:101:PHE:CE2  | 2.56                     | 0.41              |
| 40:1o:92:LEU:O     | 40:1o:96:LYS:HG3   | 2.20                     | 0.41              |
| 40:1o:96:LYS:O     | 40:1o:100:GLU:HG2  | 2.21                     | 0.41              |
| 41:1p:8:VAL:HG13   | 41:1p:9:TYR:CD1    | 2.56                     | 0.41              |
| 42:1q:25:ARG:HD2   | 42:1q:74:PHE:CZ    | 2.54                     | 0.41              |
| 46:3B:306:PRO:HA   | 49:3I:52:ARG:HB2   | 2.02                     | 0.41              |
| 47:3C:223:TYR:HB3  | 48:3D:316:TRP:CZ2  | 2.56                     | 0.41              |
| 50:3F:87:LEU:O     | 50:3F:92:TRP:NE1   | 2.43                     | 0.41              |
| 46:3O:340:ALA:O    | 46:3O:344:VAL:HG23 | 2.21                     | 0.41              |
| 49:3R:110:ARG:HD2  | 51:3T:21:PHE:O     | 2.21                     | 0.41              |
| 56:4B:49:LYS:O     | 56:4B:49:LYS:HG2   | 2.21                     | 0.41              |
| 56:4B:105:TYR:HB2  | 56:4B:120:SER:O    | 2.20                     | 0.41              |
| 57:4C:92:LEU:HD13  | 57:4C:92:LEU:HA    | 1.95                     | 0.41              |
| 57:4C:132:LEU:HD12 | 61:4G:31:CYS:C     | 2.45                     | 0.41              |
| 57:4C:141:GLY:O    | 57:4C:144:ILE:HG22 | 2.21                     | 0.41              |
| 58:4D:33:LEU:HB3   | 58:4D:38:LYS:HG3   | 2.03                     | 0.41              |
| 58:4D:82:VAL:HG22  | 75:4D:201:CDL:OB7  | 2.21                     | 0.41              |
| 75:4D:201:CDL:HB61 | 75:4D:201:CDL:H711 | 1.48                     | 0.41              |
| 60:4F:51:SER:HB3   | 60:4F:91:LEU:HD22  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:4F:90:LYS:NZ    | 60:4F:90:LYS:HB3   | 2.36                     | 0.41              |
| 55:8A:244:TYR:HB3  | 55:8A:248:LEU:HD11 | 2.02                     | 0.41              |
| 55:8A:351:GLY:HA3  | 55:8A:380:VAL:HG13 | 2.02                     | 0.41              |
| 55:8A:376:HIS:O    | 55:8A:380:VAL:HG22 | 2.20                     | 0.41              |
| 55:8A:377:PHE:HB2  | 88:8A:605:HEA:C2D  | 2.51                     | 0.41              |
| 57:8C:63:ARG:CD    | 64:8J:12:PHE:HE2   | 2.33                     | 0.41              |
| 57:8C:101:PHE:CZ   | 57:8C:256:ILE:HA   | 2.56                     | 0.41              |
| 58:8D:100:LYS:HG2  | 65:8K:36:ILE:HG21  | 2.03                     | 0.41              |
| 59:8E:44:GLU:CD    | 59:8E:46:LYS:HB2   | 2.46                     | 0.41              |
| 63:8I:28:SER:O     | 63:8I:31:VAL:HG22  | 2.20                     | 0.41              |
| 63:8I:43:ARG:O     | 63:8I:47:TYR:CD1   | 2.71                     | 0.41              |
| 1:1A:37:TYR:CD1    | 1:1A:37:TYR:C      | 2.99                     | 0.41              |
| 1:1A:73:LEU:HD13   | 8:1H:103:LEU:HD21  | 2.03                     | 0.41              |
| 2:1B:45:LEU:O      | 2:1B:47:PRO:HD3    | 2.21                     | 0.41              |
| 2:1B:144:ILE:HD12  | 2:1B:162:GLN:HG2   | 2.02                     | 0.41              |
| 3:1C:35:LYS:HD3    | 3:1C:36:TYR:CZ     | 2.55                     | 0.41              |
| 6:1F:429:ARG:HE    | 6:1F:429:ARG:HB2   | 1.65                     | 0.41              |
| 7:1G:113:GLU:HA    | 17:1Q:46:GLN:NE2   | 2.35                     | 0.41              |
| 7:1G:366:THR:CB    | 7:1G:450:MET:HE2   | 2.51                     | 0.41              |
| 9:1I:43:ARG:HG2    | 43:1r:11:ARG:HH21  | 1.86                     | 0.41              |
| 12:1L:556:ILE:HD13 | 12:1L:556:ILE:HA   | 1.91                     | 0.41              |
| 69:1M:502:3PE:H321 | 69:1M:502:3PE:H31  | 1.21                     | 0.41              |
| 14:1N:131:LEU:HD12 | 14:1N:216:PHE:HE2  | 1.86                     | 0.41              |
| 14:1N:310:ASN:HB2  | 15:1O:274:THR:HG22 | 2.02                     | 0.41              |
| 19:1S:87:THR:O     | 19:1S:91:GLU:CD    | 2.64                     | 0.41              |
| 20:1T:52:MET:HA    | 20:1T:55:GLU:CG    | 2.51                     | 0.41              |
| 20:1U:60:PHE:HE1   | 20:1U:80:ILE:HG13  | 1.86                     | 0.41              |
| 20:1U:61:GLU:OE2   | 39:1n:84:SER:OG    | 2.25                     | 0.41              |
| 27:1b:38:THR:O     | 27:1b:42:ILE:HG13  | 2.21                     | 0.41              |
| 29:1d:63:LEU:HD23  | 75:1d:203:CDL:HA62 | 2.02                     | 0.41              |
| 36:1k:29:GLU:O     | 36:1k:33:GLU:HG2   | 2.20                     | 0.41              |
| 38:1m:106:THR:O    | 38:1m:110:LYS:HG3  | 2.21                     | 0.41              |
| 45:3A:87:ASN:ND2   | 45:3A:98:TYR:OH    | 2.41                     | 0.41              |
| 46:3B:232:LEU:HD12 | 46:3B:232:LEU:HA   | 1.81                     | 0.41              |
| 47:3C:50:PHE:CE2   | 49:3E:140:MET:HE2  | 2.56                     | 0.41              |
| 49:3E:195:LEU:HD11 | 49:3E:248:ARG:HD2  | 2.03                     | 0.41              |
| 45:3N:21:ASN:ND2   | 45:3N:216:PHE:O    | 2.54                     | 0.41              |
| 45:3N:214:LYS:HE2  | 45:3N:214:LYS:HB2  | 1.86                     | 0.41              |
| 49:3R:177:ARG:HH21 | 49:3R:245:ALA:HA   | 1.86                     | 0.41              |
| 51:3T:50:PRO:O     | 51:3T:54:VAL:HG13  | 2.21                     | 0.41              |
| 55:4A:127:THR:HB   | 55:4A:129:TYR:CE1  | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:4B:4:PRO:HB3    | 65:4K:41:ASN:OD1   | 2.21                     | 0.41              |
| 75:4D:201:CDL:H581 | 75:4D:201:CDL:H621 | 2.02                     | 0.41              |
| 59:4E:49:ASP:C     | 59:4E:49:ASP:OD1   | 2.62                     | 0.41              |
| 59:4E:72:LYS:HB2   | 59:4E:82:TYR:CE2   | 2.56                     | 0.41              |
| 55:8A:53:ILE:O     | 55:8A:56:VAL:HG22  | 2.20                     | 0.41              |
| 56:8B:102:HIS:HB2  | 56:8B:105:TYR:CE1  | 2.56                     | 0.41              |
| 56:8B:147:GLU:C    | 56:8B:185:MET:HE1  | 2.46                     | 0.41              |
| 58:8D:34:SER:CB    | 58:8D:37:GLN:OE1   | 2.69                     | 0.41              |
| 63:8I:34:PHE:CD1   | 63:8I:34:PHE:C     | 2.99                     | 0.41              |
| 5:1E:23:PHE:HA     | 5:1E:57:GLN:HE22   | 1.87                     | 0.40              |
| 5:1E:192:SER:OG    | 5:1E:193:CYS:N     | 2.53                     | 0.40              |
| 6:1F:15:LEU:HB2    | 6:1F:271:GLU:HB2   | 2.03                     | 0.40              |
| 6:1F:47:GLU:O      | 6:1F:51:LYS:HG2    | 2.21                     | 0.40              |
| 6:1F:126:GLY:HA3   | 6:1F:173:PHE:CE1   | 2.56                     | 0.40              |
| 7:1G:94:MET:HE3    | 7:1G:120:SER:N     | 2.35                     | 0.40              |
| 8:1H:74:ALA:HB3    | 8:1H:75:PRO:HD3    | 2.03                     | 0.40              |
| 8:1H:144:VAL:O     | 8:1H:148:ILE:HG13  | 2.21                     | 0.40              |
| 10:1J:171:ILE:HG23 | 14:1N:45:MET:SD    | 2.61                     | 0.40              |
| 11:1K:41:PHE:HD1   | 11:1K:42:ILE:HD13  | 1.85                     | 0.40              |
| 12:1L:355:ASP:OD2  | 12:1L:357:ARG:NH2  | 2.54                     | 0.40              |
| 14:1N:155:LEU:HD22 | 14:1N:278:MET:HE2  | 2.02                     | 0.40              |
| 15:1O:146:LYS:O    | 15:1O:149:VAL:HG22 | 2.22                     | 0.40              |
| 17:1Q:85:THR:HG23  | 21:1V:115:ILE:HD11 | 2.03                     | 0.40              |
| 26:1a:26:ILE:HD13  | 26:1a:26:ILE:N     | 2.36                     | 0.40              |
| 36:1k:15:LEU:H     | 36:1k:15:LEU:HD12  | 1.86                     | 0.40              |
| 37:1l:62:TYR:HD1   | 37:1l:63:ASP:N     | 2.19                     | 0.40              |
| 44:1s:33:PHE:CD1   | 44:1s:33:PHE:C     | 2.99                     | 0.40              |
| 45:3A:260:PRO:HB2  | 45:3A:264:ASN:HB3  | 2.03                     | 0.40              |
| 45:3A:342:TRP:CZ3  | 45:3A:441:MET:HE1  | 2.56                     | 0.40              |
| 45:3N:145:MET:HE1  | 45:3N:250:LEU:O    | 2.22                     | 0.40              |
| 45:3N:316:GLU:OE1  | 45:3N:316:GLU:N    | 2.54                     | 0.40              |
| 49:3R:267:SER:O    | 49:3R:271:VAL:HB   | 2.21                     | 0.40              |
| 69:3R:302:3PE:H3B1 | 70:3R:303:PC1:H3F1 | 2.03                     | 0.40              |
| 52:3U:49:GLN:C     | 52:3U:49:GLN:CD    | 2.89                     | 0.40              |
| 55:4A:8:TYR:O      | 57:4C:13:PRO:HB3   | 2.21                     | 0.40              |
| 55:4A:202:LEU:HD22 | 55:4A:238:PHE:CE2  | 2.56                     | 0.40              |
| 56:4B:62:GLU:HG3   | 68:4N:14:SER:OG    | 2.21                     | 0.40              |
| 75:4B:303:CDL:HA61 | 75:4B:303:CDL:H311 | 1.69                     | 0.40              |
| 57:4C:129:VAL:HB   | 57:4C:130:PRO:HD3  | 2.03                     | 0.40              |
| 58:4D:122:ARG:HG3  | 65:4K:53:TRP:CD2   | 2.56                     | 0.40              |
| 55:8A:25:TRP:HB2   | 87:8L:101:PGV:H281 | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:8A:601:PGV:H321 | 87:8A:601:PGV:H292 | 1.83                     | 0.40              |
| 56:8B:148:MET:N    | 56:8B:148:MET:SD   | 2.94                     | 0.40              |
| 57:8C:23:SER:O     | 57:8C:27:MET:HG3   | 2.21                     | 0.40              |
| 57:8C:175:LEU:HD13 | 87:8C:305:PGV:H221 | 2.03                     | 0.40              |
| 58:8D:77:GLU:O     | 58:8D:80:THR:OG1   | 2.33                     | 0.40              |
| 59:8E:24:ILE:CD1   | 59:8E:28:GLU:HB2   | 2.51                     | 0.40              |
| 2:1B:47:PRO:HD2    | 2:1B:75:VAL:O      | 2.21                     | 0.40              |
| 2:1B:53:ALA:HB3    | 71:1B:201:SF4:S2   | 2.61                     | 0.40              |
| 3:1C:58:ILE:HD12   | 3:1C:118:GLU:HG2   | 2.03                     | 0.40              |
| 3:1C:147:ASP:OD1   | 3:1C:147:ASP:N     | 2.54                     | 0.40              |
| 4:1D:237:ASN:CB    | 8:1H:284:GLN:OE1   | 2.68                     | 0.40              |
| 6:1F:397:LYS:HA    | 6:1F:397:LYS:HD2   | 1.87                     | 0.40              |
| 7:1G:195:LEU:HD11  | 7:1G:393:ALA:HB2   | 2.02                     | 0.40              |
| 7:1G:349:PHE:H     | 7:1G:509:PRO:HB2   | 1.86                     | 0.40              |
| 12:1L:116:ARG:HD3  | 75:1L:702:CDL:OB3  | 2.20                     | 0.40              |
| 12:1L:341:MET:CE   | 12:1L:457:LEU:HD12 | 2.50                     | 0.40              |
| 12:1L:545:SER:OG   | 13:1M:274:SER:HB3  | 2.22                     | 0.40              |
| 69:1L:703:3PE:H281 | 75:1h:202:CDL:HB62 | 2.04                     | 0.40              |
| 13:1M:325:MET:CE   | 13:1M:441:ILE:HB   | 2.51                     | 0.40              |
| 14:1N:122:ILE:HD12 | 14:1N:126:ALA:HB1  | 2.03                     | 0.40              |
| 15:1O:101:TYR:CE1  | 15:1O:128:ILE:HG23 | 2.48                     | 0.40              |
| 17:1Q:27:GLU:HG2   | 17:1Q:28:GLU:OE1   | 2.21                     | 0.40              |
| 19:1S:17:GLU:HB2   | 19:1S:51:PRO:HB2   | 2.03                     | 0.40              |
| 25:1Z:131:GLU:HG3  | 25:1Z:132:GLU:N    | 2.35                     | 0.40              |
| 28:1c:45:ARG:HE    | 28:1c:45:ARG:HB2   | 1.69                     | 0.40              |
| 33:1h:11:ILE:HG22  | 39:1n:98:VAL:HG12  | 2.03                     | 0.40              |
| 33:1h:56:PRO:HD3   | 41:1p:63:TYR:HE2   | 1.84                     | 0.40              |
| 35:1j:69:ASP:CG    | 40:1o:117:ARG:HH22 | 2.28                     | 0.40              |
| 42:1q:44:TYR:OH    | 42:1q:113:HIS:N    | 2.55                     | 0.40              |
| 45:3A:40:TRP:CZ2   | 45:3A:377:GLU:HA   | 2.57                     | 0.40              |
| 46:3B:181:TYR:CZ   | 46:3B:182:ARG:HG2  | 2.56                     | 0.40              |
| 47:3C:226:ILE:HD12 | 47:3C:226:ILE:HA   | 1.98                     | 0.40              |
| 51:3G:36:ILE:HB    | 51:3G:37:PRO:HD3   | 2.02                     | 0.40              |
| 53:3J:23:THR:N     | 54:3Y:23:MET:SD    | 2.95                     | 0.40              |
| 53:3J:56:TRP:HA    | 53:3J:59:ILE:HG12  | 2.03                     | 0.40              |
| 45:3N:445:ARG:NH2  | 69:3N:501:3PE:O22  | 2.54                     | 0.40              |
| 47:3P:72:ASP:CG    | 48:3Q:49:ARG:HH22  | 2.29                     | 0.40              |
| 75:3P:504:CDL:OA9  | 75:3P:504:CDL:H341 | 2.21                     | 0.40              |
| 55:4A:233:HIS:HB3  | 57:4C:99:TRP:CZ2   | 2.56                     | 0.40              |
| 57:4C:22:LEU:O     | 57:4C:26:LEU:HG    | 2.21                     | 0.40              |
| 57:4C:151:LEU:HD12 | 57:4C:151:LEU:HA   | 1.91                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:4C:305:CDL:H651 | 75:4C:305:CDL:H261 | 2.04                     | 0.40              |
| 62:4H:75:ARG:HB3   | 62:4H:80:THR:O     | 2.21                     | 0.40              |
| 65:4K:42:LEU:HD12  | 87:4K:101:PGV:H221 | 2.02                     | 0.40              |
| 68:4N:14:SER:O     | 68:4N:17:PRO:HD2   | 2.22                     | 0.40              |
| 55:8A:28:MET:HG3   | 66:8L:29:PHE:CD1   | 2.54                     | 0.40              |
| 55:8A:253:MET:O    | 55:8A:257:ILE:HG12 | 2.20                     | 0.40              |
| 55:8A:289:ALA:HB1  | 55:8A:297:MET:HE1  | 2.03                     | 0.40              |
| 56:8B:41:ILE:CG2   | 56:8B:45:MET:CE    | 2.98                     | 0.40              |
| 56:8B:136:LEU:HD22 | 56:8B:193:TYR:HB3  | 2.03                     | 0.40              |
| 56:8B:145:PRO:HA   | 56:8B:214:VAL:O    | 2.20                     | 0.40              |
| 4:1D:237:ASN:HB3   | 8:1H:284:GLN:OE1   | 2.21                     | 0.40              |
| 6:1F:29:HIS:HA     | 44:1s:39:ARG:HH11  | 1.87                     | 0.40              |
| 6:1F:57:LEU:HD23   | 6:1F:57:LEU:HA     | 1.96                     | 0.40              |
| 7:1G:255:HIS:CE1   | 7:1G:257:ASP:HB2   | 2.57                     | 0.40              |
| 8:1H:90:PRO:HG3    | 8:1H:162:LEU:HB3   | 2.04                     | 0.40              |
| 8:1H:149:ILE:HG12  | 8:1H:181:LEU:HD22  | 2.04                     | 0.40              |
| 9:1I:135:PRO:HB2   | 42:1q:93:MET:HE1   | 2.03                     | 0.40              |
| 10:1J:127:ILE:HG21 | 11:1K:2:PRO:HG3    | 2.03                     | 0.40              |
| 12:1L:127:THR:HA   | 12:1L:130:ILE:HD12 | 2.04                     | 0.40              |
| 12:1L:292:ALA:HB2  | 12:1L:304:PHE:CB   | 2.51                     | 0.40              |
| 12:1L:516:PRO:HB3  | 39:1n:29:TRP:CH2   | 2.57                     | 0.40              |
| 13:1M:410:MET:HA   | 13:1M:413:THR:HG22 | 2.03                     | 0.40              |
| 14:1N:149:ILE:CD1  | 14:1N:154:MET:CE   | 2.99                     | 0.40              |
| 14:1N:284:MET:HE3  | 14:1N:284:MET:HB3  | 1.92                     | 0.40              |
| 16:1P:81:ILE:O     | 16:1P:85:VAL:HB    | 2.22                     | 0.40              |
| 16:1P:116:ALA:O    | 16:1P:120:VAL:HG23 | 2.21                     | 0.40              |
| 17:1Q:69:LEU:HA    | 18:1R:27:ARG:HH12  | 1.87                     | 0.40              |
| 20:1U:52:MET:HE1   | 39:1n:23:LEU:HD12  | 2.02                     | 0.40              |
| 21:1V:93:MET:CE    | 21:1V:98:PRO:HG2   | 2.51                     | 0.40              |
| 26:1a:55:SER:HB2   | 26:1a:62:VAL:HG13  | 2.03                     | 0.40              |
| 32:1g:90:ARG:HA    | 32:1g:90:ARG:HD3   | 1.91                     | 0.40              |
| 41:1p:10:PRO:HD2   | 41:1p:108:ARG:HG2  | 2.03                     | 0.40              |
| 45:3A:270:LEU:HD22 | 45:3A:320:LEU:HD21 | 2.03                     | 0.40              |
| 69:3A:503:3PE:N    | 47:3C:3:ASN:OD1    | 2.34                     | 0.40              |
| 47:3C:152:ALA:HB2  | 47:3C:287:LYS:HG2  | 2.03                     | 0.40              |
| 45:3N:444:LEU:HA   | 53:3W:17:THR:HG21  | 2.03                     | 0.40              |
| 46:3O:109:VAL:HB   | 46:3O:119:LEU:HD12 | 2.04                     | 0.40              |
| 47:3P:318:ARG:O    | 47:3P:322:GLN:HG3  | 2.22                     | 0.40              |
| 51:3T:10:MET:HE2   | 51:3T:10:MET:HB2   | 1.90                     | 0.40              |
| 75:3T:101:CDL:HB61 | 75:3T:101:CDL:H711 | 1.49                     | 0.40              |
| 52:3U:47:ARG:HG3   | 52:3U:49:GLN:H     | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:4A:191:THR:CG2  | 55:4A:245:ILE:HG23 | 2.51                     | 0.40              |
| 55:4A:508:PRO:HG2  | 60:4F:32:ASN:ND2   | 2.36                     | 0.40              |
| 87:4A:602:PGV:H181 | 57:4C:31:LEU:HD12  | 2.02                     | 0.40              |
| 56:4B:7:LEU:HD11   | 75:4B:303:CDL:H761 | 2.02                     | 0.40              |
| 56:4B:155:SER:OG   | 56:4B:156:SER:N    | 2.55                     | 0.40              |
| 57:4C:109:THR:OG1  | 87:4C:303:PGV:H062 | 2.21                     | 0.40              |
| 60:4F:62:CYS:HB3   | 60:4F:85:CYS:HB3   | 2.02                     | 0.40              |
| 60:4F:76:LYS:HD3   | 60:4F:76:LYS:C     | 2.47                     | 0.40              |
| 66:4L:38:PHE:HD1   | 66:4L:41:ARG:HD2   | 1.85                     | 0.40              |
| 55:8A:52:GLN:OE1   | 55:8A:56:VAL:CG1   | 2.69                     | 0.40              |
| 59:8E:61:PHE:CE1   | 59:8E:65:VAL:CG2   | 3.05                     | 0.40              |
| 62:8H:6:THR:CA     | 62:8H:9:LYS:HZ2    | 2.29                     | 0.40              |
| 3:1C:49:GLU:HG2    | 3:1C:106:ARG:NE    | 2.36                     | 0.40              |
| 3:1C:177:ASP:OD1   | 3:1C:180:VAL:HG22  | 2.20                     | 0.40              |
| 4:1D:128:ILE:CG1   | 4:1D:325:VAL:HG21  | 2.51                     | 0.40              |
| 5:1E:120:ILE:HG22  | 5:1E:139:LEU:HD22  | 2.02                     | 0.40              |
| 7:1G:521:VAL:HG22  | 7:1G:542:PHE:HB3   | 2.03                     | 0.40              |
| 9:1I:95:GLU:HG3    | 9:1I:108:ARG:HD2   | 2.04                     | 0.40              |
| 10:1J:162:LEU:O    | 10:1J:166:VAL:HG23 | 2.22                     | 0.40              |
| 14:1N:21:MET:HE1   | 70:1d:202:PC1:H3B2 | 2.03                     | 0.40              |
| 14:1N:49:ASN:O     | 14:1N:53:THR:HG23  | 2.22                     | 0.40              |
| 14:1N:258:SER:HB3  | 14:1N:333:SER:O    | 2.22                     | 0.40              |
| 15:1O:100:LEU:HD23 | 15:1O:100:LEU:HA   | 1.90                     | 0.40              |
| 15:1O:136:GLU:O    | 15:1O:140:ARG:HG2  | 2.22                     | 0.40              |
| 17:1Q:82:LEU:HD12  | 17:1Q:82:LEU:HA    | 1.87                     | 0.40              |
| 20:1U:45:LEU:O     | 20:1U:49:GLU:HG3   | 2.21                     | 0.40              |
| 24:1Y:11:ILE:H     | 24:1Y:11:ILE:HG12  | 1.75                     | 0.40              |
| 29:1d:85:LEU:HD23  | 29:1d:85:LEU:HA    | 1.92                     | 0.40              |
| 32:1g:33:GLU:H     | 32:1g:33:GLU:CD    | 2.30                     | 0.40              |
| 35:1j:69:ASP:CB    | 40:1o:117:ARG:HH12 | 2.34                     | 0.40              |
| 37:1l:54:SER:OG    | 37:1l:55:GLN:N     | 2.54                     | 0.40              |
| 40:1o:73:PHE:CG    | 40:1o:74:PRO:HA    | 2.56                     | 0.40              |
| 41:1p:49:GLU:O     | 41:1p:53:GLN:HG2   | 2.21                     | 0.40              |
| 45:3A:154:HIS:NE2  | 45:3A:314:TYR:OH   | 2.39                     | 0.40              |
| 45:3A:436:ARG:HD3  | 47:3C:222:PRO:HD3  | 2.03                     | 0.40              |
| 46:3B:36:ALA:O     | 46:3B:207:ILE:HA   | 2.20                     | 0.40              |
| 48:3D:108:SER:HB2  | 48:3D:288:ASP:CG   | 2.46                     | 0.40              |
| 49:3E:175:PHE:CZ   | 49:3E:215:GLY:HA3  | 2.56                     | 0.40              |
| 49:3E:235:TYR:HA   | 49:3E:243:TYR:H    | 1.87                     | 0.40              |
| 47:3P:344:GLU:HG3  | 51:3T:66:PHE:HE1   | 1.85                     | 0.40              |
| 48:3Q:33:TYR:HA    | 48:3Q:37:CYS:SG    | 2.61                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:3Q:41:HIS:CE1   | 86:3Q:501:HEC:NA   | 2.89                     | 0.40              |
| 49:3R:195:LEU:HD23 | 49:3R:195:LEU:HA   | 1.83                     | 0.40              |
| 52:3U:19:THR:O     | 52:3U:23:GLN:OE1   | 2.39                     | 0.40              |
| 55:4A:217:THR:HB   | 57:4C:195:SER:HB3  | 2.03                     | 0.40              |
| 56:4B:40:TYR:HD2   | 63:4I:24:ALA:HA    | 1.85                     | 0.40              |
| 87:4B:302:PGV:C20  | 87:4C:303:PGV:H62  | 2.52                     | 0.40              |
| 57:4C:181:TYR:HE2  | 93:4C:307:PEK:H22  | 1.87                     | 0.40              |
| 75:4C:305:CDL:H462 | 68:4N:1:MET:HG3    | 2.04                     | 0.40              |
| 58:4D:67:SER:CB    | 59:4E:106:LEU:HB3  | 2.50                     | 0.40              |
| 58:4D:110:THR:HG22 | 58:4D:115:TRP:NE1  | 2.37                     | 0.40              |
| 58:4D:120:THR:O    | 58:4D:124:LEU:HD22 | 2.22                     | 0.40              |
| 66:4L:45:LEU:HD21  | 67:4M:40:TYR:CD2   | 2.56                     | 0.40              |
| 55:8A:119:GLU:OE1  | 55:8A:119:GLU:HA   | 2.22                     | 0.40              |
| 55:8A:220:PHE:CE1  | 55:8A:231:TYR:HB2  | 2.57                     | 0.40              |
| 55:8A:334:TRP:HB2  | 75:8D:201:CDL:H752 | 2.04                     | 0.40              |
| 75:8B:303:CDL:H861 | 75:8B:303:CDL:H202 | 2.04                     | 0.40              |
| 57:8C:76:GLN:NE2   | 57:8C:231:HIS:CE1  | 2.89                     | 0.40              |
| 68:8N:44:CYS:HB2   | 68:8N:53:PRO:HG3   | 2.02                     | 0.40              |
| 2:1B:116:MET:SD    | 2:1B:156:LEU:HD22  | 2.61                     | 0.40              |
| 4:1D:417:ILE:O     | 4:1D:420:THR:HG22  | 2.22                     | 0.40              |
| 5:1E:187:ARG:HA    | 5:1E:187:ARG:HD3   | 1.82                     | 0.40              |
| 6:1F:52:GLY:O      | 6:1F:56:ILE:HG13   | 2.21                     | 0.40              |
| 6:1F:270:GLU:HG3   | 6:1F:271:GLU:N     | 2.36                     | 0.40              |
| 6:1F:391:SER:OG    | 43:1r:48:LEU:HB3   | 2.21                     | 0.40              |
| 7:1G:53:ARG:CZ     | 7:1G:56:LEU:HD11   | 2.51                     | 0.40              |
| 7:1G:201:ASP:OD2   | 7:1G:268:ARG:NH1   | 2.54                     | 0.40              |
| 7:1G:508:LYS:H     | 7:1G:508:LYS:HG2   | 1.69                     | 0.40              |
| 70:1H:402:PC1:O12  | 9:1I:24:THR:HG23   | 2.22                     | 0.40              |
| 12:1L:364:LYS:O    | 35:1j:17:LEU:HD21  | 2.22                     | 0.40              |
| 12:1L:483:PRO:HB2  | 12:1L:485:TYR:CD1  | 2.56                     | 0.40              |
| 13:1M:133:ILE:HG12 | 13:1M:223:ALA:HB2  | 2.02                     | 0.40              |
| 13:1M:225:ILE:HD13 | 13:1M:331:ASN:HB2  | 2.02                     | 0.40              |
| 14:1N:73:ALA:HB3   | 14:1N:98:MET:HE3   | 2.04                     | 0.40              |
| 14:1N:198:THR:O    | 14:1N:202:ILE:HG13 | 2.22                     | 0.40              |
| 14:1N:323:MET:H    | 14:1N:323:MET:HG2  | 1.71                     | 0.40              |
| 16:1P:57:MET:HA    | 16:1P:60:ARG:HE    | 1.85                     | 0.40              |
| 16:1P:253:PHE:O    | 16:1P:254:LEU:HD23 | 2.22                     | 0.40              |
| 17:1Q:69:LEU:HD11  | 42:1q:126:PRO:HG2  | 2.03                     | 0.40              |
| 19:1S:32:VAL:O     | 19:1S:36:ILE:HG12  | 2.21                     | 0.40              |
| 20:1T:37:MET:HE2   | 20:1T:37:MET:HB2   | 1.70                     | 0.40              |
| 75:1X:201:CDL:H382 | 29:1d:32:VAL:HG12  | 2.04                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:1Z:57:ARG:HA    | 25:1Z:60:LEU:HD12  | 2.03                     | 0.40              |
| 29:1d:34:MET:HE1   | 75:1d:203:CDL:H441 | 2.04                     | 0.40              |
| 40:1o:93:ASP:C     | 40:1o:93:ASP:OD1   | 2.64                     | 0.40              |
| 42:1q:8:ARG:HG2    | 42:1q:12:GLN:HE21  | 1.86                     | 0.40              |
| 45:3A:64:PHE:CD1   | 45:3A:86:LEU:HD21  | 2.56                     | 0.40              |
| 49:3E:174:LEU:HD12 | 49:3E:213:LEU:O    | 2.21                     | 0.40              |
| 49:3E:195:LEU:O    | 49:3E:195:LEU:HD12 | 2.22                     | 0.40              |
| 49:3E:226:ALA:HA   | 49:3E:234:TYR:CD1  | 2.56                     | 0.40              |
| 70:3J:101:PC1:H2C1 | 54:3Y:31:GLY:HA3   | 2.02                     | 0.40              |
| 45:3N:373:THR:HB   | 45:3N:374:PRO:HD3  | 2.03                     | 0.40              |
| 48:3Q:98:PRO:O     | 48:3Q:102:ARG:HG3  | 2.20                     | 0.40              |
| 49:3R:150:SER:HB3  | 49:3R:170:ARG:N    | 2.30                     | 0.40              |
| 49:3R:184:ILE:H    | 49:3R:184:ILE:HG13 | 1.68                     | 0.40              |
| 51:3T:32:LYS:HB2   | 51:3T:32:LYS:HE2   | 1.75                     | 0.40              |
| 55:4A:495:LEU:HD22 | 60:4F:73:TRP:CD1   | 2.57                     | 0.40              |
| 56:4B:89:GLU:OE2   | 68:4N:68:VAL:CB    | 2.67                     | 0.40              |
| 60:4F:82:CYS:SG    | 60:4F:83:PRO:CD    | 3.10                     | 0.40              |
| 87:8B:301:PGV:H342 | 87:8B:301:PGV:H302 | 2.04                     | 0.40              |
| 57:8C:6:HIS:CD2    | 57:8C:8:TYR:HB2    | 2.56                     | 0.40              |
| 57:8C:63:ARG:CD    | 64:8J:12:PHE:CE2   | 3.04                     | 0.40              |
| 87:8G:101:PGV:H202 | 87:8G:101:PGV:H012 | 1.18                     | 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   | 1A    | 113/115 (98%) | 103 (91%) | 8 (7%)  | 2 (2%)   | 6           | 6   |
| 2   | 1B    | 153/258 (59%) | 145 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 3   | 1C    | 207/264 (78%) | 199 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 4   | 1D    | 427/476 (90%) | 412 (96%) | 15 (4%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|------------|---------|----------|-------------|-----|
| 5   | 1E    | 212/249 (85%)  | 200 (94%)  | 11 (5%) | 1 (0%)   | 24          | 31  |
| 6   | 1F    | 430/464 (93%)  | 402 (94%)  | 25 (6%) | 3 (1%)   | 18          | 23  |
| 7   | 1G    | 697/727 (96%)  | 668 (96%)  | 28 (4%) | 1 (0%)   | 48          | 60  |
| 8   | 1H    | 316/318 (99%)  | 294 (93%)  | 20 (6%) | 2 (1%)   | 21          | 27  |
| 9   | 1I    | 174/239 (73%)  | 167 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 10  | 1J    | 172/175 (98%)  | 161 (94%)  | 10 (6%) | 1 (1%)   | 21          | 27  |
| 11  | 1K    | 96/98 (98%)    | 93 (97%)   | 2 (2%)  | 1 (1%)   | 12          | 15  |
| 12  | 1L    | 604/606 (100%) | 563 (93%)  | 41 (7%) | 0        | 100         | 100 |
| 13  | 1M    | 457/459 (100%) | 448 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 14  | 1N    | 345/347 (99%)  | 335 (97%)  | 9 (3%)  | 1 (0%)   | 36          | 46  |
| 15  | 1O    | 318/357 (89%)  | 305 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 16  | 1P    | 340/377 (90%)  | 326 (96%)  | 14 (4%) | 0        | 100         | 100 |
| 17  | 1Q    | 127/175 (73%)  | 118 (93%)  | 9 (7%)  | 0        | 100         | 100 |
| 18  | 1R    | 94/123 (76%)   | 89 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 19  | 1S    | 85/99 (86%)    | 80 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 20  | 1T    | 83/156 (53%)   | 82 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 20  | 1U    | 84/156 (54%)   | 79 (94%)   | 5 (6%)  | 0        | 100         | 100 |
| 21  | 1V    | 113/116 (97%)  | 110 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 22  | 1W    | 113/128 (88%)  | 106 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 23  | 1X    | 169/172 (98%)  | 163 (96%)  | 5 (3%)  | 1 (1%)   | 21          | 27  |
| 24  | 1Y    | 137/141 (97%)  | 135 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 25  | 1Z    | 139/144 (96%)  | 137 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 26  | 1a    | 68/70 (97%)    | 68 (100%)  | 0       | 0        | 100         | 100 |
| 27  | 1b    | 81/84 (96%)    | 74 (91%)   | 7 (9%)  | 0        | 100         | 100 |
| 28  | 1c    | 47/76 (62%)    | 46 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 29  | 1d    | 117/122 (96%)  | 113 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 30  | 1e    | 97/106 (92%)   | 92 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 31  | 1f    | 55/135 (41%)   | 50 (91%)   | 5 (9%)  | 0        | 100         | 100 |
| 32  | 1g    | 98/154 (64%)   | 90 (92%)   | 8 (8%)  | 0        | 100         | 100 |
| 33  | 1h    | 136/189 (72%)  | 136 (100%) | 0       | 0        | 100         | 100 |
| 34  | 1i    | 126/128 (98%)  | 118 (94%)  | 8 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 35  | 1j    | 69/105 (66%)   | 67 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 36  | 1k    | 79/98 (81%)    | 76 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 37  | 1l    | 154/186 (83%)  | 146 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 38  | 1m    | 126/129 (98%)  | 122 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 39  | 1n    | 170/179 (95%)  | 161 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 40  | 1o    | 120/137 (88%)  | 114 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 41  | 1p    | 171/176 (97%)  | 170 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 42  | 1q    | 143/145 (99%)  | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 43  | 1r    | 90/113 (80%)   | 87 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 44  | 1s    | 43/471 (9%)    | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 45  | 3A    | 436/480 (91%)  | 428 (98%) | 6 (1%)  | 2 (0%)   | 24          | 31  |
| 45  | 3N    | 444/480 (92%)  | 427 (96%) | 16 (4%) | 1 (0%)   | 43          | 55  |
| 46  | 3B    | 414/453 (91%)  | 403 (97%) | 11 (3%) | 0        | 100         | 100 |
| 46  | 3O    | 413/453 (91%)  | 404 (98%) | 8 (2%)  | 1 (0%)   | 43          | 55  |
| 47  | 3C    | 377/379 (100%) | 366 (97%) | 11 (3%) | 0        | 100         | 100 |
| 47  | 3P    | 377/379 (100%) | 369 (98%) | 8 (2%)  | 0        | 100         | 100 |
| 48  | 3D    | 235/326 (72%)  | 229 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 48  | 3Q    | 237/326 (73%)  | 231 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 49  | 3E    | 194/274 (71%)  | 177 (91%) | 16 (8%) | 1 (0%)   | 24          | 31  |
| 49  | 3I    | 45/274 (16%)   | 43 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 49  | 3R    | 194/274 (71%)  | 172 (89%) | 18 (9%) | 4 (2%)   | 5           | 4   |
| 49  | 3V    | 29/274 (11%)   | 29 (100%) | 0       | 0        | 100         | 100 |
| 50  | 3F    | 96/111 (86%)   | 95 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 50  | 3S    | 96/111 (86%)   | 96 (100%) | 0       | 0        | 100         | 100 |
| 51  | 3G    | 72/82 (88%)    | 71 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 51  | 3T    | 72/82 (88%)    | 71 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 52  | 3H    | 63/91 (69%)    | 62 (98%)  | 0       | 1 (2%)   | 7           | 7   |
| 52  | 3U    | 63/91 (69%)    | 62 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 53  | 3J    | 54/60 (90%)    | 52 (96%)  | 1 (2%)  | 1 (2%)   | 6           | 5   |
| 53  | 3W    | 54/60 (90%)    | 53 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 54  | 3X    | 50/56 (89%)    | 47 (94%)  | 3 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 54  | 3Y    | 49/56 (88%)       | 45 (92%)    | 4 (8%)   | 0        | 100         | 100 |
| 55  | 4A    | 512/514 (100%)    | 497 (97%)   | 14 (3%)  | 1 (0%)   | 43          | 55  |
| 55  | 8A    | 512/514 (100%)    | 497 (97%)   | 13 (2%)  | 2 (0%)   | 30          | 38  |
| 56  | 4B    | 225/229 (98%)     | 215 (96%)   | 10 (4%)  | 0        | 100         | 100 |
| 56  | 8B    | 225/229 (98%)     | 216 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 57  | 4C    | 257/261 (98%)     | 251 (98%)   | 6 (2%)   | 0        | 100         | 100 |
| 57  | 8C    | 257/261 (98%)     | 248 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 58  | 4D    | 137/169 (81%)     | 126 (92%)   | 11 (8%)  | 0        | 100         | 100 |
| 58  | 8D    | 137/169 (81%)     | 132 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 59  | 4E    | 103/152 (68%)     | 101 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 59  | 8E    | 103/152 (68%)     | 101 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 60  | 4F    | 95/128 (74%)      | 92 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 60  | 8F    | 95/128 (74%)      | 92 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 61  | 4G    | 73/97 (75%)       | 70 (96%)    | 3 (4%)   | 0        | 100         | 100 |
| 61  | 8G    | 73/97 (75%)       | 69 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| 62  | 4H    | 80/86 (93%)       | 75 (94%)    | 5 (6%)   | 0        | 100         | 100 |
| 62  | 8H    | 80/86 (93%)       | 74 (92%)    | 6 (8%)   | 0        | 100         | 100 |
| 63  | 4I    | 65/75 (87%)       | 64 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 63  | 8I    | 65/75 (87%)       | 64 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 64  | 4J    | 56/80 (70%)       | 55 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 64  | 8J    | 56/80 (70%)       | 54 (96%)    | 2 (4%)   | 0        | 100         | 100 |
| 65  | 4K    | 47/80 (59%)       | 44 (94%)    | 3 (6%)   | 0        | 100         | 100 |
| 65  | 8K    | 47/80 (59%)       | 46 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 66  | 4L    | 44/63 (70%)       | 43 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 66  | 8L    | 44/63 (70%)       | 44 (100%)   | 0        | 0        | 100         | 100 |
| 67  | 4M    | 41/70 (59%)       | 41 (100%)   | 0        | 0        | 100         | 100 |
| 67  | 8M    | 41/70 (59%)       | 41 (100%)   | 0        | 0        | 100         | 100 |
| 68  | 4N    | 80/82 (98%)       | 72 (90%)    | 7 (9%)   | 1 (1%)   | 9           | 10  |
| 68  | 8N    | 80/82 (98%)       | 70 (88%)    | 9 (11%)  | 1 (1%)   | 9           | 10  |
| All | All   | 15889/19086 (83%) | 15257 (96%) | 603 (4%) | 29 (0%)  | 44          | 55  |

All (29) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | 1H    | 92  | PRO  |
| 10  | 1J    | 66  | VAL  |
| 23  | 1X    | 28  | ALA  |
| 49  | 3E    | 271 | VAL  |
| 53  | 3J    | 57  | LYS  |
| 45  | 3N    | 224 | VAL  |
| 1   | 1A    | 52  | SER  |
| 8   | 1H    | 208 | VAL  |
| 49  | 3R    | 181 | LYS  |
| 49  | 3R    | 228 | ALA  |
| 68  | 8N    | 33  | VAL  |
| 1   | 1A    | 109 | LYS  |
| 6   | 1F    | 249 | ARG  |
| 6   | 1F    | 297 | VAL  |
| 49  | 3R    | 273 | VAL  |
| 68  | 4N    | 33  | VAL  |
| 46  | 3O    | 171 | ALA  |
| 49  | 3R    | 150 | SER  |
| 7   | 1G    | 654 | GLN  |
| 11  | 1K    | 2   | PRO  |
| 45  | 3A    | 231 | PHE  |
| 5   | 1E    | 215 | ALA  |
| 6   | 1F    | 207 | PRO  |
| 45  | 3A    | 350 | THR  |
| 52  | 3H    | 79  | ASP  |
| 55  | 8A    | 128 | VAL  |
| 55  | 4A    | 128 | VAL  |
| 55  | 8A    | 3   | VAL  |
| 14  | 1N    | 110 | 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   | 1A    | 99/99 (100%)  | 99 (100%)  | 0        | 100         | 100 |
| 2   | 1B    | 131/212 (62%) | 130 (99%)  | 1 (1%)   | 73          | 86  |
| 3   | 1C    | 190/227 (84%) | 190 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | 1D    | 371/405 (92%)  | 370 (100%) | 1 (0%)   | 86          | 93  |
| 5   | 1E    | 183/207 (88%)  | 183 (100%) | 0        | 100         | 100 |
| 6   | 1F    | 346/368 (94%)  | 344 (99%)  | 2 (1%)   | 78          | 89  |
| 7   | 1G    | 588/610 (96%)  | 587 (100%) | 1 (0%)   | 87          | 94  |
| 8   | 1H    | 274/274 (100%) | 273 (100%) | 1 (0%)   | 84          | 92  |
| 9   | 1I    | 151/201 (75%)  | 151 (100%) | 0        | 100         | 100 |
| 10  | 1J    | 140/141 (99%)  | 139 (99%)  | 1 (1%)   | 76          | 87  |
| 11  | 1K    | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 12  | 1L    | 539/539 (100%) | 539 (100%) | 0        | 100         | 100 |
| 13  | 1M    | 408/408 (100%) | 407 (100%) | 1 (0%)   | 87          | 94  |
| 14  | 1N    | 310/310 (100%) | 310 (100%) | 0        | 100         | 100 |
| 15  | 1O    | 283/307 (92%)  | 283 (100%) | 0        | 100         | 100 |
| 16  | 1P    | 296/323 (92%)  | 296 (100%) | 0        | 100         | 100 |
| 17  | 1Q    | 117/152 (77%)  | 117 (100%) | 0        | 100         | 100 |
| 18  | 1R    | 79/97 (81%)    | 78 (99%)   | 1 (1%)   | 61          | 77  |
| 19  | 1S    | 77/82 (94%)    | 77 (100%)  | 0        | 100         | 100 |
| 20  | 1T    | 79/133 (59%)   | 79 (100%)  | 0        | 100         | 100 |
| 20  | 1U    | 79/133 (59%)   | 79 (100%)  | 0        | 100         | 100 |
| 21  | 1V    | 100/101 (99%)  | 100 (100%) | 0        | 100         | 100 |
| 22  | 1W    | 107/112 (96%)  | 107 (100%) | 0        | 100         | 100 |
| 23  | 1X    | 153/154 (99%)  | 153 (100%) | 0        | 100         | 100 |
| 24  | 1Y    | 101/102 (99%)  | 101 (100%) | 0        | 100         | 100 |
| 25  | 1Z    | 123/124 (99%)  | 123 (100%) | 0        | 100         | 100 |
| 26  | 1a    | 58/58 (100%)   | 58 (100%)  | 0        | 100         | 100 |
| 27  | 1b    | 69/70 (99%)    | 69 (100%)  | 0        | 100         | 100 |
| 28  | 1c    | 45/66 (68%)    | 45 (100%)  | 0        | 100         | 100 |
| 29  | 1d    | 106/109 (97%)  | 105 (99%)  | 1 (1%)   | 70          | 84  |
| 30  | 1e    | 87/94 (93%)    | 87 (100%)  | 0        | 100         | 100 |
| 31  | 1f    | 54/113 (48%)   | 54 (100%)  | 0        | 100         | 100 |
| 32  | 1g    | 92/129 (71%)   | 91 (99%)   | 1 (1%)   | 65          | 81  |
| 33  | 1h    | 121/158 (77%)  | 120 (99%)  | 1 (1%)   | 73          | 86  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 34  | 1i    | 120/120 (100%) | 119 (99%)  | 1 (1%)   | 73          | 86  |
| 35  | 1j    | 62/84 (74%)    | 62 (100%)  | 0        | 100         | 100 |
| 36  | 1k    | 63/76 (83%)    | 63 (100%)  | 0        | 100         | 100 |
| 37  | 1l    | 141/161 (88%)  | 141 (100%) | 0        | 100         | 100 |
| 38  | 1m    | 113/114 (99%)  | 112 (99%)  | 1 (1%)   | 70          | 84  |
| 39  | 1n    | 156/160 (98%)  | 156 (100%) | 0        | 100         | 100 |
| 40  | 1o    | 110/119 (92%)  | 110 (100%) | 0        | 100         | 100 |
| 41  | 1p    | 154/156 (99%)  | 153 (99%)  | 1 (1%)   | 78          | 89  |
| 42  | 1q    | 131/131 (100%) | 131 (100%) | 0        | 100         | 100 |
| 43  | 1r    | 85/98 (87%)    | 85 (100%)  | 0        | 100         | 100 |
| 44  | 1s    | 44/351 (12%)   | 44 (100%)  | 0        | 100         | 100 |
| 45  | 3A    | 367/397 (92%)  | 366 (100%) | 1 (0%)   | 86          | 93  |
| 45  | 3N    | 372/397 (94%)  | 370 (100%) | 2 (0%)   | 81          | 90  |
| 46  | 3B    | 328/355 (92%)  | 327 (100%) | 1 (0%)   | 86          | 93  |
| 46  | 3O    | 327/355 (92%)  | 327 (100%) | 0        | 100         | 100 |
| 47  | 3C    | 332/332 (100%) | 332 (100%) | 0        | 100         | 100 |
| 47  | 3P    | 332/332 (100%) | 330 (99%)  | 2 (1%)   | 78          | 89  |
| 48  | 3D    | 202/259 (78%)  | 202 (100%) | 0        | 100         | 100 |
| 48  | 3Q    | 204/259 (79%)  | 203 (100%) | 1 (0%)   | 81          | 90  |
| 49  | 3E    | 166/226 (74%)  | 165 (99%)  | 1 (1%)   | 78          | 89  |
| 49  | 3I    | 37/226 (16%)   | 37 (100%)  | 0        | 100         | 100 |
| 49  | 3R    | 166/226 (74%)  | 165 (99%)  | 1 (1%)   | 78          | 89  |
| 49  | 3V    | 24/226 (11%)   | 23 (96%)   | 1 (4%)   | 26          | 40  |
| 50  | 3F    | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 50  | 3S    | 90/99 (91%)    | 90 (100%)  | 0        | 100         | 100 |
| 51  | 3G    | 67/73 (92%)    | 67 (100%)  | 0        | 100         | 100 |
| 51  | 3T    | 67/73 (92%)    | 67 (100%)  | 0        | 100         | 100 |
| 52  | 3H    | 62/85 (73%)    | 62 (100%)  | 0        | 100         | 100 |
| 52  | 3U    | 62/85 (73%)    | 62 (100%)  | 0        | 100         | 100 |
| 53  | 3J    | 46/48 (96%)    | 46 (100%)  | 0        | 100         | 100 |
| 53  | 3W    | 46/48 (96%)    | 46 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 54  | 3X    | 42/46 (91%)       | 42 (100%)    | 0        | 100         | 100 |
| 54  | 3Y    | 41/46 (89%)       | 41 (100%)    | 0        | 100         | 100 |
| 55  | 4A    | 424/424 (100%)    | 423 (100%)   | 1 (0%)   | 87          | 94  |
| 55  | 8A    | 424/424 (100%)    | 423 (100%)   | 1 (0%)   | 87          | 94  |
| 56  | 4B    | 210/211 (100%)    | 208 (99%)    | 2 (1%)   | 68          | 82  |
| 56  | 8B    | 210/211 (100%)    | 208 (99%)    | 2 (1%)   | 68          | 82  |
| 57  | 4C    | 223/225 (99%)     | 223 (100%)   | 0        | 100         | 100 |
| 57  | 8C    | 223/225 (99%)     | 222 (100%)   | 1 (0%)   | 84          | 92  |
| 58  | 4D    | 124/149 (83%)     | 124 (100%)   | 0        | 100         | 100 |
| 58  | 8D    | 124/149 (83%)     | 124 (100%)   | 0        | 100         | 100 |
| 59  | 4E    | 92/124 (74%)      | 92 (100%)    | 0        | 100         | 100 |
| 59  | 8E    | 92/124 (74%)      | 91 (99%)     | 1 (1%)   | 65          | 81  |
| 60  | 4F    | 80/100 (80%)      | 79 (99%)     | 1 (1%)   | 61          | 77  |
| 60  | 8F    | 80/100 (80%)      | 80 (100%)    | 0        | 100         | 100 |
| 61  | 4G    | 65/80 (81%)       | 65 (100%)    | 0        | 100         | 100 |
| 61  | 8G    | 65/80 (81%)       | 65 (100%)    | 0        | 100         | 100 |
| 62  | 4H    | 73/76 (96%)       | 72 (99%)     | 1 (1%)   | 59          | 76  |
| 62  | 8H    | 73/76 (96%)       | 73 (100%)    | 0        | 100         | 100 |
| 63  | 4I    | 54/61 (88%)       | 54 (100%)    | 0        | 100         | 100 |
| 63  | 8I    | 54/61 (88%)       | 54 (100%)    | 0        | 100         | 100 |
| 64  | 4J    | 49/68 (72%)       | 47 (96%)     | 2 (4%)   | 27          | 41  |
| 64  | 8J    | 49/68 (72%)       | 48 (98%)     | 1 (2%)   | 48          | 67  |
| 65  | 4K    | 38/66 (58%)       | 38 (100%)    | 0        | 100         | 100 |
| 65  | 8K    | 38/66 (58%)       | 36 (95%)     | 2 (5%)   | 20          | 30  |
| 66  | 4L    | 39/55 (71%)       | 38 (97%)     | 1 (3%)   | 40          | 59  |
| 66  | 8L    | 39/55 (71%)       | 39 (100%)    | 0        | 100         | 100 |
| 67  | 4M    | 37/57 (65%)       | 36 (97%)     | 1 (3%)   | 39          | 58  |
| 67  | 8M    | 37/57 (65%)       | 36 (97%)     | 1 (3%)   | 39          | 58  |
| 68  | 4N    | 70/70 (100%)      | 70 (100%)    | 0        | 100         | 100 |
| 68  | 8N    | 70/70 (100%)      | 70 (100%)    | 0        | 100         | 100 |
| All | All   | 13845/16096 (86%) | 13802 (100%) | 43 (0%)  | 84          | 93  |

All (43) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1B    | 134 | ARG  |
| 4   | 1D    | 337 | GLU  |
| 6   | 1F    | 21  | ILE  |
| 6   | 1F    | 247 | ARG  |
| 7   | 1G    | 651 | LEU  |
| 8   | 1H    | 127 | TYR  |
| 10  | 1J    | 66  | VAL  |
| 13  | 1M    | 114 | GLU  |
| 18  | 1R    | 89  | LEU  |
| 29  | 1d    | 64  | TYR  |
| 32  | 1g    | 54  | ASP  |
| 33  | 1h    | 79  | PHE  |
| 34  | 1i    | 16  | GLU  |
| 38  | 1m    | 117 | GLU  |
| 41  | 1p    | 34  | LYS  |
| 45  | 3A    | 146 | ARG  |
| 46  | 3B    | 400 | GLN  |
| 49  | 3E    | 218 | THR  |
| 45  | 3N    | 112 | LEU  |
| 45  | 3N    | 117 | VAL  |
| 47  | 3P    | 254 | ASP  |
| 47  | 3P    | 345 | HIS  |
| 48  | 3Q    | 97  | ASN  |
| 49  | 3R    | 152 | ILE  |
| 49  | 3V    | 76  | VAL  |
| 55  | 4A    | 101 | SER  |
| 56  | 4B    | 45  | MET  |
| 56  | 4B    | 55  | THR  |
| 60  | 4F    | 51  | SER  |
| 62  | 4H    | 31  | GLN  |
| 64  | 4J    | 15  | ASP  |
| 64  | 4J    | 49  | CYS  |
| 66  | 4L    | 46  | LYS  |
| 67  | 4M    | 25  | SER  |
| 55  | 8A    | 69  | MET  |
| 56  | 8B    | 158 | ASP  |
| 56  | 8B    | 181 | GLN  |
| 57  | 8C    | 92  | LEU  |
| 59  | 8E    | 33  | MET  |
| 64  | 8J    | 57  | HIS  |
| 65  | 8K    | 15  | ASN  |
| 65  | 8K    | 52  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 67  | 8M    | 4   | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1B    | 106 | GLN  |
| 2   | 1B    | 162 | GLN  |
| 2   | 1B    | 164 | GLN  |
| 3   | 1C    | 39  | GLN  |
| 3   | 1C    | 41  | GLN  |
| 3   | 1C    | 144 | ASN  |
| 4   | 1D    | 129 | GLN  |
| 4   | 1D    | 201 | GLN  |
| 4   | 1D    | 316 | ASN  |
| 5   | 1E    | 15  | ASN  |
| 5   | 1E    | 27  | ASN  |
| 5   | 1E    | 37  | ASN  |
| 6   | 1F    | 250 | ASN  |
| 7   | 1G    | 51  | ASN  |
| 7   | 1G    | 101 | HIS  |
| 7   | 1G    | 259 | ASN  |
| 7   | 1G    | 476 | ASN  |
| 7   | 1G    | 646 | ASN  |
| 8   | 1H    | 157 | ASN  |
| 8   | 1H    | 304 | HIS  |
| 9   | 1I    | 144 | HIS  |
| 9   | 1I    | 150 | ASN  |
| 11  | 1K    | 92  | ASN  |
| 12  | 1L    | 23  | ASN  |
| 12  | 1L    | 30  | ASN  |
| 12  | 1L    | 194 | ASN  |
| 12  | 1L    | 351 | ASN  |
| 12  | 1L    | 506 | ASN  |
| 12  | 1L    | 603 | ASN  |
| 13  | 1M    | 51  | ASN  |
| 13  | 1M    | 168 | GLN  |
| 13  | 1M    | 220 | HIS  |
| 13  | 1M    | 331 | ASN  |
| 14  | 1N    | 174 | GLN  |
| 14  | 1N    | 204 | ASN  |
| 14  | 1N    | 322 | GLN  |
| 14  | 1N    | 347 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | 1O    | 114 | HIS  |
| 15  | 1O    | 120 | GLN  |
| 15  | 1O    | 251 | GLN  |
| 15  | 1O    | 288 | GLN  |
| 16  | 1P    | 136 | ASN  |
| 16  | 1P    | 321 | HIS  |
| 19  | 1S    | 47  | ASN  |
| 19  | 1S    | 72  | GLN  |
| 19  | 1S    | 85  | GLN  |
| 20  | 1U    | 33  | ASN  |
| 21  | 1V    | 75  | GLN  |
| 22  | 1W    | 51  | GLN  |
| 22  | 1W    | 70  | ASN  |
| 22  | 1W    | 99  | GLN  |
| 23  | 1X    | 98  | HIS  |
| 24  | 1Y    | 78  | GLN  |
| 24  | 1Y    | 88  | ASN  |
| 26  | 1a    | 25  | HIS  |
| 29  | 1d    | 46  | ASN  |
| 30  | 1e    | 44  | HIS  |
| 32  | 1g    | 103 | ASN  |
| 34  | 1i    | 47  | ASN  |
| 34  | 1i    | 51  | GLN  |
| 34  | 1i    | 127 | HIS  |
| 38  | 1m    | 51  | ASN  |
| 39  | 1n    | 12  | GLN  |
| 39  | 1n    | 13  | GLN  |
| 40  | 1o    | 81  | HIS  |
| 40  | 1o    | 116 | GLN  |
| 41  | 1p    | 106 | GLN  |
| 41  | 1p    | 123 | ASN  |
| 42  | 1q    | 123 | GLN  |
| 43  | 1r    | 35  | GLN  |
| 44  | 1s    | 44  | HIS  |
| 44  | 1s    | 65  | GLN  |
| 44  | 1s    | 71  | GLN  |
| 44  | 1s    | 75  | HIS  |
| 45  | 3A    | 94  | HIS  |
| 45  | 3A    | 159 | GLN  |
| 46  | 3B    | 305 | GLN  |
| 46  | 3B    | 354 | ASN  |
| 46  | 3B    | 358 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | 3C    | 54  | HIS  |
| 47  | 3C    | 85  | ASN  |
| 47  | 3C    | 341 | GLN  |
| 48  | 3D    | 102 | HIS  |
| 48  | 3D    | 193 | ASN  |
| 49  | 3E    | 131 | ASN  |
| 49  | 3E    | 164 | ASN  |
| 49  | 3E    | 199 | GLN  |
| 50  | 3F    | 34  | ASN  |
| 51  | 3G    | 25  | GLN  |
| 51  | 3G    | 75  | ASN  |
| 45  | 3N    | 9   | GLN  |
| 45  | 3N    | 69  | ASN  |
| 45  | 3N    | 159 | GLN  |
| 46  | 3O    | 143 | GLN  |
| 46  | 3O    | 351 | ASN  |
| 46  | 3O    | 354 | ASN  |
| 47  | 3P    | 54  | HIS  |
| 47  | 3P    | 85  | ASN  |
| 47  | 3P    | 341 | GLN  |
| 49  | 3R    | 257 | ASN  |
| 55  | 4A    | 214 | ASN  |
| 55  | 4A    | 491 | ASN  |
| 57  | 4C    | 50  | ASN  |
| 57  | 4C    | 76  | GLN  |
| 57  | 4C    | 231 | HIS  |
| 58  | 4D    | 29  | HIS  |
| 58  | 4D    | 72  | ASN  |
| 58  | 4D    | 76  | ASN  |
| 59  | 4E    | 78  | HIS  |
| 60  | 4F    | 32  | ASN  |
| 60  | 4F    | 94  | HIS  |
| 61  | 4G    | 41  | HIS  |
| 61  | 4G    | 43  | HIS  |
| 62  | 4H    | 22  | ASN  |
| 62  | 4H    | 28  | ASN  |
| 66  | 4L    | 17  | ASN  |
| 66  | 4L    | 42  | HIS  |
| 68  | 4N    | 8   | GLN  |
| 68  | 4N    | 55  | ASN  |
| 55  | 8A    | 328 | HIS  |
| 55  | 8A    | 406 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 55  | 8A    | 413 | HIS  |
| 55  | 8A    | 422 | ASN  |
| 56  | 8B    | 6   | GLN  |
| 56  | 8B    | 24  | HIS  |
| 57  | 8C    | 6   | HIS  |
| 57  | 8C    | 38  | ASN  |
| 57  | 8C    | 50  | ASN  |
| 57  | 8C    | 76  | GLN  |
| 57  | 8C    | 122 | HIS  |
| 59  | 8E    | 78  | HIS  |
| 59  | 8E    | 94  | ASN  |
| 60  | 8F    | 66  | ASN  |
| 62  | 8H    | 12  | GLN  |
| 62  | 8H    | 25  | GLN  |
| 62  | 8H    | 28  | ASN  |
| 64  | 8J    | 29  | ASN  |
| 65  | 8K    | 41  | ASN  |
| 68  | 8N    | 12  | HIS  |
| 68  | 8N    | 50  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 14  | FME  | 1N    | 1   | 14   | 8,9,10       | 0.56 | 0           | 8,9,11      | 1.02 | 1 (12%)     |
| 1   | FME  | 1A    | 1   | 1    | 8,9,10       | 0.54 | 0           | 8,9,11      | 1.07 | 1 (12%)     |
| 56  | FME  | 4B    | 1   | 56   | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.99 | 1 (12%)     |
| 13  | FME  | 1M    | 1   | 13   | 8,9,10       | 0.56 | 0           | 8,9,11      | 1.04 | 1 (12%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 55  | FME  | 8A    | 1   | 55   | 8,9,10       | 0.55 | 0        | 8,9,11      | 1.16 | 1 (12%)  |
| 12  | FME  | 1L    | 1   | 12   | 8,9,10       | 0.57 | 0        | 8,9,11      | 0.90 | 1 (12%)  |
| 11  | FME  | 1K    | 1   | 11   | 8,9,10       | 0.55 | 0        | 8,9,11      | 0.98 | 1 (12%)  |
| 56  | FME  | 8B    | 1   | 56   | 8,9,10       | 0.56 | 0        | 8,9,11      | 0.83 | 1 (12%)  |
| 8   | FME  | 1H    | 1   | 8    | 8,9,10       | 0.56 | 0        | 8,9,11      | 1.01 | 1 (12%)  |
| 55  | FME  | 4A    | 1   | 55   | 8,9,10       | 0.55 | 0        | 8,9,11      | 1.01 | 1 (12%)  |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 14  | FME  | 1N    | 1   | 14   | -       | 1/7/9/11 | -     |
| 1   | FME  | 1A    | 1   | 1    | -       | 0/7/9/11 | -     |
| 56  | FME  | 4B    | 1   | 56   | -       | 3/7/9/11 | -     |
| 13  | FME  | 1M    | 1   | 13   | -       | 0/7/9/11 | -     |
| 55  | FME  | 8A    | 1   | 55   | -       | 1/7/9/11 | -     |
| 12  | FME  | 1L    | 1   | 12   | -       | 1/7/9/11 | -     |
| 11  | FME  | 1K    | 1   | 11   | -       | 3/7/9/11 | -     |
| 56  | FME  | 8B    | 1   | 56   | -       | 1/7/9/11 | -     |
| 8   | FME  | 1H    | 1   | 8    | -       | 1/7/9/11 | -     |
| 55  | FME  | 4A    | 1   | 55   | -       | 1/7/9/11 | -     |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13  | 1M    | 1   | FME  | O-C-CA | -2.63 | 118.01      | 124.77   |
| 11  | 1K    | 1   | FME  | O-C-CA | -2.61 | 118.07      | 124.77   |
| 1   | 1A    | 1   | FME  | O-C-CA | -2.60 | 118.08      | 124.77   |
| 8   | 1H    | 1   | FME  | O-C-CA | -2.57 | 118.17      | 124.77   |
| 55  | 8A    | 1   | FME  | O-C-CA | -2.48 | 118.38      | 124.77   |
| 14  | 1N    | 1   | FME  | O-C-CA | -2.46 | 118.44      | 124.77   |
| 55  | 4A    | 1   | FME  | O-C-CA | -2.44 | 118.50      | 124.77   |
| 56  | 4B    | 1   | FME  | O-C-CA | -2.38 | 118.65      | 124.77   |
| 12  | 1L    | 1   | FME  | O-C-CA | -2.38 | 118.66      | 124.77   |
| 56  | 8B    | 1   | FME  | O-C-CA | -2.29 | 118.87      | 124.77   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | 1H    | 1   | FME  | O1-CN-N-CA  |
| 14  | 1N    | 1   | FME  | O1-CN-N-CA  |
| 56  | 4B    | 1   | FME  | O1-CN-N-CA  |
| 56  | 4B    | 1   | FME  | CB-CA-N-CN  |
| 56  | 8B    | 1   | FME  | O1-CN-N-CA  |
| 55  | 4A    | 1   | FME  | CA-CB-CG-SD |
| 11  | 1K    | 1   | FME  | N-CA-CB-CG  |
| 55  | 8A    | 1   | FME  | CA-CB-CG-SD |
| 11  | 1K    | 1   | FME  | C-CA-CB-CG  |
| 11  | 1K    | 1   | FME  | CB-CG-SD-CE |
| 12  | 1L    | 1   | FME  | CB-CA-N-CN  |
| 56  | 4B    | 1   | FME  | CA-CB-CG-SD |

There are no ring outliers.

8 monomers are involved in 14 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | 1N    | 1   | FME  | 2       | 0            |
| 1   | 1A    | 1   | FME  | 3       | 0            |
| 56  | 4B    | 1   | FME  | 2       | 0            |
| 13  | 1M    | 1   | FME  | 1       | 0            |
| 55  | 8A    | 1   | FME  | 1       | 0            |
| 11  | 1K    | 1   | FME  | 3       | 0            |
| 56  | 8B    | 1   | FME  | 1       | 0            |
| 55  | 4A    | 1   | FME  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 11 are monoatomic - leaving 135 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 |
| 87  | PGV  | 4C    | 301 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.74 | 1 (1%)   |
| 73  | FMN  | 1F    | 501 | -    | 33,33,33     | 0.60 | 0        | 48,50,50    | 0.67 | 1 (2%)   |
| 94  | PO4  | 4H    | 101 | -    | 4,4,4        | 0.97 | 0        | 6,6,6       | 0.47 | 0        |
| 75  | CDL  | 1h    | 202 | -    | 79,79,99     | 0.31 | 0        | 85,91,111   | 0.42 | 0        |
| 87  | PGV  | 4A    | 603 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.35 | 0        |
| 70  | PC1  | 1I    | 203 | -    | 43,43,53     | 0.29 | 0        | 49,51,61    | 0.32 | 0        |
| 75  | CDL  | 3G    | 103 | -    | 55,55,99     | 0.34 | 0        | 61,67,111   | 0.48 | 0        |
| 92  | PSC  | 8B    | 305 | -    | 51,51,51     | 0.29 | 0        | 57,59,59    | 0.42 | 0        |
| 70  | PC1  | 1A    | 202 | -    | 34,34,53     | 0.37 | 0        | 40,42,61    | 0.44 | 0        |
| 69  | 3PE  | 3N    | 503 | -    | 24,24,50     | 0.37 | 0        | 27,29,55    | 0.56 | 0        |
| 70  | PC1  | 1B    | 203 | -    | 47,47,53     | 0.29 | 0        | 53,55,61    | 0.42 | 0        |
| 70  | PC1  | 1P    | 401 | -    | 32,32,53     | 0.33 | 0        | 38,40,61    | 0.37 | 0        |
| 71  | SF4  | 1F    | 502 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 75  | CDL  | 3G    | 102 | -    | 51,51,99     | 0.35 | 0        | 57,63,111   | 0.56 | 0        |
| 87  | PGV  | 4J    | 101 | -    | 50,50,50     | 0.30 | 0        | 53,56,56    | 0.38 | 0        |
| 69  | 3PE  | 1M    | 502 | -    | 47,47,50     | 0.27 | 0        | 50,52,55    | 0.33 | 0        |
| 69  | 3PE  | 1Y    | 206 | -    | 26,26,50     | 0.35 | 0        | 29,31,55    | 0.55 | 0        |
| 91  | CUA  | 4B    | 304 | 56   | 0,1,1        | -    | -        | -           |      |          |
| 94  | PO4  | 8H    | 101 | -    | 4,4,4        | 0.97 | 0        | 6,6,6       | 0.44 | 0        |
| 75  | CDL  | 1N    | 902 | -    | 61,61,99     | 0.31 | 0        | 67,73,111   | 0.69 | 1 (1%)   |
| 87  | PGV  | 4C    | 304 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.47 | 1 (1%)   |
| 87  | PGV  | 8C    | 304 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.38 | 0        |
| 87  | PGV  | 4A    | 601 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.40 | 0        |
| 87  | PGV  | 4L    | 101 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.38 | 0        |
| 69  | 3PE  | 3C    | 503 | -    | 34,34,50     | 0.32 | 0        | 37,39,55    | 0.45 | 0        |
| 69  | 3PE  | 1d    | 201 | -    | 48,48,50     | 0.27 | 0        | 51,53,55    | 0.36 | 0        |
| 69  | 3PE  | 3A    | 503 | -    | 31,31,50     | 0.41 | 0        | 34,36,55    | 0.48 | 0        |
| 75  | CDL  | 1q    | 203 | -    | 60,60,99     | 0.34 | 0        | 66,72,111   | 0.42 | 0        |
| 84  | MYR  | 1l    | 201 | -    | 13,14,15     | 0.31 | 0        | 12,13,15    | 0.29 | 0        |
| 70  | PC1  | 1M    | 505 | -    | 43,43,53     | 0.31 | 0        | 49,51,61    | 0.40 | 0        |
| 81  | AYA  | 1Y    | 201 | -    | 6,7,8        | 0.64 | 0        | 6,8,10      | 0.86 | 0        |
| 72  | FES  | 1E    | 301 | 5    | 0,4,4        | -    | -        | -           |      |          |
| 76  | GTP  | 1O    | 401 | 77   | 33,34,34     | 0.56 | 0        | 50,54,54    | 0.57 | 0        |
| 87  | PGV  | 4K    | 101 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.31 | 0        |
| 75  | CDL  | 4C    | 305 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.39 | 0        |
| 70  | PC1  | 1H    | 403 | -    | 47,47,53     | 0.29 | 0        | 53,55,61    | 0.36 | 0        |
| 87  | PGV  | 8C    | 301 | -    | 50,50,50     | 0.27 | 0        | 53,56,56    | 0.35 | 0        |
| 85  | HEM  | 3P    | 501 | 47   | 50,50,50     | 1.57 | 8 (16%)  | 67,82,82    | 1.61 | 11 (16%) |
| 69  | 3PE  | 1j    | 101 | -    | 43,43,50     | 0.29 | 0        | 46,48,55    | 0.44 | 0        |
| 92  | PSC  | 4B    | 305 | -    | 51,51,51     | 0.29 | 0        | 57,59,59    | 0.47 | 1 (1%)   |
| 86  | HEC  | 3D    | 501 | 48   | 44,49,50     | 2.68 | 27 (61%) | 56,80,82    | 2.03 | 16 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 72  | FES  | 3E    | 301 | 49   | 0,4,4        | -    | -        | -           |      |          |
| 70  | PC1  | 1d    | 202 | -    | 38,38,53     | 0.31 | 0        | 44,46,61    | 0.47 | 0        |
| 70  | PC1  | 1Y    | 207 | -    | 45,45,53     | 0.29 | 0        | 51,53,61    | 0.34 | 0        |
| 87  | PGV  | 4A    | 602 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.32 | 0        |
| 87  | PGV  | 4C    | 303 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.39 | 0        |
| 69  | 3PE  | 3D    | 502 | -    | 32,32,50     | 0.33 | 0        | 35,37,55    | 0.49 | 0        |
| 75  | CDL  | 8D    | 201 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.41 | 0        |
| 69  | 3PE  | 3P    | 503 | -    | 32,32,50     | 0.33 | 0        | 35,37,55    | 0.37 | 0        |
| 69  | 3PE  | 1M    | 501 | -    | 44,44,50     | 0.29 | 0        | 47,49,55    | 0.34 | 0        |
| 69  | 3PE  | 3R    | 302 | -    | 46,46,50     | 0.28 | 0        | 49,51,55    | 0.36 | 0        |
| 80  | EHZ  | 1T    | 101 | 20   | 31,36,37     | 0.20 | 0        | 36,44,47    | 1.12 | 1 (2%)   |
| 70  | PC1  | 1h    | 203 | -    | 46,46,53     | 0.28 | 0        | 52,54,61    | 0.30 | 0        |
| 81  | AYA  | 1q    | 202 | -    | 6,7,8        | 0.62 | 0        | 6,8,10      | 0.89 | 0        |
| 93  | PEK  | 8G    | 102 | -    | 52,52,52     | 0.26 | 0        | 55,57,57    | 0.40 | 0        |
| 75  | CDL  | 1X    | 201 | -    | 85,85,99     | 0.29 | 0        | 91,97,111   | 0.39 | 0        |
| 86  | HEC  | 3Q    | 501 | 48   | 46,50,50     | 2.62 | 27 (58%) | 58,82,82    | 2.01 | 16 (27%) |
| 82  | AME  | 1h    | 201 | -    | 9,10,11      | 0.51 | 0        | 9,11,13     | 0.99 | 1 (11%)  |
| 87  | PGV  | 8B    | 302 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.37 | 0        |
| 71  | SF4  | 1G    | 801 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 69  | 3PE  | 3A    | 502 | -    | 26,26,50     | 0.36 | 0        | 29,31,55    | 0.64 | 1 (3%)   |
| 75  | CDL  | 1H    | 401 | -    | 50,50,99     | 0.36 | 0        | 56,62,111   | 0.60 | 1 (1%)   |
| 69  | 3PE  | 1m    | 201 | -    | 40,40,50     | 0.29 | 0        | 43,45,55    | 0.40 | 0        |
| 80  | EHZ  | 1n    | 201 | -    | 31,36,37     | 0.18 | 0        | 36,44,47    | 1.05 | 1 (2%)   |
| 70  | PC1  | 1H    | 402 | -    | 53,53,53     | 0.28 | 0        | 59,61,61    | 0.35 | 0        |
| 87  | PGV  | 8K    | 101 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.32 | 0        |
| 87  | PGV  | 8B    | 301 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.32 | 0        |
| 70  | PC1  | 1A    | 203 | -    | 34,34,53     | 0.33 | 0        | 40,42,61    | 0.39 | 0        |
| 69  | 3PE  | 3N    | 501 | -    | 31,31,50     | 0.33 | 0        | 34,36,55    | 0.49 | 0        |
| 69  | 3PE  | 1L    | 703 | -    | 44,44,50     | 0.29 | 0        | 47,49,55    | 0.34 | 0        |
| 69  | 3PE  | 3Y    | 101 | -    | 29,29,50     | 0.34 | 0        | 32,34,55    | 0.42 | 0        |
| 87  | PGV  | 8C    | 307 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.35 | 0        |
| 69  | 3PE  | 1L    | 701 | -    | 45,45,50     | 0.28 | 0        | 48,50,55    | 0.33 | 0        |
| 75  | CDL  | 3P    | 504 | -    | 55,55,99     | 0.35 | 0        | 61,67,111   | 0.52 | 0        |
| 69  | 3PE  | 1M    | 506 | -    | 49,49,50     | 0.28 | 0        | 52,54,55    | 0.33 | 0        |
| 69  | 3PE  | 3G    | 101 | -    | 28,28,50     | 0.33 | 0        | 31,33,55    | 0.37 | 0        |
| 70  | PC1  | 1M    | 503 | -    | 34,34,53     | 0.32 | 0        | 40,42,61    | 0.52 | 0        |
| 93  | PEK  | 4G    | 102 | -    | 52,52,52     | 0.26 | 0        | 55,57,57    | 0.40 | 0        |
| 69  | 3PE  | 1P    | 403 | -    | 34,34,50     | 0.31 | 0        | 37,39,55    | 0.43 | 0        |
| 69  | 3PE  | 1Y    | 204 | -    | 29,29,50     | 0.34 | 0        | 32,34,55    | 0.80 | 1 (3%)   |
| 75  | CDL  | 1d    | 203 | -    | 64,64,99     | 0.32 | 0        | 70,76,111   | 0.41 | 0        |
| 75  | CDL  | 8C    | 306 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.40 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 93  | PEK  | 4C    | 307 | -    | 51,51,52     | 0.26 | 0        | 54,56,57    | 0.42 | 0        |
| 87  | PGV  | 8C    | 305 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.46 | 1 (1%)   |
| 75  | CDL  | 4B    | 303 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.30 | 0        |
| 69  | 3PE  | 1M    | 504 | -    | 50,50,50     | 0.28 | 0        | 53,55,55    | 0.46 | 0        |
| 69  | 3PE  | 1Y    | 203 | -    | 39,39,50     | 0.31 | 0        | 42,44,55    | 0.50 | 0        |
| 71  | SF4  | 1B    | 201 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 87  | PGV  | 8A    | 601 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.41 | 0        |
| 87  | PGV  | 4B    | 302 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.36 | 0        |
| 75  | CDL  | 8B    | 303 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.30 | 0        |
| 87  | PGV  | 4C    | 302 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.31 | 0        |
| 87  | PGV  | 8L    | 101 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.41 | 0        |
| 75  | CDL  | 3T    | 101 | -    | 56,56,99     | 0.35 | 0        | 62,68,111   | 0.48 | 0        |
| 87  | PGV  | 8J    | 101 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.40 | 0        |
| 93  | PEK  | 8C    | 308 | -    | 51,51,52     | 0.26 | 0        | 54,56,57    | 0.41 | 0        |
| 69  | 3PE  | 3C    | 504 | -    | 33,33,50     | 0.33 | 0        | 36,38,55    | 0.41 | 0        |
| 72  | FES  | 1G    | 803 | 7    | 0,4,4        | -    | -        | -           |      |          |
| 88  | HEA  | 8A    | 604 | 55   | 67,67,67     | 2.45 | 26 (38%) | 81,103,103  | 2.54 | 33 (40%) |
| 70  | PC1  | 3J    | 101 | -    | 46,46,53     | 0.28 | 0        | 52,54,61    | 0.32 | 0        |
| 75  | CDL  | 1L    | 702 | -    | 75,75,99     | 0.29 | 0        | 81,87,111   | 0.37 | 0        |
| 70  | PC1  | 3X    | 101 | -    | 28,28,53     | 0.36 | 0        | 34,36,61    | 0.48 | 0        |
| 87  | PGV  | 4M    | 101 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.30 | 0        |
| 87  | PGV  | 4G    | 101 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.45 | 1 (1%)   |
| 75  | CDL  | 4D    | 201 | -    | 99,99,99     | 0.27 | 0        | 105,111,111 | 0.43 | 0        |
| 87  | PGV  | 8C    | 303 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.32 | 0        |
| 70  | PC1  | 3R    | 303 | -    | 44,44,53     | 0.29 | 0        | 50,52,61    | 0.36 | 0        |
| 71  | SF4  | 1I    | 201 | 9    | 0,12,12      | -    | -        | -           |      |          |
| 85  | HEM  | 3C    | 501 | 47   | 50,50,50     | 1.56 | 8 (16%)  | 67,82,82    | 1.62 | 11 (16%) |
| 75  | CDL  | 3N    | 502 | -    | 42,42,99     | 0.37 | 0        | 48,54,111   | 0.52 | 0        |
| 87  | PGV  | 8C    | 302 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.72 | 1 (1%)   |
| 83  | CHD  | 1i    | 201 | -    | 32,32,32     | 0.51 | 0        | 51,51,51    | 0.57 | 0        |
| 72  | FES  | 3R    | 301 | 49   | 0,4,4        | -    | -        | -           |      |          |
| 87  | PGV  | 4C    | 306 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.36 | 0        |
| 88  | HEA  | 4A    | 605 | 55   | 67,67,67     | 2.45 | 26 (38%) | 81,103,103  | 2.55 | 34 (41%) |
| 70  | PC1  | 1q    | 201 | -    | 48,48,53     | 0.28 | 0        | 54,56,61    | 0.33 | 0        |
| 85  | HEM  | 3P    | 502 | 47   | 50,50,50     | 1.56 | 8 (16%)  | 67,82,82    | 1.59 | 12 (17%) |
| 70  | PC1  | 1B    | 202 | -    | 45,45,53     | 0.28 | 0        | 51,53,61    | 0.35 | 0        |
| 88  | HEA  | 8A    | 605 | 55   | 67,67,67     | 2.45 | 26 (38%) | 81,103,103  | 2.53 | 34 (41%) |
| 69  | 3PE  | 1N    | 901 | -    | 48,48,50     | 0.28 | 0        | 51,53,55    | 0.36 | 0        |
| 87  | PGV  | 8A    | 603 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.33 | 0        |
| 69  | 3PE  | 1K    | 101 | -    | 43,43,50     | 0.30 | 0        | 46,48,55    | 0.34 | 0        |
| 75  | CDL  | 3A    | 501 | -    | 57,57,99     | 0.33 | 0        | 63,69,111   | 0.42 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 87  | PGV  | 4B    | 301 | -    | 50,50,50     | 0.27 | 0        | 53,56,56    | 0.31 | 0        |
| 87  | PGV  | 8G    | 101 | -    | 50,50,50     | 0.29 | 0        | 53,56,56    | 0.45 | 1 (1%)   |
| 88  | HEA  | 4A    | 604 | 55   | 67,67,67     | 2.45 | 25 (37%) | 81,103,103  | 2.55 | 35 (43%) |
| 87  | PGV  | 8A    | 602 | -    | 50,50,50     | 0.28 | 0        | 53,56,56    | 0.30 | 0        |
| 91  | CUA  | 8B    | 304 | 56   | 0,1,1        | -    | -        | -           |      |          |
| 69  | 3PE  | 1A    | 201 | -    | 46,46,50     | 0.28 | 0        | 49,51,55    | 0.36 | 0        |
| 69  | 3PE  | 1Y    | 202 | -    | 30,30,50     | 0.32 | 0        | 33,35,55    | 0.53 | 0        |
| 69  | 3PE  | 1Y    | 205 | -    | 32,32,50     | 0.32 | 0        | 35,37,55    | 0.52 | 0        |
| 71  | SF4  | 1G    | 802 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 85  | HEM  | 3C    | 502 | -    | 50,50,50     | 1.56 | 9 (18%)  | 67,82,82    | 1.58 | 12 (17%) |
| 71  | SF4  | 1I    | 202 | 9    | 0,12,12      | -    | -        | -           |      |          |
| 78  | NDP  | 1P    | 402 | -    | 51,52,52     | 0.50 | 0        | 71,80,80    | 0.83 | 2 (2%)   |

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   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 87  | PGV  | 4C    | 301 | -    | -       | 11/55/55/55  | -       |
| 73  | FMN  | 1F    | 501 | -    | -       | 2/18/18/18   | 0/3/3/3 |
| 75  | CDL  | 1h    | 202 | -    | -       | 19/90/90/110 | -       |
| 87  | PGV  | 4A    | 603 | -    | -       | 3/55/55/55   | -       |
| 70  | PC1  | 1I    | 203 | -    | -       | 5/47/47/57   | -       |
| 75  | CDL  | 3G    | 103 | -    | -       | 8/66/66/110  | -       |
| 92  | PSC  | 8B    | 305 | -    | -       | 16/55/55/55  | -       |
| 70  | PC1  | 1A    | 202 | -    | -       | 4/38/38/57   | -       |
| 69  | 3PE  | 3N    | 503 | -    | -       | 5/28/28/54   | -       |
| 70  | PC1  | 1B    | 203 | -    | -       | 10/51/51/57  | -       |
| 70  | PC1  | 1P    | 401 | -    | -       | 5/36/36/57   | -       |
| 71  | SF4  | 1F    | 502 | 6    | -       | -            | 0/6/5/5 |
| 75  | CDL  | 3G    | 102 | -    | -       | 8/62/62/110  | -       |
| 87  | PGV  | 4J    | 101 | -    | -       | 7/55/55/55   | -       |
| 69  | 3PE  | 1M    | 502 | -    | -       | 13/51/51/54  | -       |
| 69  | 3PE  | 1Y    | 206 | -    | -       | 5/30/30/54   | -       |
| 75  | CDL  | 1N    | 902 | -    | -       | 15/71/71/110 | -       |
| 87  | PGV  | 4C    | 304 | -    | -       | 4/55/55/55   | -       |
| 87  | PGV  | 8C    | 304 | -    | -       | 13/55/55/55  | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 87  | PGV  | 4A    | 601 | -    | -       | 14/55/55/55    | -       |
| 87  | PGV  | 4L    | 101 | -    | -       | 5/55/55/55     | -       |
| 69  | 3PE  | 3C    | 503 | -    | -       | 11/38/38/54    | -       |
| 69  | 3PE  | 1d    | 201 | -    | -       | 7/52/52/54     | -       |
| 69  | 3PE  | 3A    | 503 | -    | -       | 6/35/35/54     | -       |
| 75  | CDL  | 1q    | 203 | -    | -       | 6/71/71/110    | -       |
| 84  | MYR  | 1l    | 201 | -    | -       | 1/12/12/13     | -       |
| 70  | PC1  | 1M    | 505 | -    | -       | 13/47/47/57    | -       |
| 81  | AYA  | 1Y    | 201 | -    | -       | 0/5/6/8        | -       |
| 72  | FES  | 1E    | 301 | 5    | -       | -              | 0/1/1/1 |
| 76  | GTP  | 1O    | 401 | 77   | -       | 4/22/38/38     | 0/3/3/3 |
| 87  | PGV  | 4K    | 101 | -    | -       | 14/55/55/55    | -       |
| 75  | CDL  | 4C    | 305 | -    | -       | 18/110/110/110 | -       |
| 70  | PC1  | 1H    | 403 | -    | -       | 4/51/51/57     | -       |
| 87  | PGV  | 8C    | 301 | -    | -       | 3/55/55/55     | -       |
| 85  | HEM  | 3P    | 501 | 47   | -       | 9/14/54/54     | -       |
| 69  | 3PE  | 1j    | 101 | -    | -       | 3/47/47/54     | -       |
| 92  | PSC  | 4B    | 305 | -    | -       | 14/55/55/55    | -       |
| 86  | HEC  | 3D    | 501 | 48   | -       | 3/13/53/54     | -       |
| 72  | FES  | 3E    | 301 | 49   | -       | -              | 0/1/1/1 |
| 70  | PC1  | 1d    | 202 | -    | -       | 7/42/42/57     | -       |
| 70  | PC1  | 1Y    | 207 | -    | -       | 8/49/49/57     | -       |
| 87  | PGV  | 4A    | 602 | -    | -       | 1/55/55/55     | -       |
| 87  | PGV  | 4C    | 303 | -    | -       | 9/55/55/55     | -       |
| 69  | 3PE  | 3D    | 502 | -    | -       | 1/36/36/54     | -       |
| 75  | CDL  | 8D    | 201 | -    | -       | 14/110/110/110 | -       |
| 69  | 3PE  | 3P    | 503 | -    | -       | 6/36/36/54     | -       |
| 69  | 3PE  | 1M    | 501 | -    | -       | 6/48/48/54     | -       |
| 69  | 3PE  | 3R    | 302 | -    | -       | 4/50/50/54     | -       |
| 80  | EHZ  | 1T    | 101 | 20   | -       | 10/42/44/45    | -       |
| 70  | PC1  | 1h    | 203 | -    | -       | 12/50/50/57    | -       |
| 81  | AYA  | 1q    | 202 | -    | -       | 0/5/6/8        | -       |
| 93  | PEK  | 8G    | 102 | -    | -       | 6/56/56/56     | -       |
| 75  | CDL  | 1X    | 201 | -    | -       | 17/96/96/110   | -       |
| 86  | HEC  | 3Q    | 501 | 48   | -       | 3/14/54/54     | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 82  | AME  | 1h    | 201 | -    | -       | 2/9/10/12      | -       |
| 87  | PGV  | 8B    | 302 | -    | -       | 5/55/55/55     | -       |
| 71  | SF4  | 1G    | 801 | 7    | -       | -              | 0/6/5/5 |
| 69  | 3PE  | 3A    | 502 | -    | -       | 7/30/30/54     | -       |
| 75  | CDL  | 1H    | 401 | -    | -       | 4/61/61/110    | -       |
| 69  | 3PE  | 1m    | 201 | -    | -       | 9/44/44/54     | -       |
| 80  | EHZ  | 1n    | 201 | -    | -       | 4/42/44/45     | -       |
| 70  | PC1  | 1H    | 402 | -    | -       | 6/57/57/57     | -       |
| 87  | PGV  | 8K    | 101 | -    | -       | 13/55/55/55    | -       |
| 87  | PGV  | 8B    | 301 | -    | -       | 7/55/55/55     | -       |
| 70  | PC1  | 1A    | 203 | -    | -       | 2/38/38/57     | -       |
| 69  | 3PE  | 3N    | 501 | -    | -       | 10/35/35/54    | -       |
| 69  | 3PE  | 1L    | 703 | -    | -       | 6/48/48/54     | -       |
| 69  | 3PE  | 3Y    | 101 | -    | -       | 5/33/33/54     | -       |
| 87  | PGV  | 8C    | 307 | -    | -       | 3/55/55/55     | -       |
| 69  | 3PE  | 1L    | 701 | -    | -       | 4/49/49/54     | -       |
| 75  | CDL  | 3P    | 504 | -    | -       | 17/66/66/110   | -       |
| 69  | 3PE  | 1M    | 506 | -    | -       | 7/53/53/54     | -       |
| 69  | 3PE  | 3G    | 101 | -    | -       | 3/32/32/54     | -       |
| 70  | PC1  | 1M    | 503 | -    | -       | 6/38/38/57     | -       |
| 93  | PEK  | 4G    | 102 | -    | -       | 6/56/56/56     | -       |
| 69  | 3PE  | 1P    | 403 | -    | -       | 5/38/38/54     | -       |
| 69  | 3PE  | 1Y    | 204 | -    | -       | 9/33/33/54     | -       |
| 75  | CDL  | 1d    | 203 | -    | -       | 11/75/75/110   | -       |
| 75  | CDL  | 8C    | 306 | -    | -       | 18/110/110/110 | -       |
| 93  | PEK  | 4C    | 307 | -    | -       | 3/55/55/56     | -       |
| 87  | PGV  | 8C    | 305 | -    | -       | 6/55/55/55     | -       |
| 75  | CDL  | 4B    | 303 | -    | -       | 14/110/110/110 | -       |
| 69  | 3PE  | 1M    | 504 | -    | -       | 10/54/54/54    | -       |
| 69  | 3PE  | 1Y    | 203 | -    | -       | 14/43/43/54    | -       |
| 71  | SF4  | 1B    | 201 | 2    | -       | -              | 0/6/5/5 |
| 87  | PGV  | 8A    | 601 | -    | -       | 11/55/55/55    | -       |
| 87  | PGV  | 4B    | 302 | -    | -       | 5/55/55/55     | -       |
| 75  | CDL  | 8B    | 303 | -    | -       | 15/110/110/110 | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions       | Rings   |
|-----|------|-------|-----|------|---------|----------------|---------|
| 87  | PGV  | 4C    | 302 | -    | -       | 9/55/55/55     | -       |
| 87  | PGV  | 8L    | 101 | -    | -       | 5/55/55/55     | -       |
| 75  | CDL  | 3T    | 101 | -    | -       | 9/67/67/110    | -       |
| 87  | PGV  | 8J    | 101 | -    | -       | 9/55/55/55     | -       |
| 93  | PEK  | 8C    | 308 | -    | -       | 2/55/55/56     | -       |
| 69  | 3PE  | 3C    | 504 | -    | -       | 8/37/37/54     | -       |
| 72  | FES  | 1G    | 803 | 7    | -       | -              | 0/1/1/1 |
| 88  | HEA  | 8A    | 604 | 55   | -       | 6/36/76/76     | -       |
| 70  | PC1  | 3J    | 101 | -    | -       | 1/50/50/57     | -       |
| 75  | CDL  | 1L    | 702 | -    | -       | 13/86/86/110   | -       |
| 70  | PC1  | 3X    | 101 | -    | -       | 2/32/32/57     | -       |
| 87  | PGV  | 4M    | 101 | -    | -       | 7/55/55/55     | -       |
| 87  | PGV  | 4G    | 101 | -    | -       | 10/55/55/55    | -       |
| 75  | CDL  | 4D    | 201 | -    | -       | 15/110/110/110 | -       |
| 87  | PGV  | 8C    | 303 | -    | -       | 10/55/55/55    | -       |
| 70  | PC1  | 3R    | 303 | -    | -       | 3/48/48/57     | -       |
| 71  | SF4  | 1I    | 201 | 9    | -       | -              | 0/6/5/5 |
| 85  | HEM  | 3C    | 501 | 47   | -       | 7/14/54/54     | -       |
| 75  | CDL  | 3N    | 502 | -    | -       | 8/53/53/110    | -       |
| 87  | PGV  | 8C    | 302 | -    | -       | 15/55/55/55    | -       |
| 83  | CHD  | 1i    | 201 | -    | -       | 2/9/74/74      | 0/4/4/4 |
| 87  | PGV  | 4C    | 306 | -    | -       | 2/55/55/55     | -       |
| 72  | FES  | 3R    | 301 | 49   | -       | -              | 0/1/1/1 |
| 88  | HEA  | 4A    | 605 | 55   | -       | 5/36/76/76     | -       |
| 70  | PC1  | 1q    | 201 | -    | -       | 3/52/52/57     | -       |
| 85  | HEM  | 3P    | 502 | 47   | -       | 8/14/54/54     | -       |
| 70  | PC1  | 1B    | 202 | -    | -       | 3/49/49/57     | -       |
| 88  | HEA  | 8A    | 605 | 55   | -       | 6/36/76/76     | -       |
| 69  | 3PE  | 1N    | 901 | -    | -       | 11/52/52/54    | -       |
| 87  | PGV  | 8A    | 603 | -    | -       | 4/55/55/55     | -       |
| 69  | 3PE  | 1K    | 101 | -    | -       | 9/47/47/54     | -       |
| 75  | CDL  | 3A    | 501 | -    | -       | 1/68/68/110    | -       |
| 87  | PGV  | 4B    | 301 | -    | -       | 2/55/55/55     | -       |
| 87  | PGV  | 8G    | 101 | -    | -       | 8/55/55/55     | -       |
| 88  | HEA  | 4A    | 604 | 55   | -       | 10/36/76/76    | -       |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 87  | PGV  | 8A    | 602 | -    | -       | 8/55/55/55 | -       |
| 69  | 3PE  | 1A    | 201 | -    | -       | 7/50/50/54 | -       |
| 69  | 3PE  | 1Y    | 202 | -    | -       | 9/34/34/54 | -       |
| 69  | 3PE  | 1Y    | 205 | -    | -       | 2/36/36/54 | -       |
| 71  | SF4  | 1G    | 802 | 7    | -       | -          | 0/6/5/5 |
| 85  | HEM  | 3C    | 502 | -    | -       | 6/14/54/54 | -       |
| 71  | SF4  | 1I    | 202 | 9    | -       | -          | 0/6/5/5 |
| 78  | NDP  | 1P    | 402 | -    | -       | 3/34/77/77 | 0/5/5/5 |

All (190) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 88  | 8A    | 604 | HEA  | FE-NB   | 5.66 | 2.12        | 1.94     |
| 88  | 4A    | 604 | HEA  | FE-ND   | 5.65 | 2.12        | 1.94     |
| 88  | 4A    | 604 | HEA  | FE-NB   | 5.64 | 2.12        | 1.94     |
| 88  | 8A    | 604 | HEA  | FE-ND   | 5.62 | 2.12        | 1.94     |
| 88  | 4A    | 605 | HEA  | FE-ND   | 5.61 | 2.12        | 1.94     |
| 88  | 8A    | 605 | HEA  | FE-ND   | 5.58 | 2.12        | 1.94     |
| 88  | 4A    | 605 | HEA  | FE-NB   | 5.54 | 2.12        | 1.94     |
| 88  | 8A    | 605 | HEA  | FE-NB   | 5.51 | 2.11        | 1.94     |
| 88  | 8A    | 604 | HEA  | C3B-C2B | 5.50 | 1.47        | 1.34     |
| 88  | 8A    | 605 | HEA  | C3B-C2B | 5.47 | 1.47        | 1.34     |
| 88  | 4A    | 604 | HEA  | C3B-C2B | 5.45 | 1.47        | 1.34     |
| 88  | 4A    | 605 | HEA  | C3B-C2B | 5.43 | 1.47        | 1.34     |
| 85  | 3C    | 501 | HEM  | FE-NB   | 5.33 | 2.11        | 1.94     |
| 85  | 3P    | 501 | HEM  | FE-NB   | 5.32 | 2.11        | 1.94     |
| 85  | 3C    | 502 | HEM  | FE-NB   | 5.20 | 2.10        | 1.94     |
| 85  | 3P    | 502 | HEM  | FE-NB   | 5.17 | 2.10        | 1.94     |
| 86  | 3D    | 501 | HEC  | C2A-C3A | 5.07 | 1.47        | 1.36     |
| 88  | 8A    | 604 | HEA  | FE-NC   | 4.97 | 2.11        | 1.95     |
| 88  | 8A    | 605 | HEA  | C3D-C2D | 4.97 | 1.47        | 1.36     |
| 86  | 3Q    | 501 | HEC  | C2A-C3A | 4.96 | 1.47        | 1.36     |
| 88  | 4A    | 604 | HEA  | FE-NC   | 4.92 | 2.11        | 1.95     |
| 88  | 4A    | 605 | HEA  | FE-NC   | 4.91 | 2.11        | 1.95     |
| 86  | 3D    | 501 | HEC  | CHD-C4C | 4.91 | 1.48        | 1.38     |
| 86  | 3Q    | 501 | HEC  | CHD-C4C | 4.90 | 1.48        | 1.38     |
| 88  | 4A    | 605 | HEA  | C3D-C2D | 4.89 | 1.47        | 1.36     |
| 88  | 8A    | 605 | HEA  | FE-NC   | 4.88 | 2.11        | 1.95     |
| 86  | 3D    | 501 | HEC  | CHB-C4A | 4.84 | 1.47        | 1.38     |
| 86  | 3Q    | 501 | HEC  | CHB-C4A | 4.84 | 1.47        | 1.38     |
| 88  | 8A    | 604 | HEA  | C3D-C2D | 4.83 | 1.47        | 1.36     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 86  | 3Q    | 501 | HEC  | CHA-C1A | 4.80 | 1.47        | 1.38     |
| 88  | 4A    | 604 | HEA  | C3D-C2D | 4.78 | 1.47        | 1.36     |
| 86  | 3D    | 501 | HEC  | CHA-C1A | 4.76 | 1.47        | 1.38     |
| 86  | 3Q    | 501 | HEC  | CHC-C4B | 4.72 | 1.47        | 1.38     |
| 86  | 3D    | 501 | HEC  | CHC-C4B | 4.71 | 1.47        | 1.38     |
| 88  | 8A    | 604 | HEA  | C3A-C2A | 4.69 | 1.47        | 1.37     |
| 88  | 4A    | 604 | HEA  | C3A-C2A | 4.63 | 1.47        | 1.37     |
| 88  | 8A    | 605 | HEA  | C3A-C2A | 4.59 | 1.47        | 1.37     |
| 88  | 4A    | 605 | HEA  | C3A-C2A | 4.54 | 1.47        | 1.37     |
| 86  | 3D    | 501 | HEC  | CAB-C3B | 4.47 | 1.49        | 1.35     |
| 88  | 8A    | 605 | HEA  | CHC-C4B | 4.46 | 1.47        | 1.38     |
| 86  | 3Q    | 501 | HEC  | CAC-C3C | 4.46 | 1.49        | 1.35     |
| 88  | 4A    | 605 | HEA  | CHD-C1D | 4.45 | 1.47        | 1.38     |
| 86  | 3Q    | 501 | HEC  | CAB-C3B | 4.45 | 1.49        | 1.35     |
| 86  | 3D    | 501 | HEC  | CAC-C3C | 4.43 | 1.49        | 1.35     |
| 88  | 4A    | 604 | HEA  | CHC-C4B | 4.42 | 1.47        | 1.38     |
| 88  | 8A    | 605 | HEA  | CHD-C1D | 4.42 | 1.47        | 1.38     |
| 88  | 4A    | 605 | HEA  | CHC-C4B | 4.41 | 1.47        | 1.38     |
| 88  | 4A    | 604 | HEA  | CHB-C4A | 4.38 | 1.47        | 1.38     |
| 88  | 4A    | 604 | HEA  | CHD-C1D | 4.36 | 1.47        | 1.38     |
| 88  | 8A    | 604 | HEA  | CHD-C1D | 4.32 | 1.47        | 1.38     |
| 88  | 4A    | 605 | HEA  | C1A-NA  | 4.31 | 1.47        | 1.39     |
| 88  | 8A    | 604 | HEA  | CHC-C4B | 4.30 | 1.47        | 1.38     |
| 88  | 8A    | 605 | HEA  | CHB-C4A | 4.29 | 1.46        | 1.38     |
| 88  | 4A    | 605 | HEA  | CHB-C4A | 4.26 | 1.46        | 1.38     |
| 88  | 4A    | 604 | HEA  | CHA-C1A | 4.26 | 1.46        | 1.38     |
| 88  | 8A    | 604 | HEA  | CHB-C4A | 4.26 | 1.46        | 1.38     |
| 88  | 8A    | 604 | HEA  | C1A-NA  | 4.25 | 1.47        | 1.39     |
| 88  | 8A    | 604 | HEA  | CHA-C1A | 4.25 | 1.46        | 1.38     |
| 85  | 3P    | 501 | HEM  | FE-NC   | 4.22 | 2.09        | 1.95     |
| 85  | 3C    | 501 | HEM  | FE-NC   | 4.22 | 2.09        | 1.95     |
| 88  | 4A    | 604 | HEA  | C1A-NA  | 4.18 | 1.47        | 1.39     |
| 85  | 3P    | 502 | HEM  | FE-NC   | 4.17 | 2.08        | 1.95     |
| 88  | 8A    | 605 | HEA  | C1A-NA  | 4.16 | 1.47        | 1.39     |
| 85  | 3C    | 502 | HEM  | FE-NC   | 4.16 | 2.08        | 1.95     |
| 88  | 8A    | 605 | HEA  | CHA-C1A | 4.06 | 1.46        | 1.38     |
| 88  | 4A    | 605 | HEA  | CHA-C1A | 4.05 | 1.46        | 1.38     |
| 88  | 8A    | 605 | HEA  | C4A-NA  | 4.00 | 1.47        | 1.39     |
| 88  | 4A    | 605 | HEA  | C4A-NA  | 4.00 | 1.47        | 1.39     |
| 88  | 8A    | 604 | HEA  | C4A-NA  | 4.00 | 1.47        | 1.39     |
| 88  | 4A    | 604 | HEA  | C4A-NA  | 3.99 | 1.47        | 1.39     |
| 86  | 3D    | 501 | HEC  | CHD-C1D | 3.83 | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 86  | 3D    | 501 | HEC  | CHA-C4D | 3.82  | 1.48        | 1.39     |
| 86  | 3Q    | 501 | HEC  | CHD-C1D | 3.81  | 1.48        | 1.39     |
| 86  | 3Q    | 501 | HEC  | CHA-C4D | 3.76  | 1.47        | 1.39     |
| 86  | 3Q    | 501 | HEC  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 86  | 3D    | 501 | HEC  | CHB-C1B | 3.73  | 1.47        | 1.39     |
| 86  | 3Q    | 501 | HEC  | CHC-C1C | 3.73  | 1.47        | 1.39     |
| 86  | 3D    | 501 | HEC  | CHC-C1C | 3.66  | 1.47        | 1.39     |
| 88  | 4A    | 605 | HEA  | CHD-C4C | 3.57  | 1.47        | 1.39     |
| 88  | 8A    | 605 | HEA  | CHC-C1C | 3.52  | 1.47        | 1.39     |
| 88  | 8A    | 605 | HEA  | CHD-C4C | 3.52  | 1.47        | 1.39     |
| 88  | 4A    | 604 | HEA  | CHC-C1C | 3.49  | 1.47        | 1.39     |
| 88  | 4A    | 605 | HEA  | CHC-C1C | 3.47  | 1.47        | 1.39     |
| 88  | 4A    | 604 | HEA  | CHD-C4C | 3.44  | 1.47        | 1.39     |
| 88  | 8A    | 604 | HEA  | CHC-C1C | 3.38  | 1.47        | 1.39     |
| 88  | 8A    | 604 | HEA  | CHD-C4C | 3.37  | 1.47        | 1.39     |
| 86  | 3D    | 501 | HEC  | C3D-C2D | 3.36  | 1.47        | 1.38     |
| 85  | 3C    | 502 | HEM  | C1B-NB  | -3.35 | 1.34        | 1.40     |
| 85  | 3P    | 502 | HEM  | C1B-NB  | -3.35 | 1.34        | 1.40     |
| 88  | 8A    | 604 | HEA  | CHA-C4D | 3.31  | 1.46        | 1.39     |
| 88  | 4A    | 604 | HEA  | CHA-C4D | 3.31  | 1.46        | 1.39     |
| 88  | 8A    | 605 | HEA  | CHB-C1B | 3.28  | 1.46        | 1.39     |
| 88  | 4A    | 605 | HEA  | CHB-C1B | 3.25  | 1.46        | 1.39     |
| 85  | 3C    | 502 | HEM  | C4D-ND  | -3.25 | 1.34        | 1.40     |
| 88  | 4A    | 604 | HEA  | CHB-C1B | 3.24  | 1.46        | 1.39     |
| 88  | 4A    | 605 | HEA  | CHA-C4D | 3.23  | 1.46        | 1.39     |
| 85  | 3P    | 502 | HEM  | C4D-ND  | -3.22 | 1.34        | 1.40     |
| 88  | 8A    | 605 | HEA  | CHA-C4D | 3.22  | 1.46        | 1.39     |
| 85  | 3P    | 501 | HEM  | C1B-NB  | -3.21 | 1.34        | 1.40     |
| 88  | 8A    | 604 | HEA  | CHB-C1B | 3.19  | 1.46        | 1.39     |
| 86  | 3Q    | 501 | HEC  | C3D-C2D | 3.17  | 1.47        | 1.38     |
| 85  | 3C    | 501 | HEM  | C1B-NB  | -3.17 | 1.34        | 1.40     |
| 85  | 3C    | 501 | HEM  | C4D-ND  | -3.16 | 1.34        | 1.40     |
| 85  | 3P    | 501 | HEM  | C4D-ND  | -3.15 | 1.34        | 1.40     |
| 88  | 4A    | 604 | HEA  | C4B-C3B | 2.80  | 1.49        | 1.44     |
| 88  | 8A    | 604 | HEA  | C4B-C3B | 2.73  | 1.49        | 1.44     |
| 88  | 8A    | 605 | HEA  | C1D-ND  | -2.69 | 1.35        | 1.40     |
| 88  | 4A    | 604 | HEA  | C1D-ND  | -2.68 | 1.35        | 1.40     |
| 88  | 8A    | 605 | HEA  | C4B-C3B | 2.66  | 1.49        | 1.44     |
| 86  | 3D    | 501 | HEC  | C1B-C2B | 2.63  | 1.49        | 1.43     |
| 86  | 3Q    | 501 | HEC  | C1B-C2B | 2.62  | 1.49        | 1.43     |
| 88  | 4A    | 605 | HEA  | C1D-ND  | -2.62 | 1.35        | 1.40     |
| 88  | 4A    | 605 | HEA  | C4B-C3B | 2.62  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 86  | 3Q    | 501 | HEC  | C1C-C2C | 2.61  | 1.49        | 1.43     |
| 88  | 8A    | 605 | HEA  | C4B-NB  | -2.60 | 1.35        | 1.40     |
| 88  | 8A    | 604 | HEA  | C1D-ND  | -2.59 | 1.35        | 1.40     |
| 88  | 4A    | 604 | HEA  | C4D-C3D | 2.57  | 1.49        | 1.45     |
| 88  | 4A    | 605 | HEA  | C4B-NB  | -2.56 | 1.35        | 1.40     |
| 86  | 3D    | 501 | HEC  | C1C-C2C | 2.54  | 1.49        | 1.43     |
| 88  | 4A    | 604 | HEA  | C4B-NB  | -2.53 | 1.35        | 1.40     |
| 88  | 8A    | 605 | HEA  | C1C-C2C | 2.53  | 1.49        | 1.43     |
| 88  | 4A    | 604 | HEA  | C1C-C2C | 2.52  | 1.49        | 1.43     |
| 88  | 8A    | 604 | HEA  | C1C-C2C | 2.52  | 1.49        | 1.43     |
| 88  | 8A    | 604 | HEA  | C4B-NB  | -2.52 | 1.35        | 1.40     |
| 88  | 4A    | 605 | HEA  | C1C-C2C | 2.51  | 1.49        | 1.43     |
| 86  | 3D    | 501 | HEC  | C1D-C2D | 2.49  | 1.49        | 1.43     |
| 85  | 3P    | 502 | HEM  | FE-ND   | -2.47 | 1.87        | 1.94     |
| 86  | 3Q    | 501 | HEC  | C1D-C2D | 2.47  | 1.48        | 1.43     |
| 85  | 3C    | 502 | HEM  | FE-ND   | -2.47 | 1.87        | 1.94     |
| 85  | 3C    | 501 | HEM  | FE-ND   | -2.45 | 1.87        | 1.94     |
| 86  | 3D    | 501 | HEC  | C4B-NB  | -2.43 | 1.35        | 1.39     |
| 88  | 8A    | 604 | HEA  | C4D-C3D | 2.43  | 1.49        | 1.45     |
| 85  | 3P    | 501 | HEM  | FE-ND   | -2.42 | 1.87        | 1.94     |
| 86  | 3Q    | 501 | HEC  | C4B-NB  | -2.40 | 1.35        | 1.39     |
| 86  | 3D    | 501 | HEC  | C1A-NA  | -2.37 | 1.35        | 1.39     |
| 86  | 3D    | 501 | HEC  | C4A-NA  | -2.36 | 1.35        | 1.39     |
| 85  | 3P    | 501 | HEM  | C1C-C2C | -2.35 | 1.40        | 1.45     |
| 85  | 3P    | 502 | HEM  | C1C-C2C | -2.35 | 1.40        | 1.45     |
| 85  | 3C    | 502 | HEM  | C1C-C2C | -2.34 | 1.40        | 1.45     |
| 86  | 3Q    | 501 | HEC  | C4A-NA  | -2.32 | 1.35        | 1.39     |
| 85  | 3C    | 501 | HEM  | C1C-C2C | -2.31 | 1.40        | 1.45     |
| 88  | 4A    | 605 | HEA  | C1D-C2D | 2.31  | 1.49        | 1.44     |
| 86  | 3D    | 501 | HEC  | C4C-NC  | -2.30 | 1.35        | 1.39     |
| 86  | 3Q    | 501 | HEC  | C4C-NC  | -2.30 | 1.35        | 1.39     |
| 88  | 8A    | 605 | HEA  | C11-C3B | -2.27 | 1.48        | 1.51     |
| 88  | 8A    | 605 | HEA  | C4D-C3D | 2.27  | 1.48        | 1.45     |
| 86  | 3Q    | 501 | HEC  | C1A-NA  | -2.26 | 1.35        | 1.39     |
| 86  | 3D    | 501 | HEC  | C1D-ND  | -2.26 | 1.35        | 1.39     |
| 86  | 3D    | 501 | HEC  | C4D-ND  | -2.25 | 1.35        | 1.39     |
| 86  | 3Q    | 501 | HEC  | C1D-ND  | -2.23 | 1.35        | 1.39     |
| 88  | 8A    | 604 | HEA  | C1A-C2A | 2.23  | 1.49        | 1.45     |
| 88  | 4A    | 605 | HEA  | C11-C3B | -2.23 | 1.48        | 1.51     |
| 88  | 8A    | 605 | HEA  | C1D-C2D | 2.22  | 1.49        | 1.44     |
| 88  | 4A    | 605 | HEA  | C4D-C3D | 2.20  | 1.48        | 1.45     |
| 86  | 3D    | 501 | HEC  | C4D-C3D | 2.20  | 1.49        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 86  | 3Q    | 501 | HEC  | C4D-ND  | -2.19 | 1.35        | 1.39     |
| 88  | 4A    | 605 | HEA  | C1A-C2A | 2.18  | 1.49        | 1.45     |
| 88  | 8A    | 604 | HEA  | C1D-C2D | 2.17  | 1.48        | 1.44     |
| 85  | 3P    | 502 | HEM  | C1D-ND  | -2.17 | 1.34        | 1.38     |
| 86  | 3D    | 501 | HEC  | C1C-NC  | -2.17 | 1.35        | 1.39     |
| 88  | 4A    | 604 | HEA  | C4C-NC  | -2.15 | 1.35        | 1.39     |
| 88  | 8A    | 605 | HEA  | C4C-NC  | -2.15 | 1.35        | 1.39     |
| 88  | 4A    | 604 | HEA  | C1A-C2A | 2.15  | 1.49        | 1.45     |
| 85  | 3P    | 501 | HEM  | C1D-ND  | -2.14 | 1.34        | 1.38     |
| 88  | 4A    | 605 | HEA  | C4C-NC  | -2.13 | 1.35        | 1.39     |
| 88  | 8A    | 605 | HEA  | C1A-C2A | 2.13  | 1.48        | 1.45     |
| 88  | 8A    | 604 | HEA  | C4C-NC  | -2.12 | 1.35        | 1.39     |
| 86  | 3Q    | 501 | HEC  | C1C-NC  | -2.11 | 1.35        | 1.39     |
| 85  | 3C    | 502 | HEM  | C1D-ND  | -2.11 | 1.34        | 1.38     |
| 85  | 3P    | 501 | HEM  | C3C-C4C | -2.10 | 1.42        | 1.46     |
| 86  | 3D    | 501 | HEC  | C1A-C2A | 2.09  | 1.48        | 1.45     |
| 86  | 3D    | 501 | HEC  | C1B-NB  | -2.08 | 1.35        | 1.39     |
| 88  | 8A    | 604 | HEA  | C1B-C2B | 2.08  | 1.48        | 1.44     |
| 88  | 4A    | 604 | HEA  | C1D-C2D | 2.06  | 1.48        | 1.44     |
| 86  | 3Q    | 501 | HEC  | C1A-C2A | 2.06  | 1.48        | 1.45     |
| 85  | 3C    | 501 | HEM  | C1D-ND  | -2.05 | 1.34        | 1.38     |
| 85  | 3P    | 502 | HEM  | C3C-C4C | -2.05 | 1.42        | 1.46     |
| 88  | 4A    | 605 | HEA  | C3C-C4C | 2.04  | 1.48        | 1.42     |
| 88  | 4A    | 604 | HEA  | C1B-C2B | 2.04  | 1.48        | 1.44     |
| 86  | 3D    | 501 | HEC  | C3B-C2B | 2.04  | 1.48        | 1.41     |
| 85  | 3C    | 502 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 85  | 3C    | 501 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 88  | 8A    | 605 | HEA  | C1B-C2B | 2.03  | 1.48        | 1.44     |
| 86  | 3D    | 501 | HEC  | C3C-C2C | 2.03  | 1.48        | 1.41     |
| 86  | 3Q    | 501 | HEC  | C3B-C2B | 2.03  | 1.48        | 1.41     |
| 86  | 3Q    | 501 | HEC  | C4D-C3D | 2.02  | 1.48        | 1.44     |
| 85  | 3C    | 502 | HEM  | C4B-NB  | -2.01 | 1.34        | 1.38     |
| 86  | 3Q    | 501 | HEC  | C3C-C2C | 2.01  | 1.48        | 1.41     |
| 86  | 3Q    | 501 | HEC  | C1B-NB  | -2.01 | 1.35        | 1.39     |
| 88  | 8A    | 604 | HEA  | C11-C3B | -2.01 | 1.48        | 1.51     |

All (231) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 88  | 4A    | 605 | HEA  | C3D-C4D-ND | 6.64 | 116.77      | 110.35   |
| 88  | 8A    | 605 | HEA  | C3D-C4D-ND | 6.63 | 116.76      | 110.35   |
| 88  | 4A    | 604 | HEA  | C3D-C4D-ND | 6.54 | 116.67      | 110.35   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | 8A    | 604 | HEA  | C3D-C4D-ND  | 6.47  | 116.60      | 110.35   |
| 80  | 1T    | 101 | EHZ  | C10-S1-C9   | 6.20  | 120.16      | 101.84   |
| 88  | 8A    | 604 | HEA  | C2B-C1B-NB  | 6.02  | 116.86      | 109.90   |
| 80  | 1n    | 201 | EHZ  | C10-S1-C9   | 5.93  | 119.36      | 101.84   |
| 88  | 4A    | 605 | HEA  | C2B-C1B-NB  | 5.89  | 116.71      | 109.90   |
| 88  | 4A    | 604 | HEA  | C2B-C1B-NB  | 5.83  | 116.64      | 109.90   |
| 88  | 8A    | 604 | HEA  | C3B-C4B-NB  | 5.79  | 116.50      | 109.84   |
| 88  | 8A    | 604 | HEA  | C3C-C4C-NC  | 5.79  | 114.67      | 109.80   |
| 88  | 8A    | 605 | HEA  | C2A-C1A-NA  | 5.73  | 115.85      | 110.32   |
| 88  | 8A    | 605 | HEA  | C2B-C1B-NB  | 5.70  | 116.49      | 109.90   |
| 88  | 4A    | 605 | HEA  | C2A-C1A-NA  | 5.66  | 115.79      | 110.32   |
| 88  | 4A    | 604 | HEA  | C2D-C1D-ND  | 5.66  | 116.34      | 109.84   |
| 88  | 8A    | 604 | HEA  | C2D-C1D-ND  | 5.64  | 116.32      | 109.84   |
| 88  | 8A    | 605 | HEA  | C2D-C1D-ND  | 5.63  | 116.31      | 109.84   |
| 88  | 4A    | 604 | HEA  | C3B-C4B-NB  | 5.59  | 116.26      | 109.84   |
| 88  | 4A    | 605 | HEA  | C3C-C2C-C1C | -5.56 | 100.61      | 107.17   |
| 88  | 8A    | 605 | HEA  | C3C-C2C-C1C | -5.54 | 100.64      | 107.17   |
| 88  | 4A    | 605 | HEA  | C3B-C4B-NB  | 5.52  | 116.19      | 109.84   |
| 88  | 4A    | 605 | HEA  | C2D-C1D-ND  | 5.52  | 116.19      | 109.84   |
| 88  | 4A    | 604 | HEA  | C3C-C2C-C1C | -5.48 | 100.71      | 107.17   |
| 88  | 8A    | 604 | HEA  | C3C-C2C-C1C | -5.43 | 100.77      | 107.17   |
| 88  | 4A    | 604 | HEA  | C3C-C4C-NC  | 5.42  | 114.37      | 109.80   |
| 88  | 8A    | 605 | HEA  | C3B-C4B-NB  | 5.38  | 116.03      | 109.84   |
| 88  | 4A    | 604 | HEA  | C2A-C1A-NA  | 5.35  | 115.49      | 110.32   |
| 86  | 3D    | 501 | HEC  | C2A-C1A-NA  | 5.32  | 115.46      | 110.32   |
| 86  | 3Q    | 501 | HEC  | C2A-C1A-NA  | 5.21  | 115.35      | 110.32   |
| 88  | 8A    | 604 | HEA  | C2A-C1A-NA  | 5.21  | 115.35      | 110.32   |
| 88  | 8A    | 605 | HEA  | C3C-C4C-NC  | 5.15  | 114.13      | 109.80   |
| 88  | 4A    | 605 | HEA  | C3C-C4C-NC  | 5.14  | 114.12      | 109.80   |
| 85  | 3C    | 501 | HEM  | CHC-C4B-NB  | 5.09  | 129.90      | 124.42   |
| 78  | 1P    | 402 | NDP  | P2B-O2B-C2B | -4.98 | 110.14      | 123.43   |
| 85  | 3P    | 501 | HEM  | CHC-C4B-NB  | 4.93  | 129.72      | 124.42   |
| 85  | 3P    | 502 | HEM  | CHC-C4B-NB  | 4.92  | 129.71      | 124.42   |
| 85  | 3C    | 502 | HEM  | CHC-C4B-NB  | 4.91  | 129.71      | 124.42   |
| 86  | 3D    | 501 | HEC  | C3D-C4D-ND  | 4.68  | 115.34      | 110.15   |
| 86  | 3Q    | 501 | HEC  | C3D-C4D-ND  | 4.54  | 115.18      | 110.15   |
| 85  | 3C    | 501 | HEM  | CHD-C1D-ND  | 4.39  | 129.15      | 124.42   |
| 88  | 4A    | 604 | HEA  | CHA-C4D-ND  | -4.35 | 119.74      | 124.42   |
| 85  | 3P    | 501 | HEM  | CHD-C1D-ND  | 4.35  | 129.10      | 124.42   |
| 85  | 3P    | 502 | HEM  | CHD-C1D-ND  | 4.29  | 129.04      | 124.42   |
| 88  | 4A    | 605 | HEA  | C1D-C2D-C3D | -4.23 | 102.53      | 106.98   |
| 88  | 8A    | 604 | HEA  | C2C-C1C-NC  | 4.22  | 116.91      | 110.14   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | 8A    | 605 | HEA  | C1D-C2D-C3D | -4.22 | 102.54      | 106.98   |
| 88  | 4A    | 605 | HEA  | C2C-C1C-NC  | 4.21  | 116.89      | 110.14   |
| 88  | 8A    | 605 | HEA  | C3A-C2A-C1A | -4.18 | 103.09      | 107.05   |
| 88  | 4A    | 605 | HEA  | C3A-C2A-C1A | -4.16 | 103.11      | 107.05   |
| 88  | 4A    | 604 | HEA  | C2C-C1C-NC  | 4.12  | 116.74      | 110.14   |
| 88  | 8A    | 605 | HEA  | C2C-C1C-NC  | 4.10  | 116.71      | 110.14   |
| 88  | 8A    | 604 | HEA  | C1D-C2D-C3D | -4.07 | 102.70      | 106.98   |
| 75  | 1N    | 902 | CDL  | OB6-CB5-C51 | 4.02  | 118.25      | 111.09   |
| 85  | 3C    | 502 | HEM  | CHD-C1D-ND  | 4.00  | 128.72      | 124.42   |
| 88  | 4A    | 604 | HEA  | C1D-C2D-C3D | -3.89 | 102.89      | 106.98   |
| 86  | 3Q    | 501 | HEC  | C2C-C1C-NC  | 3.87  | 116.34      | 110.14   |
| 86  | 3D    | 501 | HEC  | C2C-C1C-NC  | 3.84  | 116.30      | 110.14   |
| 88  | 8A    | 604 | HEA  | C3A-C2A-C1A | -3.83 | 103.42      | 107.05   |
| 88  | 4A    | 604 | HEA  | C3A-C2A-C1A | -3.83 | 103.42      | 107.05   |
| 87  | 4C    | 301 | PGV  | O01-C1-C2   | 3.82  | 119.74      | 111.48   |
| 88  | 8A    | 605 | HEA  | CHA-C4D-ND  | -3.80 | 120.33      | 124.42   |
| 86  | 3D    | 501 | HEC  | C2B-C1B-NB  | 3.78  | 116.20      | 110.14   |
| 86  | 3Q    | 501 | HEC  | C2B-C1B-NB  | 3.76  | 116.16      | 110.14   |
| 88  | 4A    | 605 | HEA  | C1B-C2B-C3B | -3.73 | 102.47      | 106.80   |
| 88  | 8A    | 604 | HEA  | C1B-C2B-C3B | -3.72 | 102.49      | 106.80   |
| 88  | 8A    | 605 | HEA  | C1B-C2B-C3B | -3.70 | 102.51      | 106.80   |
| 87  | 8C    | 302 | PGV  | O01-C1-C2   | 3.58  | 119.23      | 111.48   |
| 88  | 4A    | 604 | HEA  | C1B-C2B-C3B | -3.58 | 102.65      | 106.80   |
| 85  | 3C    | 501 | HEM  | CHA-C4D-ND  | 3.53  | 128.73      | 124.37   |
| 86  | 3D    | 501 | HEC  | C1A-C2A-C3A | -3.49 | 102.51      | 107.11   |
| 86  | 3D    | 501 | HEC  | C1D-C2D-C3D | -3.48 | 102.83      | 106.82   |
| 88  | 4A    | 604 | HEA  | CAD-C3D-C4D | 3.47  | 130.75      | 124.70   |
| 88  | 4A    | 605 | HEA  | C4A-NA-C1A  | -3.46 | 100.17      | 105.82   |
| 85  | 3P    | 502 | HEM  | C1B-NB-C4B  | 3.45  | 109.30      | 105.21   |
| 85  | 3P    | 501 | HEM  | CHB-C1B-NB  | 3.44  | 128.62      | 124.37   |
| 88  | 4A    | 604 | HEA  | C4D-C3D-C2D | -3.44 | 101.89      | 106.89   |
| 85  | 3C    | 502 | HEM  | C1B-NB-C4B  | 3.44  | 109.28      | 105.21   |
| 88  | 8A    | 604 | HEA  | CHA-C4D-ND  | -3.44 | 120.73      | 124.42   |
| 85  | 3P    | 501 | HEM  | CHA-C4D-ND  | 3.43  | 128.62      | 124.37   |
| 86  | 3Q    | 501 | HEC  | C1D-C2D-C3D | -3.42 | 102.89      | 106.82   |
| 88  | 8A    | 605 | HEA  | C4A-NA-C1A  | -3.40 | 100.27      | 105.82   |
| 86  | 3Q    | 501 | HEC  | C1A-C2A-C3A | -3.38 | 102.66      | 107.11   |
| 85  | 3C    | 502 | HEM  | CHA-C4D-ND  | 3.37  | 128.53      | 124.37   |
| 88  | 8A    | 605 | HEA  | C13-C12-C11 | -3.36 | 109.03      | 114.39   |
| 88  | 4A    | 605 | HEA  | CHA-C4D-ND  | -3.34 | 120.83      | 124.42   |
| 88  | 4A    | 605 | HEA  | C13-C12-C11 | -3.33 | 109.07      | 114.39   |
| 88  | 8A    | 604 | HEA  | C13-C14-C15 | -3.30 | 120.06      | 127.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | 8A    | 605 | HEA  | C4D-C3D-C2D | -3.30 | 102.08      | 106.89   |
| 88  | 4A    | 604 | HEA  | C13-C14-C15 | -3.28 | 120.11      | 127.62   |
| 85  | 3C    | 501 | HEM  | CHB-C1B-NB  | 3.27  | 128.41      | 124.37   |
| 88  | 8A    | 604 | HEA  | C4D-C3D-C2D | -3.27 | 102.13      | 106.89   |
| 88  | 4A    | 604 | HEA  | C4A-NA-C1A  | -3.25 | 100.52      | 105.82   |
| 88  | 4A    | 605 | HEA  | C4D-C3D-C2D | -3.23 | 102.19      | 106.89   |
| 85  | 3P    | 502 | HEM  | CHA-C4D-ND  | 3.22  | 128.35      | 124.37   |
| 85  | 3C    | 501 | HEM  | C1B-NB-C4B  | 3.19  | 108.99      | 105.21   |
| 85  | 3P    | 501 | HEM  | C1B-NB-C4B  | 3.19  | 108.98      | 105.21   |
| 88  | 8A    | 604 | HEA  | C4B-C3B-C2B | -3.18 | 102.09      | 107.44   |
| 88  | 8A    | 605 | HEA  | C13-C14-C15 | -3.17 | 120.36      | 127.62   |
| 88  | 8A    | 604 | HEA  | C4A-NA-C1A  | -3.17 | 100.65      | 105.82   |
| 88  | 4A    | 604 | HEA  | C4B-C3B-C2B | -3.16 | 102.12      | 107.44   |
| 86  | 3D    | 501 | HEC  | C2D-C1D-ND  | 3.16  | 115.20      | 110.14   |
| 88  | 4A    | 605 | HEA  | C13-C14-C15 | -3.15 | 120.41      | 127.62   |
| 88  | 8A    | 604 | HEA  | CHB-C1B-NB  | -3.12 | 121.07      | 124.42   |
| 86  | 3D    | 501 | HEC  | C3A-C4A-NA  | 3.10  | 115.37      | 109.64   |
| 85  | 3P    | 502 | HEM  | CHB-C1B-NB  | 3.10  | 128.20      | 124.37   |
| 69  | 1Y    | 204 | 3PE  | O21-C21-C22 | 3.07  | 118.13      | 111.48   |
| 86  | 3Q    | 501 | HEC  | C3A-C4A-NA  | 3.06  | 115.31      | 109.64   |
| 85  | 3C    | 502 | HEM  | CHB-C1B-NB  | 3.05  | 128.14      | 124.37   |
| 86  | 3Q    | 501 | HEC  | C2D-C1D-ND  | 3.05  | 115.03      | 110.14   |
| 88  | 4A    | 605 | HEA  | C4B-C3B-C2B | -3.03 | 102.34      | 107.44   |
| 88  | 4A    | 604 | HEA  | C26-C15-C16 | 3.00  | 120.44      | 115.23   |
| 88  | 8A    | 604 | HEA  | C26-C15-C16 | 3.00  | 120.44      | 115.23   |
| 88  | 8A    | 604 | HEA  | CAD-C3D-C4D | 3.00  | 129.92      | 124.70   |
| 88  | 8A    | 605 | HEA  | C4B-C3B-C2B | -2.99 | 102.41      | 107.44   |
| 88  | 4A    | 604 | HEA  | CHB-C1B-NB  | -2.86 | 121.34      | 124.42   |
| 88  | 8A    | 605 | HEA  | CHA-C1A-NA  | -2.85 | 121.35      | 124.45   |
| 86  | 3D    | 501 | HEC  | C4A-C3A-C2A | -2.83 | 102.77      | 106.97   |
| 88  | 4A    | 604 | HEA  | CHA-C1A-NA  | -2.83 | 121.37      | 124.45   |
| 85  | 3P    | 502 | HEM  | C3B-C4B-NB  | -2.83 | 107.44      | 109.47   |
| 86  | 3Q    | 501 | HEC  | C4A-C3A-C2A | -2.82 | 102.79      | 106.97   |
| 82  | 1h    | 201 | AME  | O-C-CA      | -2.80 | 117.58      | 124.77   |
| 85  | 3C    | 502 | HEM  | C3B-C4B-NB  | -2.78 | 107.47      | 109.47   |
| 88  | 4A    | 605 | HEA  | C26-C15-C16 | 2.78  | 120.05      | 115.23   |
| 86  | 3D    | 501 | HEC  | C4D-C3D-C2D | -2.75 | 102.62      | 106.87   |
| 86  | 3Q    | 501 | HEC  | CMD-C2D-C1D | 2.72  | 129.56      | 125.42   |
| 88  | 4A    | 605 | HEA  | CHA-C1A-NA  | -2.71 | 121.50      | 124.45   |
| 88  | 4A    | 605 | HEA  | C17-C18-C19 | -2.69 | 121.46      | 127.62   |
| 88  | 8A    | 605 | HEA  | C26-C15-C16 | 2.68  | 119.88      | 115.23   |
| 78  | 1P    | 402 | NDP  | O4D-C1D-C2D | -2.66 | 100.92      | 106.62   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 85  | 3P    | 501 | HEM  | CHD-C4C-NC  | 2.66  | 127.35      | 124.45   |
| 88  | 8A    | 604 | HEA  | C4B-NB-C1B  | -2.66 | 102.06      | 105.21   |
| 88  | 4A    | 605 | HEA  | CHB-C1B-NB  | -2.66 | 121.56      | 124.42   |
| 88  | 8A    | 605 | HEA  | C27-C19-C20 | 2.65  | 119.82      | 115.23   |
| 85  | 3P    | 501 | HEM  | CHD-C1D-C2D | -2.61 | 120.90      | 125.03   |
| 86  | 3Q    | 501 | HEC  | C4D-C3D-C2D | -2.60 | 102.85      | 106.87   |
| 85  | 3C    | 501 | HEM  | CHD-C1D-C2D | -2.59 | 120.93      | 125.03   |
| 88  | 4A    | 605 | HEA  | C27-C19-C20 | 2.59  | 119.72      | 115.23   |
| 88  | 8A    | 605 | HEA  | CHB-C1B-NB  | -2.59 | 121.64      | 124.42   |
| 88  | 4A    | 604 | HEA  | CMC-C2C-C1C | 2.56  | 129.32      | 125.42   |
| 85  | 3C    | 501 | HEM  | CHD-C4C-NC  | 2.56  | 127.24      | 124.45   |
| 85  | 3P    | 501 | HEM  | C3B-C4B-NB  | -2.55 | 107.64      | 109.47   |
| 88  | 8A    | 604 | HEA  | CHC-C1C-C2C | -2.55 | 120.04      | 127.43   |
| 88  | 8A    | 605 | HEA  | C17-C18-C19 | -2.54 | 121.81      | 127.62   |
| 88  | 4A    | 605 | HEA  | CHC-C1C-C2C | -2.53 | 120.08      | 127.43   |
| 85  | 3C    | 501 | HEM  | C3B-C4B-NB  | -2.53 | 107.65      | 109.47   |
| 88  | 4A    | 604 | HEA  | C1D-ND-C4D  | -2.53 | 102.21      | 105.21   |
| 88  | 8A    | 604 | HEA  | C17-C18-C19 | -2.52 | 121.86      | 127.62   |
| 88  | 8A    | 604 | HEA  | C1D-ND-C4D  | -2.50 | 102.24      | 105.21   |
| 85  | 3P    | 502 | HEM  | CHD-C1D-C2D | -2.49 | 121.10      | 125.03   |
| 88  | 4A    | 605 | HEA  | C4B-NB-C1B  | -2.47 | 102.28      | 105.21   |
| 88  | 8A    | 605 | HEA  | C1D-ND-C4D  | -2.45 | 102.31      | 105.21   |
| 88  | 8A    | 605 | HEA  | C1A-CHA-C4D | -2.45 | 120.82      | 126.02   |
| 88  | 4A    | 604 | HEA  | CHC-C1C-C2C | -2.44 | 120.33      | 127.43   |
| 88  | 4A    | 604 | HEA  | C4B-NB-C1B  | -2.44 | 102.32      | 105.21   |
| 88  | 4A    | 605 | HEA  | C1D-ND-C4D  | -2.43 | 102.33      | 105.21   |
| 88  | 4A    | 605 | HEA  | C25-C23-C24 | 2.43  | 120.18      | 114.59   |
| 88  | 8A    | 605 | HEA  | CHC-C1C-C2C | -2.43 | 120.38      | 127.43   |
| 88  | 8A    | 604 | HEA  | CBA-CAA-C2A | -2.40 | 105.89      | 112.53   |
| 85  | 3C    | 502 | HEM  | C4C-CHD-C1D | -2.40 | 120.92      | 126.02   |
| 88  | 4A    | 604 | HEA  | C17-C18-C19 | -2.39 | 122.15      | 127.62   |
| 88  | 8A    | 604 | HEA  | CMC-C2C-C1C | 2.38  | 129.04      | 125.42   |
| 88  | 4A    | 605 | HEA  | CMB-C2B-C1B | 2.37  | 128.74      | 125.03   |
| 86  | 3Q    | 501 | HEC  | CAA-CBA-CGA | -2.37 | 107.37      | 113.67   |
| 88  | 4A    | 604 | HEA  | CMB-C2B-C1B | 2.37  | 128.74      | 125.03   |
| 88  | 8A    | 604 | HEA  | CMB-C2B-C1B | 2.37  | 128.73      | 125.03   |
| 88  | 4A    | 605 | HEA  | CMC-C2C-C1C | 2.36  | 129.01      | 125.42   |
| 88  | 8A    | 605 | HEA  | CMC-C2C-C1C | 2.35  | 129.00      | 125.42   |
| 86  | 3D    | 501 | HEC  | CMC-C2C-C3C | 2.35  | 132.08      | 126.55   |
| 88  | 8A    | 604 | HEA  | CHD-C1D-C2D | -2.35 | 120.28      | 126.95   |
| 88  | 4A    | 604 | HEA  | CHD-C1D-C2D | -2.34 | 120.28      | 126.95   |
| 85  | 3P    | 502 | HEM  | C4C-CHD-C1D | -2.34 | 121.04      | 126.02   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 88  | 4A    | 604 | HEA  | C1A-CHA-C4D | -2.33 | 121.06      | 126.02   |
| 88  | 4A    | 604 | HEA  | C27-C19-C20 | 2.33  | 119.26      | 115.23   |
| 86  | 3Q    | 501 | HEC  | CMC-C2C-C3C | 2.32  | 132.00      | 126.55   |
| 92  | 4B    | 305 | PSC  | O01-C1-C2   | 2.30  | 116.46      | 111.48   |
| 88  | 8A    | 605 | HEA  | CAD-C3D-C4D | 2.29  | 128.69      | 124.70   |
| 88  | 4A    | 604 | HEA  | C13-C12-C11 | -2.29 | 110.73      | 114.39   |
| 88  | 8A    | 605 | HEA  | CMB-C2B-C1B | 2.28  | 128.59      | 125.03   |
| 86  | 3Q    | 501 | HEC  | CMB-C2B-C3B | 2.27  | 131.90      | 126.55   |
| 69  | 3A    | 502 | 3PE  | O21-C21-C22 | 2.27  | 116.40      | 111.48   |
| 88  | 8A    | 604 | HEA  | C25-C23-C24 | 2.27  | 119.81      | 114.59   |
| 88  | 8A    | 604 | HEA  | CHA-C1A-NA  | -2.27 | 121.99      | 124.45   |
| 85  | 3C    | 502 | HEM  | CHD-C1D-C2D | -2.26 | 121.45      | 125.03   |
| 86  | 3D    | 501 | HEC  | CMB-C2B-C3B | 2.26  | 131.87      | 126.55   |
| 85  | 3P    | 501 | HEM  | C1A-CHA-C4D | -2.26 | 120.94      | 126.25   |
| 88  | 8A    | 605 | HEA  | C25-C23-C24 | 2.26  | 119.78      | 114.59   |
| 88  | 4A    | 605 | HEA  | CAD-C3D-C4D | 2.26  | 128.63      | 124.70   |
| 88  | 4A    | 605 | HEA  | C1A-CHA-C4D | -2.26 | 121.22      | 126.02   |
| 85  | 3P    | 502 | HEM  | C1A-CHA-C4D | -2.25 | 120.95      | 126.25   |
| 88  | 8A    | 604 | HEA  | CMD-C2D-C1D | 2.25  | 128.54      | 125.03   |
| 85  | 3C    | 502 | HEM  | C1A-CHA-C4D | -2.24 | 120.97      | 126.25   |
| 88  | 8A    | 605 | HEA  | C4B-NB-C1B  | -2.24 | 102.55      | 105.21   |
| 88  | 4A    | 605 | HEA  | CMD-C2D-C1D | 2.24  | 128.53      | 125.03   |
| 85  | 3P    | 502 | HEM  | CHD-C4C-NC  | 2.23  | 126.88      | 124.45   |
| 88  | 8A    | 605 | HEA  | CHD-C1D-C2D | -2.21 | 120.67      | 126.95   |
| 88  | 4A    | 604 | HEA  | C25-C23-C24 | 2.20  | 119.65      | 114.59   |
| 88  | 4A    | 604 | HEA  | CMD-C2D-C1D | 2.19  | 128.46      | 125.03   |
| 85  | 3C    | 502 | HEM  | C4A-CHB-C1B | -2.19 | 121.09      | 126.25   |
| 88  | 4A    | 605 | HEA  | CHD-C1D-C2D | -2.18 | 120.75      | 126.95   |
| 88  | 8A    | 604 | HEA  | CHB-C4A-NA  | -2.18 | 122.08      | 124.45   |
| 86  | 3Q    | 501 | HEC  | CAD-C3D-C4D | 2.17  | 129.18      | 124.94   |
| 85  | 3P    | 502 | HEM  | C4D-ND-C1D  | 2.17  | 107.77      | 105.21   |
| 88  | 4A    | 604 | HEA  | CBA-CAA-C2A | -2.16 | 106.55      | 112.53   |
| 85  | 3C    | 501 | HEM  | C1A-CHA-C4D | -2.15 | 121.19      | 126.25   |
| 86  | 3D    | 501 | HEC  | CHC-C1C-C2C | -2.14 | 121.21      | 127.43   |
| 85  | 3C    | 501 | HEM  | CHA-C4D-C3D | -2.14 | 121.28      | 125.23   |
| 86  | 3Q    | 501 | HEC  | CHC-C1C-C2C | -2.14 | 121.22      | 127.43   |
| 87  | 8G    | 101 | PGV  | O01-C1-C2   | 2.12  | 116.06      | 111.48   |
| 88  | 8A    | 604 | HEA  | C21-C22-C23 | -2.11 | 120.59      | 127.64   |
| 87  | 4G    | 101 | PGV  | O01-C1-C2   | 2.11  | 116.04      | 111.48   |
| 88  | 4A    | 604 | HEA  | CHB-C4A-NA  | -2.10 | 122.16      | 124.45   |
| 85  | 3C    | 502 | HEM  | C4D-ND-C1D  | 2.10  | 107.70      | 105.21   |
| 73  | 1F    | 501 | FMN  | C4-N3-C2    | -2.10 | 121.92      | 125.64   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 85  | 3P    | 502 | HEM  | C4A-CHB-C1B | -2.10 | 121.31      | 126.25   |
| 88  | 4A    | 605 | HEA  | CHB-C1B-C2B | -2.09 | 121.72      | 125.03   |
| 75  | 1H    | 401 | CDL  | OB6-CB5-C51 | 2.09  | 116.00      | 111.48   |
| 87  | 4C    | 304 | PGV  | O01-C1-C2   | 2.09  | 116.00      | 111.48   |
| 86  | 3D    | 501 | HEC  | CAA-CBA-CGA | -2.08 | 108.14      | 113.67   |
| 85  | 3P    | 501 | HEM  | CHA-C4D-C3D | -2.08 | 121.39      | 125.23   |
| 88  | 8A    | 605 | HEA  | CMD-C2D-C1D | 2.06  | 128.26      | 125.03   |
| 88  | 8A    | 604 | HEA  | C4C-C3C-C2C | -2.05 | 104.75      | 107.30   |
| 87  | 8C    | 305 | PGV  | O01-C1-C2   | 2.05  | 115.92      | 111.48   |
| 88  | 8A    | 605 | HEA  | C21-C22-C23 | -2.05 | 120.82      | 127.64   |
| 85  | 3C    | 502 | HEM  | CHD-C4C-NC  | 2.04  | 126.67      | 124.45   |
| 88  | 4A    | 605 | HEA  | C21-C22-C23 | -2.03 | 120.86      | 127.64   |
| 85  | 3C    | 501 | HEM  | CHA-C1A-NA  | 2.03  | 127.54      | 123.86   |
| 85  | 3P    | 501 | HEM  | CHB-C1B-C2B | -2.03 | 121.18      | 126.95   |
| 88  | 4A    | 604 | HEA  | C21-C22-C23 | -2.03 | 120.88      | 127.64   |
| 86  | 3D    | 501 | HEC  | CMD-C2D-C1D | 2.03  | 128.50      | 125.42   |
| 86  | 3D    | 501 | HEC  | CAD-C3D-C4D | 2.02  | 128.88      | 124.94   |
| 88  | 8A    | 605 | HEA  | CHB-C1B-C2B | -2.00 | 121.86      | 125.03   |

There are no chirality outliers.

All (887) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 69  | 1A    | 201 | 3PE  | C11-O13-P-O12  |
| 69  | 1K    | 101 | 3PE  | C1-O11-P-O13   |
| 69  | 1K    | 101 | 3PE  | C1-O11-P-O14   |
| 69  | 1L    | 701 | 3PE  | O32-C31-O31-C3 |
| 69  | 1L    | 701 | 3PE  | C32-C31-O31-C3 |
| 69  | 1L    | 703 | 3PE  | C2-C1-O11-P    |
| 69  | 1M    | 501 | 3PE  | C11-O13-P-O14  |
| 69  | 1M    | 502 | 3PE  | C1-O11-P-O12   |
| 69  | 1M    | 502 | 3PE  | C2-C1-O11-P    |
| 69  | 1M    | 502 | 3PE  | O32-C31-O31-C3 |
| 69  | 1M    | 502 | 3PE  | C32-C31-O31-C3 |
| 69  | 1M    | 504 | 3PE  | C2-C1-O11-P    |
| 69  | 1M    | 506 | 3PE  | C1-O11-P-O14   |
| 69  | 1N    | 901 | 3PE  | C1-O11-P-O12   |
| 69  | 1N    | 901 | 3PE  | C1-O11-P-O13   |
| 69  | 1N    | 901 | 3PE  | C1-O11-P-O14   |
| 69  | 1P    | 403 | 3PE  | C1-O11-P-O12   |
| 69  | 1Y    | 202 | 3PE  | C1-O11-P-O13   |
| 69  | 1Y    | 202 | 3PE  | C2-C1-O11-P    |

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| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 69  | 1Y    | 203 | 3PE  | C1-O11-P-O13   |
| 69  | 1Y    | 203 | 3PE  | C1-O11-P-O14   |
| 69  | 1Y    | 203 | 3PE  | C2-C1-O11-P    |
| 69  | 1Y    | 203 | 3PE  | O22-C21-O21-C2 |
| 69  | 1Y    | 203 | 3PE  | C22-C21-O21-C2 |
| 69  | 1Y    | 204 | 3PE  | O22-C21-O21-C2 |
| 69  | 1Y    | 204 | 3PE  | C22-C21-O21-C2 |
| 69  | 1Y    | 206 | 3PE  | C11-O13-P-O14  |
| 69  | 1Y    | 206 | 3PE  | C12-C11-O13-P  |
| 69  | 1j    | 101 | 3PE  | O22-C21-O21-C2 |
| 69  | 1j    | 101 | 3PE  | C22-C21-O21-C2 |
| 69  | 1m    | 201 | 3PE  | O32-C31-O31-C3 |
| 69  | 1m    | 201 | 3PE  | C32-C31-O31-C3 |
| 69  | 3A    | 502 | 3PE  | O32-C31-O31-C3 |
| 69  | 3A    | 502 | 3PE  | C32-C31-O31-C3 |
| 69  | 3A    | 502 | 3PE  | O22-C21-O21-C2 |
| 69  | 3A    | 502 | 3PE  | C22-C21-O21-C2 |
| 69  | 3A    | 503 | 3PE  | C1-O11-P-O14   |
| 69  | 3A    | 503 | 3PE  | C2-C1-O11-P    |
| 69  | 3C    | 503 | 3PE  | C11-O13-P-O11  |
| 69  | 3C    | 503 | 3PE  | C11-O13-P-O12  |
| 69  | 3C    | 503 | 3PE  | C11-O13-P-O14  |
| 69  | 3C    | 504 | 3PE  | O21-C2-C3-O31  |
| 69  | 3G    | 101 | 3PE  | O32-C31-O31-C3 |
| 69  | 3G    | 101 | 3PE  | C32-C31-O31-C3 |
| 69  | 3N    | 501 | 3PE  | C1-O11-P-O13   |
| 69  | 3N    | 501 | 3PE  | C1-O11-P-O14   |
| 69  | 3N    | 501 | 3PE  | C2-C1-O11-P    |
| 69  | 3N    | 503 | 3PE  | O22-C21-O21-C2 |
| 69  | 3N    | 503 | 3PE  | C22-C21-O21-C2 |
| 69  | 3P    | 503 | 3PE  | C11-O13-P-O11  |
| 69  | 3P    | 503 | 3PE  | C11-O13-P-O12  |
| 69  | 3P    | 503 | 3PE  | C11-O13-P-O14  |
| 69  | 3Y    | 101 | 3PE  | C2-C1-O11-P    |
| 70  | 1B    | 203 | PC1  | O22-C21-O21-C2 |
| 70  | 1B    | 203 | PC1  | C22-C21-O21-C2 |
| 70  | 1I    | 203 | PC1  | C1-O11-P-O14   |
| 70  | 1M    | 503 | PC1  | C11-O13-P-O11  |
| 70  | 1M    | 503 | PC1  | O22-C21-O21-C2 |
| 70  | 1M    | 503 | PC1  | C22-C21-O21-C2 |
| 70  | 1M    | 505 | PC1  | C1-O11-P-O12   |
| 70  | 1d    | 202 | PC1  | O22-C21-O21-C2 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 70  | 1d    | 202 | PC1  | C22-C21-O21-C2  |
| 70  | 1h    | 203 | PC1  | C11-O13-P-O14   |
| 70  | 1h    | 203 | PC1  | O32-C31-O31-C3  |
| 70  | 1h    | 203 | PC1  | C32-C31-O31-C3  |
| 70  | 3R    | 303 | PC1  | O32-C31-O31-C3  |
| 70  | 3R    | 303 | PC1  | C32-C31-O31-C3  |
| 70  | 3X    | 101 | PC1  | C1-O11-P-O14    |
| 75  | 1H    | 401 | CDL  | CA4-CA3-OA5-PA1 |
| 75  | 1H    | 401 | CDL  | OB7-CB5-OB6-CB4 |
| 75  | 1H    | 401 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 1L    | 702 | CDL  | OA6-CA4-CA6-OA8 |
| 75  | 1L    | 702 | CDL  | CB3-OB5-PB2-OB4 |
| 75  | 1N    | 902 | CDL  | OA6-CA4-CA6-OA8 |
| 75  | 1N    | 902 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 1X    | 201 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 1X    | 201 | CDL  | CA2-OA2-PA1-OA4 |
| 75  | 1X    | 201 | CDL  | C1-CB2-OB2-PB2  |
| 75  | 1h    | 202 | CDL  | CA2-OA2-PA1-OA4 |
| 75  | 1h    | 202 | CDL  | CA2-OA2-PA1-OA5 |
| 75  | 1h    | 202 | CDL  | C1-CB2-OB2-PB2  |
| 75  | 1h    | 202 | CDL  | CB2-OB2-PB2-OB3 |
| 75  | 1h    | 202 | CDL  | OB7-CB5-OB6-CB4 |
| 75  | 1h    | 202 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 1h    | 202 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 1h    | 202 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 3G    | 102 | CDL  | CB2-OB2-PB2-OB3 |
| 75  | 3G    | 102 | CDL  | CB2-OB2-PB2-OB4 |
| 75  | 3G    | 102 | CDL  | CB2-OB2-PB2-OB5 |
| 75  | 3G    | 103 | CDL  | CB2-OB2-PB2-OB4 |
| 75  | 3G    | 103 | CDL  | CB2-OB2-PB2-OB5 |
| 75  | 3P    | 504 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 3P    | 504 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 75  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA4 |
| 75  | 3T    | 101 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 3T    | 101 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 4B    | 303 | CDL  | OA9-CA7-OA8-CA6 |
| 75  | 4B    | 303 | CDL  | C31-CA7-OA8-CA6 |
| 75  | 4B    | 303 | CDL  | CB3-OB5-PB2-OB2 |
| 75  | 4B    | 303 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 4C    | 305 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 4C    | 305 | CDL  | OB7-CB5-OB6-CB4 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 75  | 4C    | 305 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 4C    | 305 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 4C    | 305 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 4D    | 201 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 4D    | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 75  | 4D    | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 4D    | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 75  | 4D    | 201 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 4D    | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 4D    | 201 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 8B    | 303 | CDL  | OA9-CA7-OA8-CA6 |
| 75  | 8B    | 303 | CDL  | C31-CA7-OA8-CA6 |
| 75  | 8B    | 303 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 8C    | 306 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 8C    | 306 | CDL  | OB7-CB5-OB6-CB4 |
| 75  | 8C    | 306 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 8C    | 306 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 8C    | 306 | CDL  | C71-CB7-OB8-CB6 |
| 75  | 8D    | 201 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 8D    | 201 | CDL  | CA3-OA5-PA1-OA3 |
| 75  | 8D    | 201 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 8D    | 201 | CDL  | OB7-CB5-OB6-CB4 |
| 75  | 8D    | 201 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 8D    | 201 | CDL  | OB9-CB7-OB8-CB6 |
| 75  | 8D    | 201 | CDL  | C71-CB7-OB8-CB6 |
| 76  | 1O    | 401 | GTP  | C5'-O5'-PA-O1A  |
| 80  | 1T    | 101 | EHZ  | N2-C15-C16-O5   |
| 84  | 1I    | 201 | MYR  | O1-C1-C2-C3     |
| 85  | 3C    | 501 | HEM  | C2B-C3B-CAB-CBB |
| 85  | 3C    | 501 | HEM  | C4B-C3B-CAB-CBB |
| 85  | 3C    | 502 | HEM  | C2B-C3B-CAB-CBB |
| 85  | 3C    | 502 | HEM  | C2C-C3C-CAC-CBC |
| 85  | 3P    | 501 | HEM  | C2B-C3B-CAB-CBB |
| 85  | 3P    | 501 | HEM  | C4B-C3B-CAB-CBB |
| 85  | 3P    | 502 | HEM  | C2B-C3B-CAB-CBB |
| 85  | 3P    | 502 | HEM  | C2C-C3C-CAC-CBC |
| 87  | 4A    | 601 | PGV  | O04-C19-O03-C01 |
| 87  | 4A    | 601 | PGV  | C20-C19-O03-C01 |
| 87  | 4A    | 603 | PGV  | C02-C03-O11-P   |
| 87  | 4C    | 301 | PGV  | C05-C04-O12-P   |
| 87  | 4C    | 301 | PGV  | O02-C1-O01-C02  |
| 87  | 4C    | 301 | PGV  | C2-C1-O01-C02   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4C    | 302 | PGV  | C03-O11-P-O14   |
| 87  | 4C    | 302 | PGV  | O04-C19-O03-C01 |
| 87  | 4C    | 302 | PGV  | C20-C19-O03-C01 |
| 87  | 4C    | 303 | PGV  | C03-O11-P-O13   |
| 87  | 4C    | 304 | PGV  | O02-C1-O01-C02  |
| 87  | 4C    | 304 | PGV  | C2-C1-O01-C02   |
| 87  | 4G    | 101 | PGV  | O02-C1-O01-C02  |
| 87  | 4G    | 101 | PGV  | C2-C1-O01-C02   |
| 87  | 4G    | 101 | PGV  | O04-C19-O03-C01 |
| 87  | 4G    | 101 | PGV  | C20-C19-O03-C01 |
| 87  | 4K    | 101 | PGV  | C03-O11-P-O12   |
| 87  | 4K    | 101 | PGV  | C03-O11-P-O14   |
| 87  | 4K    | 101 | PGV  | O04-C19-O03-C01 |
| 87  | 4K    | 101 | PGV  | C20-C19-O03-C01 |
| 87  | 8A    | 601 | PGV  | O04-C19-O03-C01 |
| 87  | 8A    | 601 | PGV  | C20-C19-O03-C01 |
| 87  | 8A    | 603 | PGV  | C02-C03-O11-P   |
| 87  | 8B    | 301 | PGV  | C03-O11-P-O12   |
| 87  | 8B    | 301 | PGV  | C03-O11-P-O13   |
| 87  | 8B    | 301 | PGV  | C04-O12-P-O11   |
| 87  | 8C    | 302 | PGV  | C04-O12-P-O11   |
| 87  | 8C    | 302 | PGV  | C04-O12-P-O13   |
| 87  | 8C    | 302 | PGV  | C05-C04-O12-P   |
| 87  | 8C    | 302 | PGV  | O02-C1-O01-C02  |
| 87  | 8C    | 302 | PGV  | C2-C1-O01-C02   |
| 87  | 8C    | 303 | PGV  | C03-O11-P-O14   |
| 87  | 8C    | 303 | PGV  | O04-C19-O03-C01 |
| 87  | 8C    | 303 | PGV  | C20-C19-O03-C01 |
| 87  | 8C    | 304 | PGV  | C03-O11-P-O12   |
| 87  | 8C    | 304 | PGV  | C03-O11-P-O13   |
| 87  | 8C    | 305 | PGV  | O02-C1-O01-C02  |
| 87  | 8C    | 305 | PGV  | C2-C1-O01-C02   |
| 87  | 8G    | 101 | PGV  | O02-C1-O01-C02  |
| 87  | 8G    | 101 | PGV  | C2-C1-O01-C02   |
| 87  | 8G    | 101 | PGV  | O04-C19-O03-C01 |
| 87  | 8G    | 101 | PGV  | C20-C19-O03-C01 |
| 87  | 8K    | 101 | PGV  | C03-O11-P-O12   |
| 87  | 8K    | 101 | PGV  | C03-O11-P-O14   |
| 87  | 8K    | 101 | PGV  | O04-C19-O03-C01 |
| 87  | 8K    | 101 | PGV  | C20-C19-O03-C01 |
| 92  | 4B    | 305 | PSC  | C03-O11-P-O12   |
| 92  | 4B    | 305 | PSC  | C03-O11-P-O13   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 92  | 4B    | 305 | PSC  | C02-C03-O11-P   |
| 92  | 4B    | 305 | PSC  | O02-C1-O01-C02  |
| 92  | 4B    | 305 | PSC  | C2-C1-O01-C02   |
| 92  | 8B    | 305 | PSC  | C03-O11-P-O12   |
| 92  | 8B    | 305 | PSC  | C03-O11-P-O13   |
| 92  | 8B    | 305 | PSC  | O02-C1-O01-C02  |
| 92  | 8B    | 305 | PSC  | C2-C1-O01-C02   |
| 80  | 1T    | 101 | EHZ  | C13-C12-N1-C11  |
| 75  | 4C    | 305 | CDL  | O1-C1-CA2-OA2   |
| 75  | 4D    | 201 | CDL  | O1-C1-CB2-OB2   |
| 75  | 8C    | 306 | CDL  | O1-C1-CA2-OA2   |
| 75  | 8D    | 201 | CDL  | O1-C1-CB2-OB2   |
| 75  | 1N    | 902 | CDL  | C51-CB5-OB6-CB4 |
| 75  | 1N    | 902 | CDL  | OB7-CB5-OB6-CB4 |
| 86  | 3D    | 501 | HEC  | C3D-CAD-CBD-CGD |
| 88  | 4A    | 604 | HEA  | C19-C20-C21-C22 |
| 88  | 8A    | 604 | HEA  | C19-C20-C21-C22 |
| 75  | 1N    | 902 | CDL  | C1-CA2-OA2-PA1  |
| 92  | 8B    | 305 | PSC  | C02-C03-O11-P   |
| 80  | 1T    | 101 | EHZ  | O3-C12-N1-C11   |
| 75  | 4C    | 305 | CDL  | CB2-C1-CA2-OA2  |
| 75  | 8C    | 306 | CDL  | CB2-C1-CA2-OA2  |
| 78  | 1P    | 402 | NDP  | O4D-C1D-N1N-C6N |
| 69  | 3C    | 503 | 3PE  | C21-C22-C23-C24 |
| 70  | 1q    | 201 | PC1  | C31-C32-C33-C34 |
| 87  | 4B    | 302 | PGV  | C1-C2-C3-C4     |
| 70  | 1Y    | 207 | PC1  | C2-C1-O11-P     |
| 70  | 1H    | 403 | PC1  | C31-C32-C33-C34 |
| 87  | 8B    | 302 | PGV  | C1-C2-C3-C4     |
| 69  | 1m    | 201 | 3PE  | C31-C32-C33-C34 |
| 87  | 4J    | 101 | PGV  | C21-C22-C23-C24 |
| 87  | 8J    | 101 | PGV  | C21-C22-C23-C24 |
| 75  | 3G    | 102 | CDL  | O1-C1-CB2-OB2   |
| 70  | 1h    | 203 | PC1  | C2-C1-O11-P     |
| 73  | 1F    | 501 | FMN  | C4'-C5'-O5'-P   |
| 69  | 1N    | 901 | 3PE  | C32-C33-C34-C35 |
| 87  | 4C    | 302 | PGV  | C5-C6-C7-C8     |
| 87  | 8C    | 303 | PGV  | C5-C6-C7-C8     |
| 75  | 1d    | 203 | CDL  | CA5-C11-C12-C13 |
| 87  | 8C    | 302 | PGV  | C26-C27-C28-C29 |
| 69  | 1L    | 703 | 3PE  | C39-C3A-C3B-C3C |
| 69  | 1M    | 501 | 3PE  | C26-C27-C28-C29 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 75  | 1q    | 203 | CDL  | C16-C17-C18-C19 |
| 69  | 3P    | 503 | 3PE  | C1-C2-C3-O31    |
| 75  | 1N    | 902 | CDL  | CB3-CB4-CB6-OB8 |
| 93  | 8C    | 308 | PEK  | C21-C22-C23-C24 |
| 69  | 1d    | 201 | 3PE  | C3C-C3D-C3E-C3F |
| 70  | 1Y    | 207 | PC1  | C23-C24-C25-C26 |
| 69  | 3A    | 503 | 3PE  | C36-C37-C38-C39 |
| 75  | 8B    | 303 | CDL  | C59-C60-C61-C62 |
| 69  | 1Y    | 204 | 3PE  | C23-C24-C25-C26 |
| 70  | 1M    | 505 | PC1  | C23-C24-C25-C26 |
| 75  | 4B    | 303 | CDL  | C59-C60-C61-C62 |
| 87  | 4B    | 301 | PGV  | C22-C23-C24-C25 |
| 69  | 3C    | 504 | 3PE  | C2-C1-O11-P     |
| 87  | 4C    | 306 | PGV  | C02-C03-O11-P   |
| 69  | 1M    | 504 | 3PE  | C38-C39-C3A-C3B |
| 85  | 3C    | 501 | HEM  | C3D-CAD-CBD-CGD |
| 69  | 3A    | 503 | 3PE  | C32-C33-C34-C35 |
| 69  | 3R    | 302 | 3PE  | C35-C36-C37-C38 |
| 69  | 1M    | 501 | 3PE  | C21-C22-C23-C24 |
| 87  | 8B    | 301 | PGV  | C22-C23-C24-C25 |
| 80  | 1T    | 101 | EHZ  | C21-C22-C23-C24 |
| 92  | 8B    | 305 | PSC  | C25-C26-C27-C28 |
| 92  | 4B    | 305 | PSC  | C25-C26-C27-C28 |
| 75  | 1d    | 203 | CDL  | C32-C33-C34-C35 |
| 75  | 1L    | 702 | CDL  | CA7-C31-C32-C33 |
| 87  | 8C    | 302 | PGV  | C7-C8-C9-C10    |
| 69  | 1d    | 201 | 3PE  | C31-C32-C33-C34 |
| 75  | 3T    | 101 | CDL  | OA5-CA3-CA4-OA6 |
| 69  | 3R    | 302 | 3PE  | C27-C28-C29-C2A |
| 87  | 8L    | 101 | PGV  | C21-C22-C23-C24 |
| 85  | 3C    | 502 | HEM  | C4B-C3B-CAB-CBB |
| 85  | 3C    | 502 | HEM  | C4C-C3C-CAC-CBC |
| 85  | 3P    | 502 | HEM  | C4B-C3B-CAB-CBB |
| 85  | 3P    | 502 | HEM  | C4C-C3C-CAC-CBC |
| 69  | 1M    | 502 | 3PE  | C22-C23-C24-C25 |
| 69  | 1A    | 201 | 3PE  | C36-C37-C38-C39 |
| 75  | 1h    | 202 | CDL  | C60-C61-C62-C63 |
| 87  | 4K    | 101 | PGV  | C02-C03-O11-P   |
| 87  | 8C    | 304 | PGV  | C02-C03-O11-P   |
| 87  | 8C    | 307 | PGV  | C02-C03-O11-P   |
| 75  | 8D    | 201 | CDL  | C71-C72-C73-C74 |
| 70  | 1B    | 203 | PC1  | C28-C29-C2A-C2B |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4L    | 101 | PGV  | C6-C7-C8-C9     |
| 87  | 4L    | 101 | PGV  | C21-C22-C23-C24 |
| 87  | 8A    | 602 | PGV  | C22-C23-C24-C25 |
| 69  | 1L    | 703 | 3PE  | C33-C34-C35-C36 |
| 80  | 1T    | 101 | EHZ  | O4-C15-C16-O5   |
| 69  | 1M    | 502 | 3PE  | C3B-C3C-C3D-C3E |
| 75  | 3T    | 101 | CDL  | OA5-CA3-CA4-CA6 |
| 75  | 4C    | 305 | CDL  | C36-C37-C38-C39 |
| 93  | 4C    | 307 | PEK  | C21-C22-C23-C24 |
| 69  | 1N    | 901 | 3PE  | C2E-C2F-C2G-C2H |
| 75  | 3T    | 101 | CDL  | C52-C53-C54-C55 |
| 87  | 8L    | 101 | PGV  | C6-C7-C8-C9     |
| 75  | 1X    | 201 | CDL  | C23-C24-C25-C26 |
| 69  | 1Y    | 203 | 3PE  | C31-C32-C33-C34 |
| 75  | 3G    | 103 | CDL  | CA5-C11-C12-C13 |
| 69  | 1L    | 703 | 3PE  | C1-C2-C3-O31    |
| 69  | 1M    | 502 | 3PE  | C1-C2-C3-O31    |
| 69  | 3C    | 504 | 3PE  | C1-C2-C3-O31    |
| 70  | 1B    | 203 | PC1  | C1-C2-C3-O31    |
| 70  | 1h    | 203 | PC1  | C1-C2-C3-O31    |
| 75  | 1N    | 902 | CDL  | CA3-CA4-CA6-OA8 |
| 75  | 8C    | 306 | CDL  | C36-C37-C38-C39 |
| 75  | 1L    | 702 | CDL  | C57-C58-C59-C60 |
| 70  | 1I    | 203 | PC1  | C24-C25-C26-C27 |
| 70  | 1h    | 203 | PC1  | C32-C33-C34-C35 |
| 75  | 8D    | 201 | CDL  | C62-C63-C64-C65 |
| 87  | 4C    | 304 | PGV  | C02-C03-O11-P   |
| 87  | 8K    | 101 | PGV  | C02-C03-O11-P   |
| 93  | 8G    | 102 | PEK  | C21-C22-C23-C24 |
| 70  | 1h    | 203 | PC1  | C2A-C2B-C2C-C2D |
| 70  | 1H    | 402 | PC1  | O11-C1-C2-O21   |
| 87  | 8B    | 302 | PGV  | C24-C25-C26-C27 |
| 87  | 8K    | 101 | PGV  | C22-C23-C24-C25 |
| 87  | 4B    | 302 | PGV  | C24-C25-C26-C27 |
| 69  | 1N    | 901 | 3PE  | O21-C2-C3-O31   |
| 87  | 8C    | 304 | PGV  | O03-C01-C02-O01 |
| 75  | 1N    | 902 | CDL  | C32-C31-CA7-OA8 |
| 87  | 8C    | 302 | PGV  | C3-C4-C5-C6     |
| 88  | 8A    | 605 | HEA  | C3B-C11-C12-C13 |
| 75  | 1L    | 702 | CDL  | C11-C12-C13-C14 |
| 75  | 4B    | 303 | CDL  | C38-C39-C40-C41 |
| 75  | 1X    | 201 | CDL  | C61-C62-C63-C64 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4C    | 301 | PGV  | C7-C8-C9-C10    |
| 75  | 1N    | 902 | CDL  | C12-C13-C14-C15 |
| 75  | 8C    | 306 | CDL  | C59-C60-C61-C62 |
| 87  | 8C    | 302 | PGV  | C27-C28-C29-C30 |
| 69  | 1N    | 901 | 3PE  | C2-C1-O11-P     |
| 75  | 3N    | 502 | CDL  | CB4-CB3-OB5-PB2 |
| 87  | 4K    | 101 | PGV  | C05-C04-O12-P   |
| 87  | 8B    | 301 | PGV  | C05-C04-O12-P   |
| 87  | 8C    | 305 | PGV  | C02-C03-O11-P   |
| 87  | 8K    | 101 | PGV  | C05-C04-O12-P   |
| 70  | 1M    | 505 | PC1  | C32-C33-C34-C35 |
| 75  | 4D    | 201 | CDL  | C71-C72-C73-C74 |
| 69  | 1M    | 506 | 3PE  | C21-C22-C23-C24 |
| 69  | 1M    | 506 | 3PE  | C27-C28-C29-C2A |
| 87  | 4A    | 601 | PGV  | C21-C22-C23-C24 |
| 69  | 1N    | 901 | 3PE  | O11-C1-C2-C3    |
| 69  | 3A    | 503 | 3PE  | O11-C1-C2-C3    |
| 69  | 3C    | 504 | 3PE  | O11-C1-C2-C3    |
| 75  | 1d    | 203 | CDL  | OA5-CA3-CA4-CA6 |
| 75  | 3P    | 504 | CDL  | OB5-CB3-CB4-CB6 |
| 87  | 8A    | 602 | PGV  | C01-C02-C03-O11 |
| 75  | 3G    | 102 | CDL  | C72-C71-CB7-OB8 |
| 93  | 4G    | 102 | PEK  | O03-C21-C22-C23 |
| 93  | 8G    | 102 | PEK  | O03-C21-C22-C23 |
| 69  | 3Y    | 101 | 3PE  | C31-C32-C33-C34 |
| 70  | 1q    | 201 | PC1  | C2A-C2B-C2C-C2D |
| 75  | 4D    | 201 | CDL  | CA2-C1-CB2-OB2  |
| 75  | 1h    | 202 | CDL  | C76-C77-C78-C79 |
| 69  | 1Y    | 202 | 3PE  | C1-C2-C3-O31    |
| 69  | 1Y    | 204 | 3PE  | C1-C2-C3-O31    |
| 69  | 3N    | 501 | 3PE  | C1-C2-C3-O31    |
| 75  | 1L    | 702 | CDL  | CA3-CA4-CA6-OA8 |
| 75  | 4B    | 303 | CDL  | CB3-CB4-CB6-OB8 |
| 75  | 8B    | 303 | CDL  | CB3-CB4-CB6-OB8 |
| 87  | 4J    | 101 | PGV  | O03-C01-C02-C03 |
| 75  | 1h    | 202 | CDL  | C34-C35-C36-C37 |
| 69  | 1d    | 201 | 3PE  | C28-C29-C2A-C2B |
| 70  | 1B    | 203 | PC1  | C35-C36-C37-C38 |
| 69  | 3G    | 101 | 3PE  | C31-C32-C33-C34 |
| 75  | 4C    | 305 | CDL  | C59-C60-C61-C62 |
| 93  | 4G    | 102 | PEK  | C21-C22-C23-C24 |
| 69  | 1M    | 504 | 3PE  | O11-C1-C2-O21   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 69  | 1m    | 201 | 3PE  | O11-C1-C2-O21   |
| 69  | 3A    | 502 | 3PE  | O11-C1-C2-O21   |
| 87  | 4C    | 302 | PGV  | O01-C02-C03-O11 |
| 87  | 8C    | 303 | PGV  | O01-C02-C03-O11 |
| 69  | 1M    | 502 | 3PE  | C34-C35-C36-C37 |
| 69  | 1Y    | 204 | 3PE  | C2-C1-O11-P     |
| 75  | 3T    | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 75  | 4B    | 303 | CDL  | C1-CA2-OA2-PA1  |
| 87  | 4G    | 101 | PGV  | C02-C03-O11-P   |
| 87  | 8G    | 101 | PGV  | C02-C03-O11-P   |
| 70  | 1M    | 505 | PC1  | C2A-C2B-C2C-C2D |
| 82  | 1h    | 201 | AME  | C-CA-N-CT1      |
| 70  | 1I    | 203 | PC1  | C37-C38-C39-C3A |
| 88  | 4A    | 605 | HEA  | C2A-CAA-CBA-CGA |
| 69  | 1Y    | 203 | 3PE  | C22-C23-C24-C25 |
| 75  | 1L    | 702 | CDL  | C33-C34-C35-C36 |
| 75  | 1q    | 203 | CDL  | C52-C51-CB5-OB6 |
| 69  | 1Y    | 204 | 3PE  | O21-C2-C3-O31   |
| 69  | 3N    | 501 | 3PE  | O21-C2-C3-O31   |
| 69  | 3N    | 503 | 3PE  | O21-C2-C3-O31   |
| 75  | 3N    | 502 | CDL  | OA6-CA4-CA6-OA8 |
| 75  | 4B    | 303 | CDL  | OB6-CB4-CB6-OB8 |
| 87  | 4C    | 303 | PGV  | O03-C01-C02-O01 |
| 87  | 8J    | 101 | PGV  | O03-C01-C02-O01 |
| 75  | 8B    | 303 | CDL  | C38-C39-C40-C41 |
| 92  | 4B    | 305 | PSC  | C9-C10-C11-C12  |
| 92  | 4B    | 305 | PSC  | C10-C11-C12-C13 |
| 92  | 8B    | 305 | PSC  | C9-C10-C11-C12  |
| 92  | 8B    | 305 | PSC  | C10-C11-C12-C13 |
| 93  | 4G    | 102 | PEK  | C5-C6-C7-C8     |
| 93  | 4G    | 102 | PEK  | C9-C10-C11-C12  |
| 93  | 8G    | 102 | PEK  | C5-C6-C7-C8     |
| 93  | 8G    | 102 | PEK  | C9-C10-C11-C12  |
| 69  | 1M    | 504 | 3PE  | C31-C32-C33-C34 |
| 87  | 4J    | 101 | PGV  | C19-C20-C21-C22 |
| 70  | 1A    | 202 | PC1  | C22-C23-C24-C25 |
| 75  | 3P    | 504 | CDL  | CA5-C11-C12-C13 |
| 75  | 1L    | 702 | CDL  | C37-C38-C39-C40 |
| 87  | 4L    | 101 | PGV  | C3-C4-C5-C6     |
| 75  | 1X    | 201 | CDL  | C36-C37-C38-C39 |
| 76  | 1O    | 401 | GTP  | PB-O3A-PA-O5'   |
| 75  | 1h    | 202 | CDL  | CB7-C71-C72-C73 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 75  | 4D    | 201 | CDL  | C59-C60-C61-C62 |
| 87  | 8J    | 101 | PGV  | C19-C20-C21-C22 |
| 75  | 4C    | 305 | CDL  | C52-C53-C54-C55 |
| 70  | 1H    | 402 | PC1  | O11-C1-C2-C3    |
| 75  | 4B    | 303 | CDL  | OA5-CA3-CA4-CA6 |
| 75  | 1X    | 201 | CDL  | C58-C59-C60-C61 |
| 87  | 4C    | 303 | PGV  | C02-C03-O11-P   |
| 87  | 8C    | 304 | PGV  | C24-C25-C26-C27 |
| 87  | 4C    | 303 | PGV  | C24-C25-C26-C27 |
| 69  | 1A    | 201 | 3PE  | O21-C21-C22-C23 |
| 70  | 1Y    | 207 | PC1  | O31-C31-C32-C33 |
| 85  | 3C    | 501 | HEM  | C2C-C3C-CAC-CBC |
| 85  | 3P    | 501 | HEM  | C2C-C3C-CAC-CBC |
| 75  | 4D    | 201 | CDL  | C62-C63-C64-C65 |
| 69  | 1Y    | 204 | 3PE  | O31-C31-C32-C33 |
| 69  | 1N    | 901 | 3PE  | O11-C1-C2-O21   |
| 75  | 1d    | 203 | CDL  | OA5-CA3-CA4-OA6 |
| 75  | 4B    | 303 | CDL  | OA5-CA3-CA4-OA6 |
| 87  | 8A    | 601 | PGV  | O01-C02-C03-O11 |
| 69  | 1M    | 501 | 3PE  | C1-C2-C3-O31    |
| 69  | 1N    | 901 | 3PE  | C1-C2-C3-O31    |
| 69  | 3N    | 503 | 3PE  | C1-C2-C3-O31    |
| 75  | 3P    | 504 | CDL  | CB3-CB4-CB6-OB8 |
| 87  | 8J    | 101 | PGV  | O03-C01-C02-C03 |
| 88  | 4A    | 604 | HEA  | O11-C11-C12-C13 |
| 88  | 8A    | 604 | HEA  | O11-C11-C12-C13 |
| 75  | 3G    | 103 | CDL  | C52-C53-C54-C55 |
| 87  | 4C    | 301 | PGV  | C26-C27-C28-C29 |
| 75  | 1h    | 202 | CDL  | C38-C39-C40-C41 |
| 69  | 1K    | 101 | 3PE  | C12-C11-O13-P   |
| 69  | 1L    | 701 | 3PE  | C12-C11-O13-P   |
| 69  | 1M    | 504 | 3PE  | C12-C11-O13-P   |
| 69  | 1Y    | 203 | 3PE  | C12-C11-O13-P   |
| 69  | 1m    | 201 | 3PE  | C12-C11-O13-P   |
| 69  | 3C    | 503 | 3PE  | C12-C11-O13-P   |
| 69  | 3C    | 504 | 3PE  | C12-C11-O13-P   |
| 69  | 3P    | 503 | 3PE  | C12-C11-O13-P   |
| 70  | 1A    | 203 | PC1  | C12-C11-O13-P   |
| 70  | 1B    | 203 | PC1  | C12-C11-O13-P   |
| 70  | 1P    | 401 | PC1  | C12-C11-O13-P   |
| 93  | 4C    | 307 | PEK  | C05-C04-O12-P   |
| 93  | 4G    | 102 | PEK  | C05-C04-O12-P   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 93  | 8C    | 308 | PEK  | C05-C04-O12-P   |
| 93  | 8G    | 102 | PEK  | C05-C04-O12-P   |
| 75  | 8C    | 306 | CDL  | C52-C53-C54-C55 |
| 69  | 1L    | 703 | 3PE  | O21-C2-C3-O31   |
| 69  | 3P    | 503 | 3PE  | O21-C2-C3-O31   |
| 70  | 1H    | 403 | PC1  | O21-C2-C3-O31   |
| 70  | 1h    | 203 | PC1  | O21-C2-C3-O31   |
| 75  | 3P    | 504 | CDL  | OB6-CB4-CB6-OB8 |
| 75  | 8B    | 303 | CDL  | OB6-CB4-CB6-OB8 |
| 87  | 4J    | 101 | PGV  | O03-C01-C02-O01 |
| 75  | 1d    | 203 | CDL  | C71-C72-C73-C74 |
| 75  | 3P    | 504 | CDL  | C31-C32-C33-C34 |
| 87  | 4K    | 101 | PGV  | C22-C23-C24-C25 |
| 75  | 1X    | 201 | CDL  | C35-C36-C37-C38 |
| 87  | 8L    | 101 | PGV  | C3-C4-C5-C6     |
| 70  | 1A    | 202 | PC1  | O13-C11-C12-N   |
| 70  | 1B    | 203 | PC1  | O13-C11-C12-N   |
| 70  | 1P    | 401 | PC1  | O13-C11-C12-N   |
| 70  | 1Y    | 207 | PC1  | O13-C11-C12-N   |
| 70  | 1h    | 203 | PC1  | O13-C11-C12-N   |
| 76  | 1O    | 401 | GTP  | PA-O3A-PB-O1B   |
| 85  | 3P    | 501 | HEM  | C3D-CAD-CBD-CGD |
| 75  | 8D    | 201 | CDL  | CA2-C1-CB2-OB2  |
| 75  | 8D    | 201 | CDL  | C59-C60-C61-C62 |
| 87  | 8B    | 302 | PGV  | C20-C21-C22-C23 |
| 70  | 1I    | 203 | PC1  | C23-C24-C25-C26 |
| 87  | 4B    | 302 | PGV  | C27-C28-C29-C30 |
| 87  | 4A    | 601 | PGV  | C11-C10-C9-C8   |
| 69  | 1M    | 504 | 3PE  | O11-C1-C2-C3    |
| 69  | 1m    | 201 | 3PE  | O11-C1-C2-C3    |
| 75  | 8B    | 303 | CDL  | OA5-CA3-CA4-CA6 |
| 87  | 4A    | 601 | PGV  | C01-C02-C03-O11 |
| 87  | 4M    | 101 | PGV  | C01-C02-C03-O11 |
| 75  | 1d    | 203 | CDL  | C1-CA2-OA2-PA1  |
| 75  | 1h    | 202 | CDL  | CB4-CB3-OB5-PB2 |
| 87  | 4A    | 601 | PGV  | C02-C03-O11-P   |
| 87  | 8A    | 601 | PGV  | C29-C30-C31-C32 |
| 80  | 1n    | 201 | EHZ  | C11-C10-S1-C9   |
| 87  | 4C    | 301 | PGV  | C3-C4-C5-C6     |
| 87  | 8B    | 302 | PGV  | C27-C28-C29-C30 |
| 69  | 3A    | 503 | 3PE  | O11-C1-C2-O21   |
| 70  | 1M    | 505 | PC1  | O11-C1-C2-O21   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 75  | 8B    | 303 | CDL  | OA5-CA3-CA4-OA6 |
| 87  | 4A    | 601 | PGV  | O01-C02-C03-O11 |
| 87  | 4M    | 101 | PGV  | O01-C02-C03-O11 |
| 87  | 8A    | 602 | PGV  | O01-C02-C03-O11 |
| 75  | 4C    | 305 | CDL  | C11-C12-C13-C14 |
| 75  | 4C    | 305 | CDL  | C16-C17-C18-C19 |
| 69  | 1Y    | 202 | 3PE  | O21-C2-C3-O31   |
| 70  | 1B    | 203 | PC1  | O21-C2-C3-O31   |
| 75  | 1N    | 902 | CDL  | OB6-CB4-CB6-OB8 |
| 70  | 1Y    | 207 | PC1  | C36-C37-C38-C39 |
| 87  | 4G    | 101 | PGV  | C22-C23-C24-C25 |
| 69  | 1M    | 502 | 3PE  | C24-C25-C26-C27 |
| 70  | 1H    | 402 | PC1  | C1-C2-C3-O31    |
| 80  | 1T    | 101 | EHZ  | C10-C11-N1-C12  |
| 80  | 1n    | 201 | EHZ  | C10-C11-N1-C12  |
| 70  | 1H    | 403 | PC1  | C39-C3A-C3B-C3C |
| 69  | 1A    | 201 | 3PE  | C11-O13-P-O11   |
| 69  | 1A    | 201 | 3PE  | C11-O13-P-O14   |
| 69  | 1K    | 101 | 3PE  | C1-O11-P-O12    |
| 69  | 1K    | 101 | 3PE  | C11-O13-P-O14   |
| 69  | 1M    | 502 | 3PE  | C1-O11-P-O13    |
| 69  | 1M    | 504 | 3PE  | C11-O13-P-O14   |
| 69  | 1M    | 506 | 3PE  | C11-O13-P-O14   |
| 69  | 1P    | 403 | 3PE  | C1-O11-P-O13    |
| 69  | 1P    | 403 | 3PE  | C1-O11-P-O14    |
| 69  | 1Y    | 202 | 3PE  | C11-O13-P-O14   |
| 69  | 1Y    | 203 | 3PE  | C11-O13-P-O14   |
| 69  | 1d    | 201 | 3PE  | C11-O13-P-O14   |
| 69  | 1j    | 101 | 3PE  | C1-O11-P-O14    |
| 69  | 1m    | 201 | 3PE  | C11-O13-P-O14   |
| 69  | 3C    | 503 | 3PE  | C1-O11-P-O14    |
| 69  | 3N    | 501 | 3PE  | C1-O11-P-O12    |
| 69  | 3N    | 501 | 3PE  | C11-O13-P-O14   |
| 69  | 3N    | 503 | 3PE  | C11-O13-P-O14   |
| 70  | 1A    | 203 | PC1  | C1-O11-P-O14    |
| 70  | 1M    | 503 | PC1  | C1-O11-P-O14    |
| 70  | 1M    | 505 | PC1  | C1-O11-P-O14    |
| 70  | 1M    | 505 | PC1  | C1-O11-P-O13    |
| 70  | 1d    | 202 | PC1  | C1-O11-P-O14    |
| 75  | 1N    | 902 | CDL  | CA3-OA5-PA1-OA3 |
| 75  | 1X    | 201 | CDL  | CA2-OA2-PA1-OA5 |
| 75  | 1X    | 201 | CDL  | CB2-OB2-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 75  | 1d    | 203 | CDL  | CB2-OB2-PB2-OB3 |
| 75  | 1h    | 202 | CDL  | CB2-OB2-PB2-OB4 |
| 75  | 1h    | 202 | CDL  | CB2-OB2-PB2-OB5 |
| 75  | 3G    | 103 | CDL  | CA2-OA2-PA1-OA3 |
| 75  | 3G    | 103 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 3N    | 502 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 3P    | 504 | CDL  | CA3-OA5-PA1-OA3 |
| 75  | 3P    | 504 | CDL  | CB3-OB5-PB2-OB3 |
| 75  | 3T    | 101 | CDL  | CA3-OA5-PA1-OA2 |
| 75  | 4B    | 303 | CDL  | CB3-OB5-PB2-OB4 |
| 75  | 4D    | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 75  | 8B    | 303 | CDL  | CB3-OB5-PB2-OB2 |
| 75  | 8B    | 303 | CDL  | CB3-OB5-PB2-OB4 |
| 75  | 8D    | 201 | CDL  | CB2-OB2-PB2-OB3 |
| 87  | 4A    | 601 | PGV  | C04-O12-P-O13   |
| 87  | 4C    | 302 | PGV  | C03-O11-P-O12   |
| 87  | 4K    | 101 | PGV  | C04-O12-P-O13   |
| 87  | 8A    | 601 | PGV  | C04-O12-P-O13   |
| 87  | 8B    | 301 | PGV  | C04-O12-P-O13   |
| 87  | 8C    | 302 | PGV  | C04-O12-P-O14   |
| 87  | 8C    | 304 | PGV  | C03-O11-P-O14   |
| 87  | 8C    | 305 | PGV  | C03-O11-P-O14   |
| 87  | 8K    | 101 | PGV  | C04-O12-P-O13   |
| 92  | 4B    | 305 | PSC  | C04-O12-P-O14   |
| 92  | 8B    | 305 | PSC  | C04-O12-P-O14   |
| 69  | 1M    | 506 | 3PE  | C28-C29-C2A-C2B |
| 70  | 1H    | 402 | PC1  | C2-C1-O11-P     |
| 70  | 1M    | 505 | PC1  | C2-C1-O11-P     |
| 75  | 1d    | 203 | CDL  | C1-CB2-OB2-PB2  |
| 75  | 3P    | 504 | CDL  | CB4-CB3-OB5-PB2 |
| 75  | 8B    | 303 | CDL  | C1-CA2-OA2-PA1  |
| 87  | 8A    | 601 | PGV  | C02-C03-O11-P   |
| 69  | 1Y    | 203 | 3PE  | C33-C34-C35-C36 |
| 70  | 1d    | 202 | PC1  | C37-C38-C39-C3A |
| 87  | 8C    | 301 | PGV  | C11-C12-C13-C14 |
| 92  | 8B    | 305 | PSC  | C12-C13-C14-C15 |
| 92  | 8B    | 305 | PSC  | C19-C20-C21-C22 |
| 75  | 1H    | 401 | CDL  | CA3-CA4-OA6-CA5 |
| 88  | 4A    | 604 | HEA  | C15-C16-C17-C18 |
| 69  | 3Y    | 101 | 3PE  | O11-C1-C2-C3    |
| 70  | 1M    | 505 | PC1  | O11-C1-C2-C3    |
| 75  | 8C    | 306 | CDL  | OB5-CB3-CB4-CB6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 8K    | 101 | PGV  | C2-C3-C4-C5     |
| 87  | 8C    | 304 | PGV  | C9-C10-C11-C12  |
| 87  | 8C    | 305 | PGV  | C9-C10-C11-C12  |
| 87  | 8K    | 101 | PGV  | C9-C10-C11-C12  |
| 69  | 1Y    | 203 | 3PE  | O11-C1-C2-O21   |
| 69  | 3C    | 504 | 3PE  | O11-C1-C2-O21   |
| 75  | 1L    | 702 | CDL  | OA5-CA3-CA4-OA6 |
| 75  | 3P    | 504 | CDL  | OB5-CB3-CB4-OB6 |
| 69  | 1m    | 201 | 3PE  | C23-C24-C25-C26 |
| 69  | 1M    | 504 | 3PE  | C24-C25-C26-C27 |
| 69  | 1Y    | 205 | 3PE  | C33-C34-C35-C36 |
| 87  | 4K    | 101 | PGV  | C2-C3-C4-C5     |
| 69  | 1M    | 502 | 3PE  | O21-C2-C3-O31   |
| 87  | 4B    | 301 | PGV  | C30-C31-C32-C33 |
| 69  | 1m    | 201 | 3PE  | O21-C21-C22-C23 |
| 69  | 3C    | 504 | 3PE  | O31-C31-C32-C33 |
| 70  | 3X    | 101 | PC1  | O21-C21-C22-C23 |
| 69  | 3C    | 503 | 3PE  | C29-C2A-C2B-C2C |
| 87  | 8C    | 301 | PGV  | C11-C10-C9-C8   |
| 88  | 4A    | 605 | HEA  | C3B-C11-C12-C13 |
| 87  | 8C    | 302 | PGV  | C1-C2-C3-C4     |
| 87  | 4C    | 303 | PGV  | C5-C6-C7-C8     |
| 87  | 4C    | 301 | PGV  | C1-C2-C3-C4     |
| 80  | 1n    | 201 | EHZ  | C7-C8-C9-O2     |
| 87  | 4K    | 101 | PGV  | C9-C10-C11-C12  |
| 87  | 4L    | 101 | PGV  | C9-C10-C11-C12  |
| 69  | 3C    | 504 | 3PE  | C23-C24-C25-C26 |
| 75  | 8C    | 306 | CDL  | C11-C12-C13-C14 |
| 75  | 8C    | 306 | CDL  | C16-C17-C18-C19 |
| 75  | 8C    | 306 | CDL  | C51-C52-C53-C54 |
| 70  | 1B    | 202 | PC1  | C36-C37-C38-C39 |
| 80  | 1T    | 101 | EHZ  | C1-C21-C22-C23  |
| 75  | 1L    | 702 | CDL  | C38-C39-C40-C41 |
| 70  | 1Y    | 207 | PC1  | C25-C26-C27-C28 |
| 87  | 4M    | 101 | PGV  | C3-C4-C5-C6     |
| 69  | 1d    | 201 | 3PE  | C2-C1-O11-P     |
| 69  | 3R    | 302 | 3PE  | C21-C22-C23-C24 |
| 87  | 4J    | 101 | PGV  | C2-C3-C4-C5     |
| 75  | 1X    | 201 | CDL  | OB5-CB3-CB4-OB6 |
| 92  | 8B    | 305 | PSC  | O01-C02-C03-O11 |
| 87  | 4A    | 602 | PGV  | C11-C12-C13-C14 |
| 87  | 4C    | 301 | PGV  | C9-C10-C11-C12  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4C    | 304 | PGV  | C9-C10-C11-C12  |
| 87  | 4M    | 101 | PGV  | C9-C10-C11-C12  |
| 87  | 8L    | 101 | PGV  | C9-C10-C11-C12  |
| 92  | 4B    | 305 | PSC  | C12-C13-C14-C15 |
| 85  | 3C    | 501 | HEM  | C4C-C3C-CAC-CBC |
| 69  | 1Y    | 202 | 3PE  | C31-C32-C33-C34 |
| 75  | 4C    | 305 | CDL  | C51-C52-C53-C54 |
| 69  | 1P    | 403 | 3PE  | C37-C38-C39-C3A |
| 87  | 8A    | 602 | PGV  | C9-C10-C11-C12  |
| 87  | 8C    | 303 | PGV  | C9-C10-C11-C12  |
| 87  | 8J    | 101 | PGV  | C9-C10-C11-C12  |
| 75  | 1X    | 201 | CDL  | C55-C56-C57-C58 |
| 69  | 3Y    | 101 | 3PE  | O21-C2-C3-O31   |
| 70  | 1M    | 505 | PC1  | O21-C2-C3-O31   |
| 87  | 8B    | 302 | PGV  | C11-C10-C9-C8   |
| 75  | 1L    | 702 | CDL  | C58-C59-C60-C61 |
| 75  | 8B    | 303 | CDL  | C11-C12-C13-C14 |
| 87  | 8C    | 304 | PGV  | C13-C14-C15-C16 |
| 87  | 4A    | 601 | PGV  | C29-C30-C31-C32 |
| 87  | 4B    | 302 | PGV  | C20-C21-C22-C23 |
| 75  | 1L    | 702 | CDL  | CA4-CA3-OA5-PA1 |
| 87  | 8C    | 304 | PGV  | C5-C6-C7-C8     |
| 69  | 1M    | 502 | 3PE  | C2A-C2B-C2C-C2D |
| 88  | 8A    | 605 | HEA  | C2A-CAA-CBA-CGA |
| 75  | 1N    | 902 | CDL  | O1-C1-CB2-OB2   |
| 69  | 3N    | 501 | 3PE  | C33-C34-C35-C36 |
| 87  | 4C    | 303 | PGV  | C9-C10-C11-C12  |
| 87  | 8A    | 603 | PGV  | C11-C12-C13-C14 |
| 87  | 8C    | 302 | PGV  | C11-C12-C13-C14 |
| 87  | 8C    | 307 | PGV  | C11-C12-C13-C14 |
| 87  | 8A    | 601 | PGV  | C24-C25-C26-C27 |
| 85  | 3C    | 501 | HEM  | CAA-CBA-CGA-O1A |
| 85  | 3C    | 501 | HEM  | CAA-CBA-CGA-O2A |
| 85  | 3P    | 501 | HEM  | CAA-CBA-CGA-O2A |
| 85  | 3P    | 502 | HEM  | CAA-CBA-CGA-O1A |
| 88  | 8A    | 604 | HEA  | CAD-CBD-CGD-O1D |
| 69  | 1Y    | 202 | 3PE  | O31-C31-C32-C33 |
| 69  | 1M    | 504 | 3PE  | C1-C2-O21-C21   |
| 69  | 1Y    | 202 | 3PE  | C1-C2-O21-C21   |
| 69  | 1Y    | 205 | 3PE  | C1-C2-O21-C21   |
| 87  | 8C    | 304 | PGV  | C01-C02-O01-C1  |
| 88  | 8A    | 604 | HEA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 70  | 1B    | 202 | PC1  | C3D-C3E-C3F-C3G |
| 75  | 1X    | 201 | CDL  | C31-C32-C33-C34 |
| 87  | 4A    | 603 | PGV  | C11-C12-C13-C14 |
| 88  | 4A    | 604 | HEA  | CAD-CBD-CGD-O1D |
| 88  | 8A    | 605 | HEA  | CAD-CBD-CGD-O1D |
| 75  | 1N    | 902 | CDL  | C32-C31-CA7-OA9 |
| 69  | 1N    | 901 | 3PE  | C23-C24-C25-C26 |
| 70  | 1h    | 203 | PC1  | C2B-C2C-C2D-C2E |
| 69  | 3C    | 503 | 3PE  | O11-C1-C2-O21   |
| 92  | 4B    | 305 | PSC  | O01-C02-C03-O11 |
| 87  | 8G    | 101 | PGV  | C7-C8-C9-C10    |
| 87  | 8A    | 603 | PGV  | C15-C16-C17-C18 |
| 69  | 1M    | 506 | 3PE  | C25-C26-C27-C28 |
| 88  | 4A    | 604 | HEA  | C2C-C3C-CAC-CBC |
| 87  | 8G    | 101 | PGV  | C9-C10-C11-C12  |
| 75  | 1N    | 902 | CDL  | C1-CB2-OB2-PB2  |
| 75  | 3N    | 502 | CDL  | C1-CB2-OB2-PB2  |
| 85  | 3C    | 502 | HEM  | CAA-CBA-CGA-O1A |
| 88  | 8A    | 605 | HEA  | C26-C15-C16-C17 |
| 75  | 4C    | 305 | CDL  | OB5-CB3-CB4-CB6 |
| 92  | 4B    | 305 | PSC  | C2-C3-C4-C5     |
| 69  | 3A    | 502 | 3PE  | O21-C2-C3-O31   |
| 75  | 1q    | 203 | CDL  | OB6-CB4-CB6-OB8 |
| 75  | 3G    | 103 | CDL  | OB6-CB4-CB6-OB8 |
| 75  | 4D    | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 85  | 3P    | 501 | HEM  | CAD-CBD-CGD-O1D |
| 85  | 3P    | 502 | HEM  | CAD-CBD-CGD-O1D |
| 87  | 4K    | 101 | PGV  | C3-C4-C5-C6     |
| 87  | 8K    | 101 | PGV  | C3-C4-C5-C6     |
| 93  | 4G    | 102 | PEK  | O04-C21-C22-C23 |
| 78  | 1P    | 402 | NDP  | O4D-C4D-C5D-O5D |
| 78  | 1P    | 402 | NDP  | C2N-C3N-C7N-N7N |
| 87  | 4M    | 101 | PGV  | C22-C23-C24-C25 |
| 88  | 4A    | 605 | HEA  | CAD-CBD-CGD-O2D |
| 75  | 1d    | 203 | CDL  | C72-C73-C74-C75 |
| 93  | 8G    | 102 | PEK  | O04-C21-C22-C23 |
| 87  | 4C    | 301 | PGV  | C11-C12-C13-C14 |
| 87  | 4M    | 101 | PGV  | C11-C12-C13-C14 |
| 87  | 8L    | 101 | PGV  | C11-C12-C13-C14 |
| 70  | 1P    | 401 | PC1  | C33-C34-C35-C36 |
| 69  | 3C    | 503 | 3PE  | C25-C26-C27-C28 |
| 75  | 3A    | 501 | CDL  | O1-C1-CA2-OA2   |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4C    | 301 | PGV  | C6-C7-C8-C9     |
| 85  | 3P    | 501 | HEM  | CAA-CBA-CGA-O1A |
| 88  | 4A    | 604 | HEA  | CAD-CBD-CGD-O2D |
| 88  | 8A    | 605 | HEA  | CAD-CBD-CGD-O2D |
| 87  | 8J    | 101 | PGV  | C5-C6-C7-C8     |
| 75  | 3N    | 502 | CDL  | CA4-CA6-OA8-CA7 |
| 69  | 3N    | 501 | 3PE  | C22-C23-C24-C25 |
| 69  | 3Y    | 101 | 3PE  | C2-C3-O31-C31   |
| 85  | 3P    | 502 | HEM  | CAD-CBD-CGD-O2D |
| 87  | 8C    | 304 | PGV  | O03-C01-C02-C03 |
| 85  | 3C    | 502 | HEM  | CAA-CBA-CGA-O2A |
| 86  | 3Q    | 501 | HEC  | CAA-CBA-CGA-O2A |
| 87  | 8C    | 307 | PGV  | C5-C6-C7-C8     |
| 87  | 4G    | 101 | PGV  | C9-C10-C11-C12  |
| 87  | 4J    | 101 | PGV  | C9-C10-C11-C12  |
| 87  | 4B    | 302 | PGV  | C11-C10-C9-C8   |
| 87  | 8A    | 603 | PGV  | C2-C3-C4-C5     |
| 75  | 1h    | 202 | CDL  | OB5-CB3-CB4-OB6 |
| 85  | 3P    | 502 | HEM  | CAA-CBA-CGA-O2A |
| 92  | 8B    | 305 | PSC  | C15-C16-C17-C18 |
| 87  | 8C    | 302 | PGV  | C6-C7-C8-C9     |
| 88  | 4A    | 604 | HEA  | C4C-C3C-CAC-CBC |
| 85  | 3P    | 501 | HEM  | CAD-CBD-CGD-O2D |
| 87  | 4A    | 601 | PGV  | C11-C12-C13-C14 |
| 87  | 4C    | 302 | PGV  | C9-C10-C11-C12  |
| 87  | 4C    | 306 | PGV  | C11-C12-C13-C14 |
| 87  | 8A    | 602 | PGV  | C11-C12-C13-C14 |
| 87  | 8C    | 302 | PGV  | C9-C10-C11-C12  |
| 69  | 1K    | 101 | 3PE  | O21-C21-C22-C23 |
| 70  | 1B    | 202 | PC1  | C3C-C3D-C3E-C3F |
| 88  | 4A    | 605 | HEA  | CAD-CBD-CGD-O1D |
| 70  | 1P    | 401 | PC1  | C24-C25-C26-C27 |
| 69  | 1Y    | 203 | 3PE  | O11-C1-C2-C3    |
| 75  | 1L    | 702 | CDL  | OA5-CA3-CA4-CA6 |
| 75  | 1h    | 202 | CDL  | OB5-CB3-CB4-CB6 |
| 88  | 4A    | 604 | HEA  | C27-C19-C20-C21 |
| 88  | 4A    | 605 | HEA  | C26-C15-C16-C17 |
| 69  | 3R    | 302 | 3PE  | C22-C23-C24-C25 |
| 69  | 1d    | 201 | 3PE  | O21-C2-C3-O31   |
| 92  | 4B    | 305 | PSC  | C19-C20-C21-C22 |
| 86  | 3D    | 501 | HEC  | CAA-CBA-CGA-O2A |
| 75  | 4B    | 303 | CDL  | C12-C11-CA5-OA6 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4C    | 303 | PGV  | C13-C14-C15-C16 |
| 87  | 8J    | 101 | PGV  | C2-C3-C4-C5     |
| 75  | 4C    | 305 | CDL  | C81-C82-C83-C84 |
| 69  | 1M    | 506 | 3PE  | C2B-C2C-C2D-C2E |
| 70  | 1M    | 505 | PC1  | C28-C29-C2A-C2B |
| 69  | 1K    | 101 | 3PE  | C24-C25-C26-C27 |
| 87  | 4K    | 101 | PGV  | C11-C12-C13-C14 |
| 87  | 8A    | 601 | PGV  | C9-C10-C11-C12  |
| 87  | 8K    | 101 | PGV  | C11-C12-C13-C14 |
| 87  | 8B    | 301 | PGV  | C30-C31-C32-C33 |
| 83  | 1i    | 201 | CHD  | C22-C23-C24-O26 |
| 69  | 3C    | 503 | 3PE  | C2C-C2D-C2E-C2F |
| 75  | 3G    | 102 | CDL  | C72-C71-CB7-OB9 |
| 86  | 3Q    | 501 | HEC  | CAA-CBA-CGA-O1A |
| 69  | 1L    | 703 | 3PE  | C29-C2A-C2B-C2C |
| 69  | 1Y    | 206 | 3PE  | C3-C2-O21-C21   |
| 69  | 3C    | 503 | 3PE  | C1-C2-O21-C21   |
| 87  | 4C    | 303 | PGV  | C01-C02-O01-C1  |
| 75  | 1X    | 201 | CDL  | C34-C35-C36-C37 |
| 69  | 3N    | 501 | 3PE  | C26-C27-C28-C29 |
| 69  | 1K    | 101 | 3PE  | C26-C27-C28-C29 |
| 75  | 3G    | 102 | CDL  | C12-C13-C14-C15 |
| 82  | 1h    | 201 | AME  | CB-CA-N-CT1     |
| 87  | 8C    | 304 | PGV  | C05-C04-O12-P   |
| 75  | 3G    | 102 | CDL  | CA2-C1-CB2-OB2  |
| 70  | 1M    | 503 | PC1  | C11-C12-N-C15   |
| 75  | 4C    | 305 | CDL  | C75-C76-C77-C78 |
| 70  | 1M    | 505 | PC1  | C1-C2-C3-O31    |
| 75  | 3N    | 502 | CDL  | CA3-CA4-CA6-OA8 |
| 85  | 3P    | 501 | HEM  | C4C-C3C-CAC-CBC |
| 70  | 3R    | 303 | PC1  | C27-C28-C29-C2A |
| 88  | 8A    | 605 | HEA  | O11-C11-C12-C13 |
| 69  | 3D    | 502 | 3PE  | C24-C25-C26-C27 |
| 87  | 4A    | 601 | PGV  | C9-C10-C11-C12  |
| 83  | 1i    | 201 | CHD  | C22-C23-C24-O25 |
| 80  | 1T    | 101 | EHZ  | C15-C16-C17-C19 |
| 70  | 1h    | 203 | PC1  | C22-C23-C24-C25 |
| 69  | 1A    | 201 | 3PE  | C2A-C2B-C2C-C2D |
| 87  | 8A    | 602 | PGV  | C3-C4-C5-C6     |
| 86  | 3D    | 501 | HEC  | CAA-CBA-CGA-O1A |
| 87  | 4C    | 303 | PGV  | C3-C4-C5-C6     |
| 93  | 4C    | 307 | PEK  | O03-C01-C02-O01 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 69  | 3A    | 502 | 3PE  | O11-C1-C2-C3    |
| 70  | 1B    | 203 | PC1  | O11-C1-C2-C3    |
| 87  | 4C    | 302 | PGV  | C01-C02-C03-O11 |
| 87  | 8C    | 303 | PGV  | C01-C02-C03-O11 |
| 92  | 4B    | 305 | PSC  | C01-C02-C03-O11 |
| 92  | 8B    | 305 | PSC  | C01-C02-C03-O11 |
| 87  | 4K    | 101 | PGV  | C1-C2-C3-C4     |
| 75  | 8C    | 306 | CDL  | C62-C63-C64-C65 |
| 87  | 4G    | 101 | PGV  | C7-C8-C9-C10    |
| 69  | 1Y    | 203 | 3PE  | C2D-C2E-C2F-C2G |
| 70  | 1M    | 505 | PC1  | C2D-C2E-C2F-C2G |
| 87  | 8C    | 303 | PGV  | C14-C15-C16-C17 |
| 76  | 1O    | 401 | GTP  | PA-O3A-PB-O2B   |
| 70  | 1A    | 202 | PC1  | C23-C24-C25-C26 |
| 80  | 1n    | 201 | EHZ  | C21-C1-C2-C3    |
| 87  | 8C    | 303 | PGV  | C26-C27-C28-C29 |
| 75  | 3G    | 103 | CDL  | C11-C12-C13-C14 |
| 75  | 8C    | 306 | CDL  | C71-C72-C73-C74 |
| 87  | 8K    | 101 | PGV  | C5-C6-C7-C8     |
| 92  | 8B    | 305 | PSC  | C4-C5-C6-C7     |
| 75  | 8C    | 306 | CDL  | C18-C19-C20-C21 |
| 87  | 4A    | 601 | PGV  | C24-C25-C26-C27 |
| 75  | 1d    | 203 | CDL  | C32-C31-CA7-OA8 |
| 87  | 8C    | 303 | PGV  | C6-C7-C8-C9     |
| 69  | 1Y    | 206 | 3PE  | O21-C21-C22-C23 |
| 87  | 8A    | 601 | PGV  | O03-C19-C20-C21 |
| 70  | 1I    | 203 | PC1  | C22-C23-C24-C25 |
| 70  | 1H    | 402 | PC1  | C31-C32-C33-C34 |
| 75  | 3P    | 504 | CDL  | C32-C31-CA7-OA8 |
| 87  | 8A    | 602 | PGV  | C21-C22-C23-C24 |
| 80  | 1T    | 101 | EHZ  | C4-C5-C6-C7     |
| 88  | 8A    | 604 | HEA  | CAA-CBA-CGA-O1A |
| 69  | 1d    | 201 | 3PE  | C35-C36-C37-C38 |
| 87  | 4C    | 301 | PGV  | C28-C29-C30-C31 |
| 70  | 1d    | 202 | PC1  | O21-C21-C22-C23 |
| 88  | 4A    | 604 | HEA  | CAA-CBA-CGA-O1A |
| 88  | 8A    | 604 | HEA  | CAA-CBA-CGA-O2A |
| 69  | 1P    | 403 | 3PE  | O21-C21-C22-C23 |
| 87  | 4A    | 601 | PGV  | O03-C19-C20-C21 |
| 75  | 4C    | 305 | CDL  | C18-C19-C20-C21 |
| 75  | 1q    | 203 | CDL  | C52-C51-CB5-OB7 |
| 88  | 4A    | 604 | HEA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 69  | 1M    | 504 | 3PE  | C32-C33-C34-C35 |
| 75  | 1X    | 201 | CDL  | OB5-CB3-CB4-CB6 |
| 73  | 1F    | 501 | FMN  | N10-C1'-C2'-O2' |
| 75  | 1X    | 201 | CDL  | CB2-C1-CA2-OA2  |
| 70  | 1H    | 402 | PC1  | C36-C37-C38-C39 |
| 75  | 8C    | 306 | CDL  | C75-C76-C77-C78 |
| 69  | 1M    | 502 | 3PE  | C29-C2A-C2B-C2C |
| 69  | 1Y    | 202 | 3PE  | C3-C2-O21-C21   |
| 75  | 3N    | 502 | CDL  | CB3-CB4-OB6-CB5 |
| 75  | 3N    | 502 | CDL  | CB6-CB4-OB6-CB5 |
| 75  | 1X    | 201 | CDL  | C63-C64-C65-C66 |
| 87  | 8J    | 101 | PGV  | C30-C31-C32-C33 |
| 87  | 8C    | 304 | PGV  | C3-C4-C5-C6     |
| 69  | 1K    | 101 | 3PE  | C34-C35-C36-C37 |
| 70  | 1P    | 401 | PC1  | C32-C33-C34-C35 |
| 75  | 3P    | 504 | CDL  | C72-C71-CB7-OB8 |
| 75  | 3P    | 504 | CDL  | C13-C14-C15-C16 |
| 87  | 8A    | 602 | PGV  | C05-C04-O12-P   |
| 70  | 1Y    | 207 | PC1  | O32-C31-C32-C33 |
| 70  | 1q    | 201 | PC1  | C32-C33-C34-C35 |
| 75  | 4C    | 305 | CDL  | C71-C72-C73-C74 |
| 69  | 1Y    | 203 | 3PE  | C27-C28-C29-C2A |
| 87  | 8G    | 101 | PGV  | C22-C23-C24-C25 |
| 75  | 1q    | 203 | CDL  | CA5-C11-C12-C13 |
| 75  | 8B    | 303 | CDL  | CB5-C51-C52-C53 |
| 75  | 1h    | 202 | CDL  | C74-C75-C76-C77 |
| 75  | 1N    | 902 | CDL  | CA7-C31-C32-C33 |
| 70  | 3J    | 101 | PC1  | C22-C23-C24-C25 |
| 70  | 1M    | 503 | PC1  | C11-C12-N-C14   |
| 75  | 4B    | 303 | CDL  | C13-C14-C15-C16 |
| 87  | 4G    | 101 | PGV  | C23-C24-C25-C26 |
| 87  | 4L    | 101 | PGV  | C11-C12-C13-C14 |
| 70  | 1d    | 202 | PC1  | O22-C21-C22-C23 |
| 69  | 1L    | 701 | 3PE  | C28-C29-C2A-C2B |
| 87  | 4A    | 603 | PGV  | C6-C7-C8-C9     |
| 69  | 1M    | 501 | 3PE  | C23-C24-C25-C26 |
| 87  | 8A    | 601 | PGV  | O04-C19-C20-C21 |
| 69  | 1M    | 501 | 3PE  | O21-C2-C3-O31   |
| 75  | 8D    | 201 | CDL  | OA6-CA4-CA6-OA8 |
| 87  | 8J    | 101 | PGV  | C27-C28-C29-C30 |
| 86  | 3Q    | 501 | HEC  | CAD-CBD-CGD-O2D |
| 75  | 1d    | 203 | CDL  | C32-C31-CA7-OA9 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 87  | 4J    | 101 | PGV  | C27-C28-C29-C30 |
| 87  | 8C    | 301 | PGV  | C26-C27-C28-C29 |
| 69  | 1A    | 201 | 3PE  | C27-C28-C29-C2A |
| 70  | 1A    | 202 | PC1  | O31-C31-C32-C33 |
| 87  | 8C    | 305 | PGV  | C7-C8-C9-C10    |
| 69  | 1Y    | 206 | 3PE  | O22-C21-C22-C23 |
| 75  | 3P    | 504 | CDL  | C32-C31-CA7-OA9 |
| 87  | 4A    | 601 | PGV  | O04-C19-C20-C21 |
| 75  | 8B    | 303 | CDL  | C12-C11-CA5-OA6 |
| 70  | 1Y    | 207 | PC1  | C3A-C3B-C3C-C3D |
| 70  | 1H    | 403 | PC1  | O11-C1-C2-C3    |
| 87  | 8A    | 601 | PGV  | C01-C02-C03-O11 |
| 75  | 1q    | 203 | CDL  | C12-C11-CA5-OA6 |
| 80  | 1T    | 101 | EHZ  | C2-C3-C4-C5     |
| 87  | 4M    | 101 | PGV  | C20-C21-C22-C23 |
| 92  | 8B    | 305 | PSC  | C2-C3-C4-C5     |
| 75  | 3P    | 504 | CDL  | C72-C71-CB7-OB9 |
| 75  | 3P    | 504 | CDL  | CB5-C51-C52-C53 |
| 70  | 1B    | 203 | PC1  | O31-C31-C32-C33 |
| 70  | 1h    | 203 | PC1  | O31-C31-C32-C33 |
| 75  | 4D    | 201 | CDL  | C32-C31-CA7-OA8 |
| 87  | 4G    | 101 | PGV  | O03-C19-C20-C21 |
| 87  | 8C    | 302 | PGV  | O03-C19-C20-C21 |
| 87  | 4K    | 101 | PGV  | C5-C6-C7-C8     |
| 69  | 1Y    | 204 | 3PE  | O22-C21-C22-C23 |
| 69  | 1Y    | 204 | 3PE  | O21-C21-C22-C23 |
| 70  | 1d    | 202 | PC1  | O31-C31-C32-C33 |
| 87  | 4C    | 302 | PGV  | C26-C27-C28-C29 |

There are no ring outliers.

121 monomers are involved in 594 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 87  | 4C    | 301 | PGV  | 2       | 0            |
| 73  | 1F    | 501 | FMN  | 4       | 0            |
| 75  | 1h    | 202 | CDL  | 14      | 0            |
| 87  | 4A    | 603 | PGV  | 10      | 0            |
| 70  | 1I    | 203 | PC1  | 3       | 0            |
| 75  | 3G    | 103 | CDL  | 6       | 0            |
| 92  | 8B    | 305 | PSC  | 8       | 0            |
| 70  | 1A    | 202 | PC1  | 7       | 0            |
| 69  | 3N    | 503 | 3PE  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 70  | 1B    | 203 | PC1  | 9       | 0            |
| 70  | 1P    | 401 | PC1  | 2       | 0            |
| 71  | 1F    | 502 | SF4  | 2       | 0            |
| 75  | 3G    | 102 | CDL  | 2       | 0            |
| 87  | 4J    | 101 | PGV  | 10      | 0            |
| 69  | 1M    | 502 | 3PE  | 12      | 0            |
| 69  | 1Y    | 206 | 3PE  | 2       | 0            |
| 91  | 4B    | 304 | CUA  | 2       | 0            |
| 94  | 8H    | 101 | PO4  | 1       | 0            |
| 75  | 1N    | 902 | CDL  | 3       | 0            |
| 87  | 4C    | 304 | PGV  | 1       | 0            |
| 87  | 8C    | 304 | PGV  | 7       | 0            |
| 87  | 4A    | 601 | PGV  | 6       | 0            |
| 87  | 4L    | 101 | PGV  | 7       | 0            |
| 69  | 3C    | 503 | 3PE  | 5       | 0            |
| 69  | 1d    | 201 | 3PE  | 5       | 0            |
| 69  | 3A    | 503 | 3PE  | 8       | 0            |
| 75  | 1q    | 203 | CDL  | 2       | 0            |
| 70  | 1M    | 505 | PC1  | 7       | 0            |
| 76  | 1O    | 401 | GTP  | 3       | 0            |
| 87  | 4K    | 101 | PGV  | 2       | 0            |
| 75  | 4C    | 305 | CDL  | 15      | 0            |
| 70  | 1H    | 403 | PC1  | 7       | 0            |
| 87  | 8C    | 301 | PGV  | 5       | 0            |
| 85  | 3P    | 501 | HEM  | 1       | 0            |
| 92  | 4B    | 305 | PSC  | 8       | 0            |
| 86  | 3D    | 501 | HEC  | 2       | 0            |
| 72  | 3E    | 301 | FES  | 2       | 0            |
| 70  | 1d    | 202 | PC1  | 8       | 0            |
| 70  | 1Y    | 207 | PC1  | 7       | 0            |
| 87  | 4A    | 602 | PGV  | 4       | 0            |
| 87  | 4C    | 303 | PGV  | 7       | 0            |
| 69  | 3D    | 502 | 3PE  | 2       | 0            |
| 75  | 8D    | 201 | CDL  | 15      | 0            |
| 69  | 1M    | 501 | 3PE  | 7       | 0            |
| 69  | 3R    | 302 | 3PE  | 5       | 0            |
| 70  | 1h    | 203 | PC1  | 1       | 0            |
| 81  | 1q    | 202 | AYA  | 2       | 0            |
| 93  | 8G    | 102 | PEK  | 5       | 0            |
| 75  | 1X    | 201 | CDL  | 12      | 0            |
| 86  | 3Q    | 501 | HEC  | 3       | 0            |
| 82  | 1h    | 201 | AME  | 1       | 0            |

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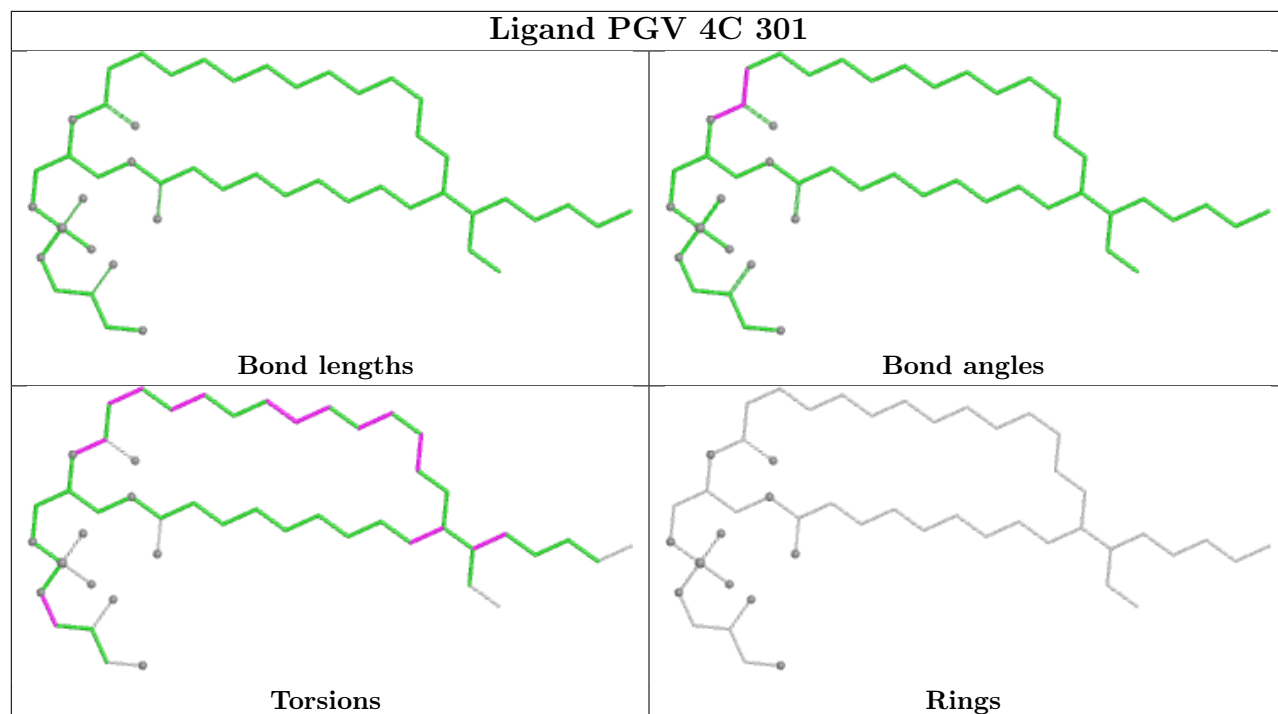
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 87  | 8B    | 302 | PGV  | 3       | 0            |
| 71  | 1G    | 801 | SF4  | 3       | 0            |
| 69  | 3A    | 502 | 3PE  | 1       | 0            |
| 75  | 1H    | 401 | CDL  | 1       | 0            |
| 80  | 1n    | 201 | EHZ  | 1       | 0            |
| 70  | 1H    | 402 | PC1  | 5       | 0            |
| 87  | 8K    | 101 | PGV  | 3       | 0            |
| 87  | 8B    | 301 | PGV  | 8       | 0            |
| 69  | 3N    | 501 | 3PE  | 5       | 0            |
| 69  | 1L    | 703 | 3PE  | 5       | 0            |
| 69  | 3Y    | 101 | 3PE  | 2       | 0            |
| 87  | 8C    | 307 | PGV  | 8       | 0            |
| 69  | 1L    | 701 | 3PE  | 3       | 0            |
| 75  | 3P    | 504 | CDL  | 9       | 0            |
| 69  | 1M    | 506 | 3PE  | 3       | 0            |
| 69  | 3G    | 101 | 3PE  | 1       | 0            |
| 70  | 1M    | 503 | PC1  | 3       | 0            |
| 93  | 4G    | 102 | PEK  | 2       | 0            |
| 69  | 1P    | 403 | 3PE  | 3       | 0            |
| 69  | 1Y    | 204 | 3PE  | 5       | 0            |
| 75  | 1d    | 203 | CDL  | 6       | 0            |
| 75  | 8C    | 306 | CDL  | 16      | 0            |
| 93  | 4C    | 307 | PEK  | 5       | 0            |
| 87  | 8C    | 305 | PGV  | 10      | 0            |
| 75  | 4B    | 303 | CDL  | 14      | 0            |
| 69  | 1M    | 504 | 3PE  | 11      | 0            |
| 69  | 1Y    | 203 | 3PE  | 9       | 0            |
| 71  | 1B    | 201 | SF4  | 2       | 0            |
| 87  | 8A    | 601 | PGV  | 10      | 0            |
| 87  | 4B    | 302 | PGV  | 4       | 0            |
| 75  | 8B    | 303 | CDL  | 10      | 0            |
| 87  | 4C    | 302 | PGV  | 5       | 0            |
| 87  | 8L    | 101 | PGV  | 7       | 0            |
| 75  | 3T    | 101 | CDL  | 9       | 0            |
| 87  | 8J    | 101 | PGV  | 4       | 0            |
| 93  | 8C    | 308 | PEK  | 5       | 0            |
| 69  | 3C    | 504 | 3PE  | 4       | 0            |
| 72  | 1G    | 803 | FES  | 2       | 0            |
| 88  | 8A    | 604 | HEA  | 8       | 0            |
| 70  | 3J    | 101 | PC1  | 4       | 0            |
| 75  | 1L    | 702 | CDL  | 6       | 0            |
| 70  | 3X    | 101 | PC1  | 2       | 0            |

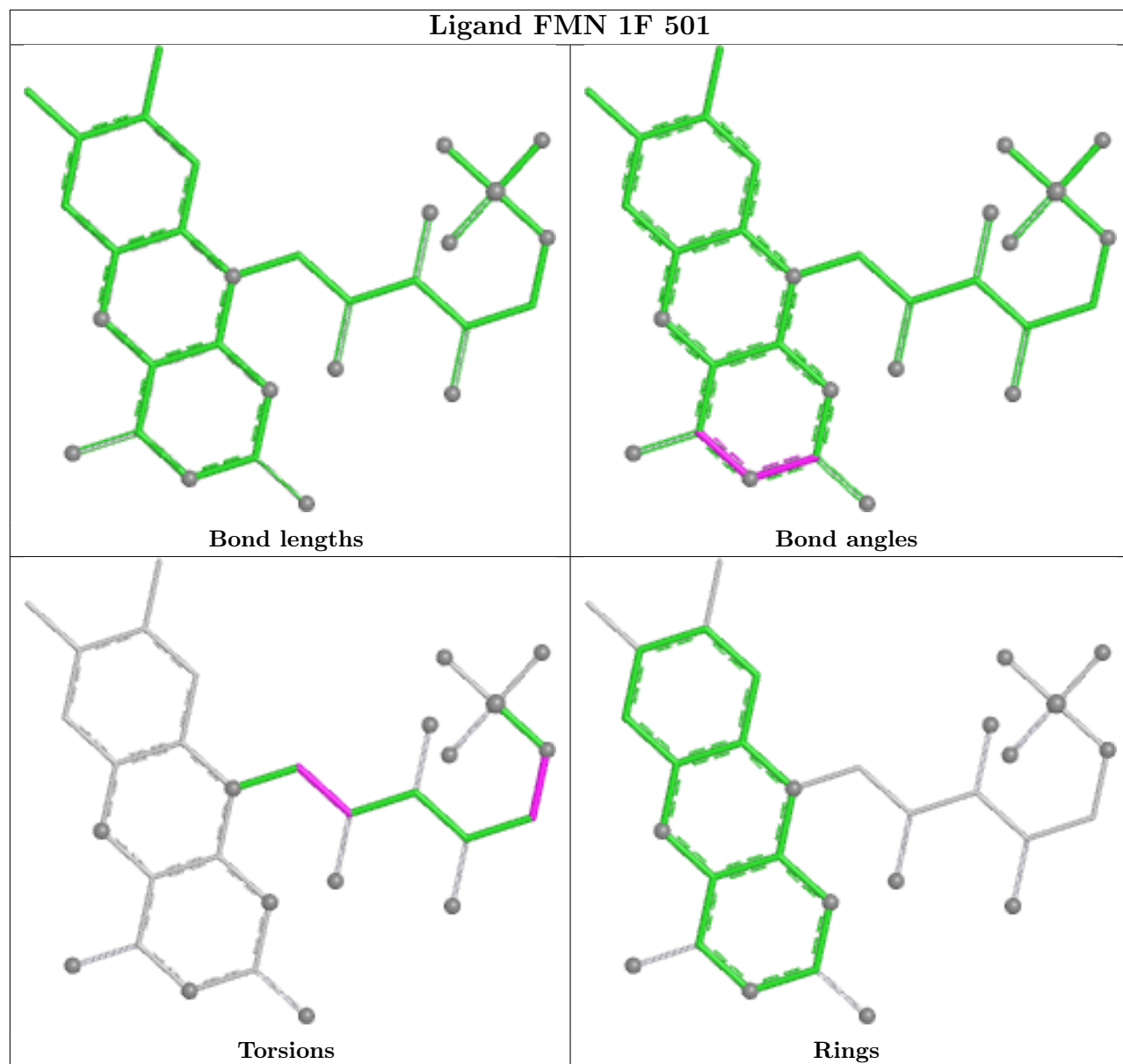
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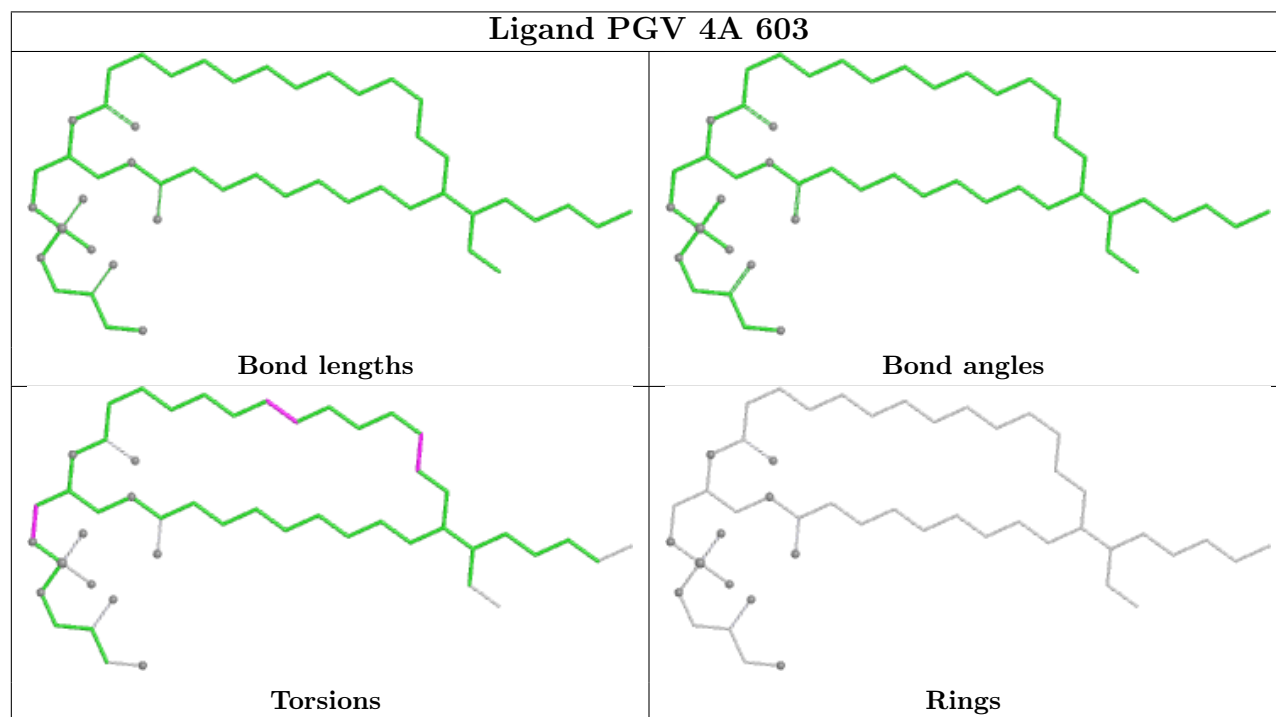
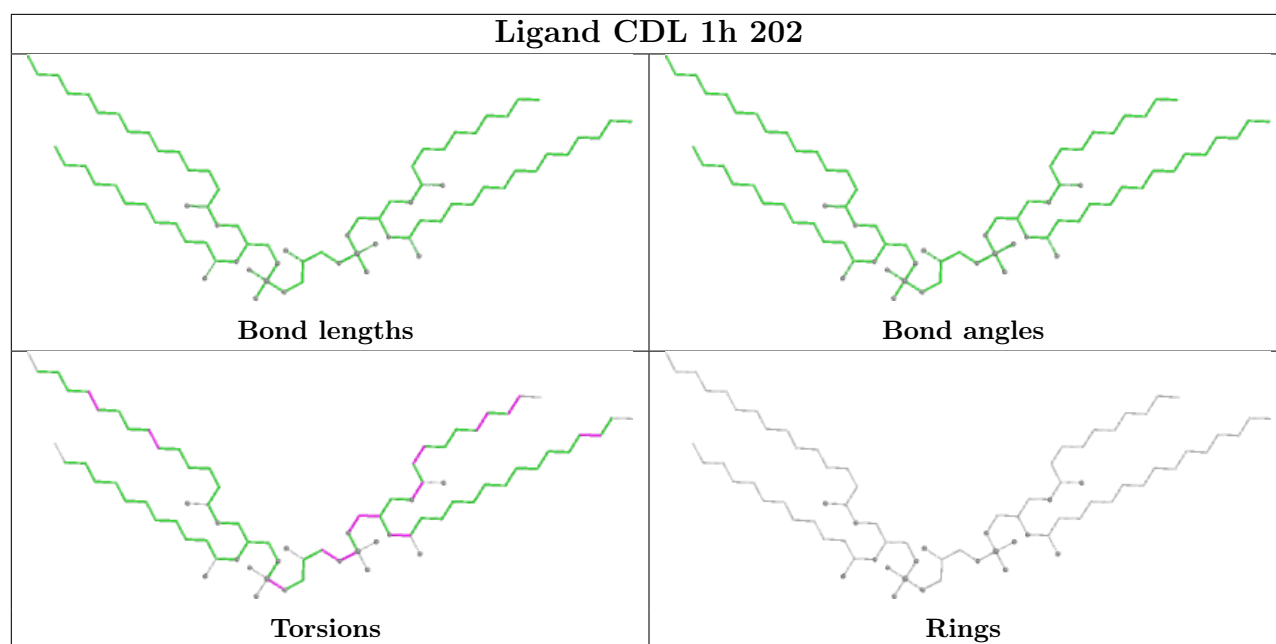
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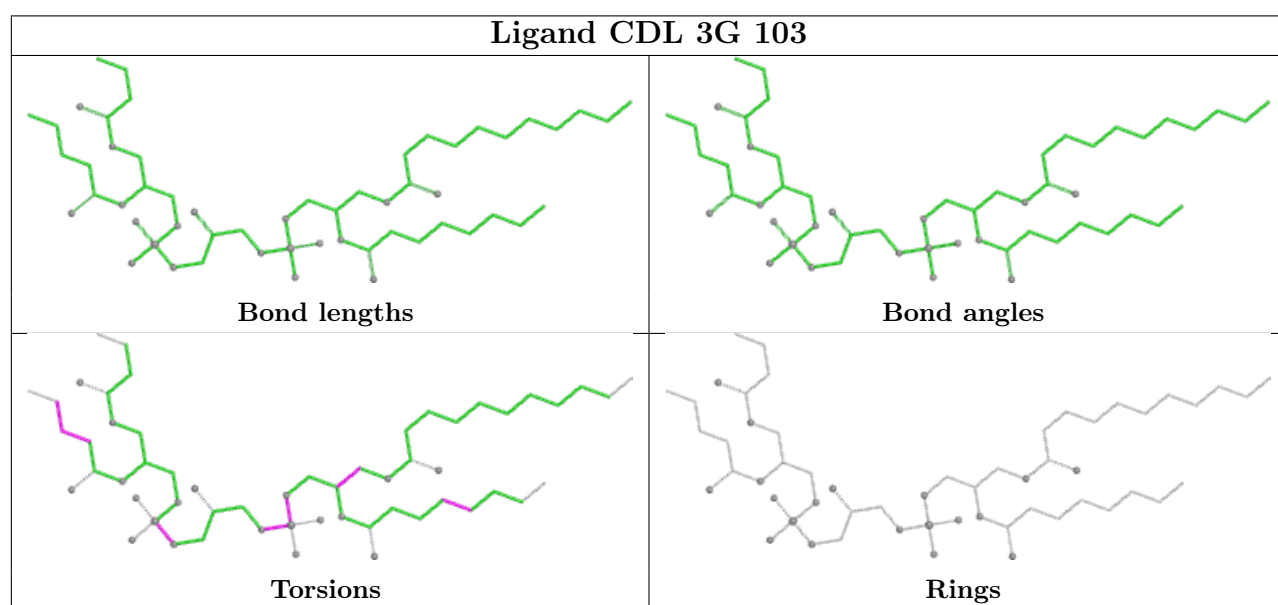
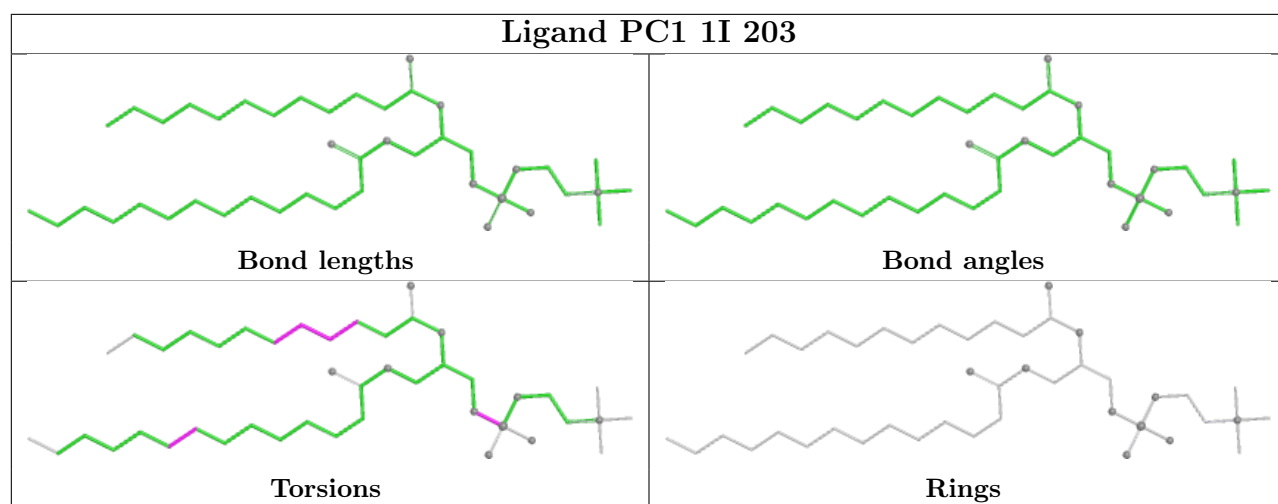
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 87  | 4M    | 101 | PGV  | 3       | 0            |
| 87  | 4G    | 101 | PGV  | 5       | 0            |
| 75  | 4D    | 201 | CDL  | 17      | 0            |
| 87  | 8C    | 303 | PGV  | 8       | 0            |
| 70  | 3R    | 303 | PC1  | 4       | 0            |
| 75  | 3N    | 502 | CDL  | 7       | 0            |
| 87  | 8C    | 302 | PGV  | 5       | 0            |
| 72  | 3R    | 301 | FES  | 2       | 0            |
| 87  | 4C    | 306 | PGV  | 8       | 0            |
| 88  | 4A    | 605 | HEA  | 4       | 0            |
| 70  | 1q    | 201 | PC1  | 4       | 0            |
| 85  | 3P    | 502 | HEM  | 3       | 0            |
| 70  | 1B    | 202 | PC1  | 7       | 0            |
| 88  | 8A    | 605 | HEA  | 4       | 0            |
| 69  | 1N    | 901 | 3PE  | 5       | 0            |
| 87  | 8A    | 603 | PGV  | 5       | 0            |
| 69  | 1K    | 101 | 3PE  | 2       | 0            |
| 75  | 3A    | 501 | CDL  | 3       | 0            |
| 87  | 4B    | 301 | PGV  | 4       | 0            |
| 87  | 8G    | 101 | PGV  | 8       | 0            |
| 88  | 4A    | 604 | HEA  | 6       | 0            |
| 87  | 8A    | 602 | PGV  | 8       | 0            |
| 91  | 8B    | 304 | CUA  | 2       | 0            |
| 69  | 1A    | 201 | 3PE  | 3       | 0            |
| 69  | 1Y    | 202 | 3PE  | 7       | 0            |
| 69  | 1Y    | 205 | 3PE  | 3       | 0            |
| 85  | 3C    | 502 | HEM  | 2       | 0            |
| 78  | 1P    | 402 | NDP  | 2       | 0            |

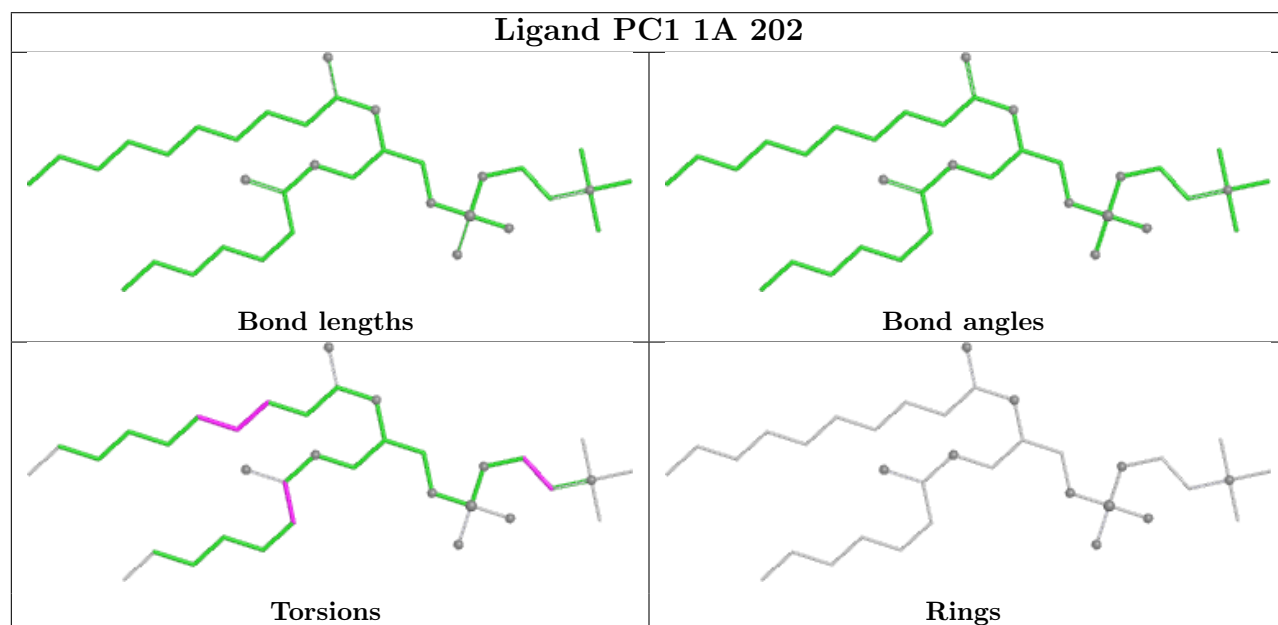
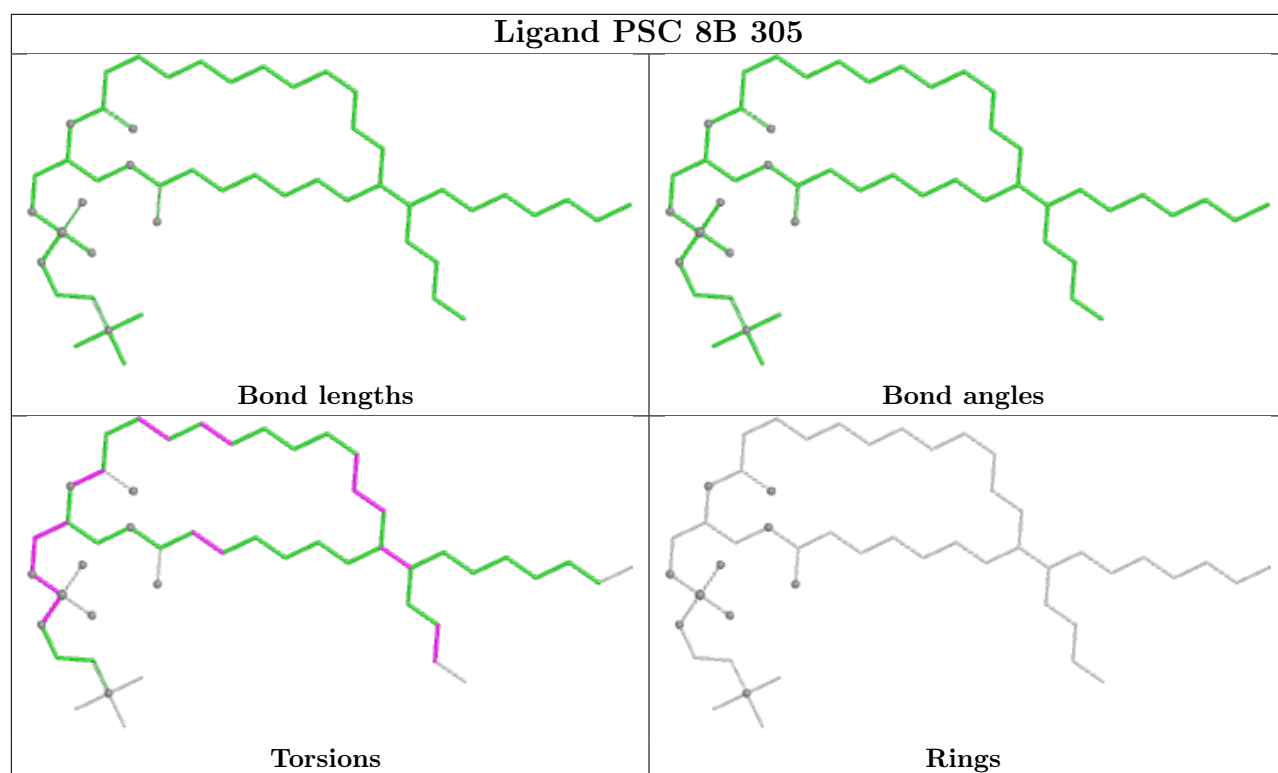
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

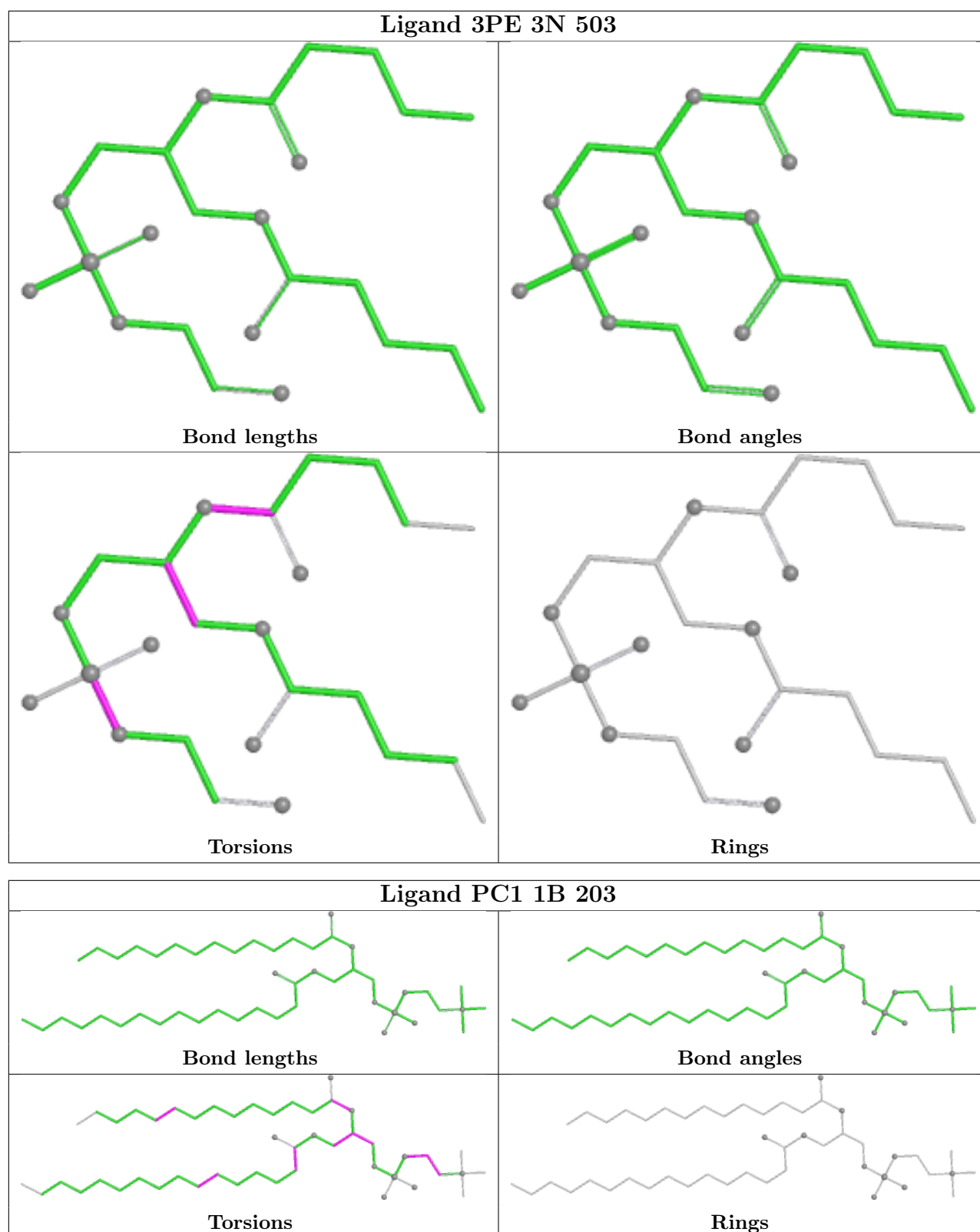


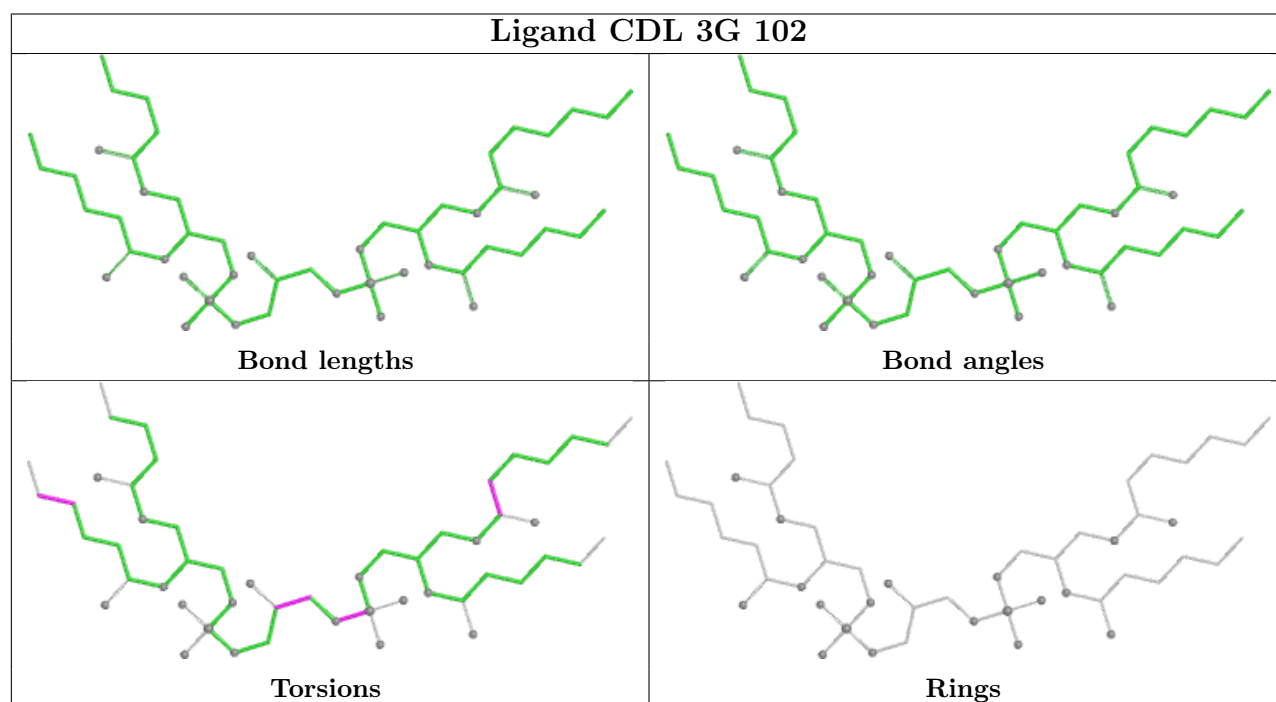
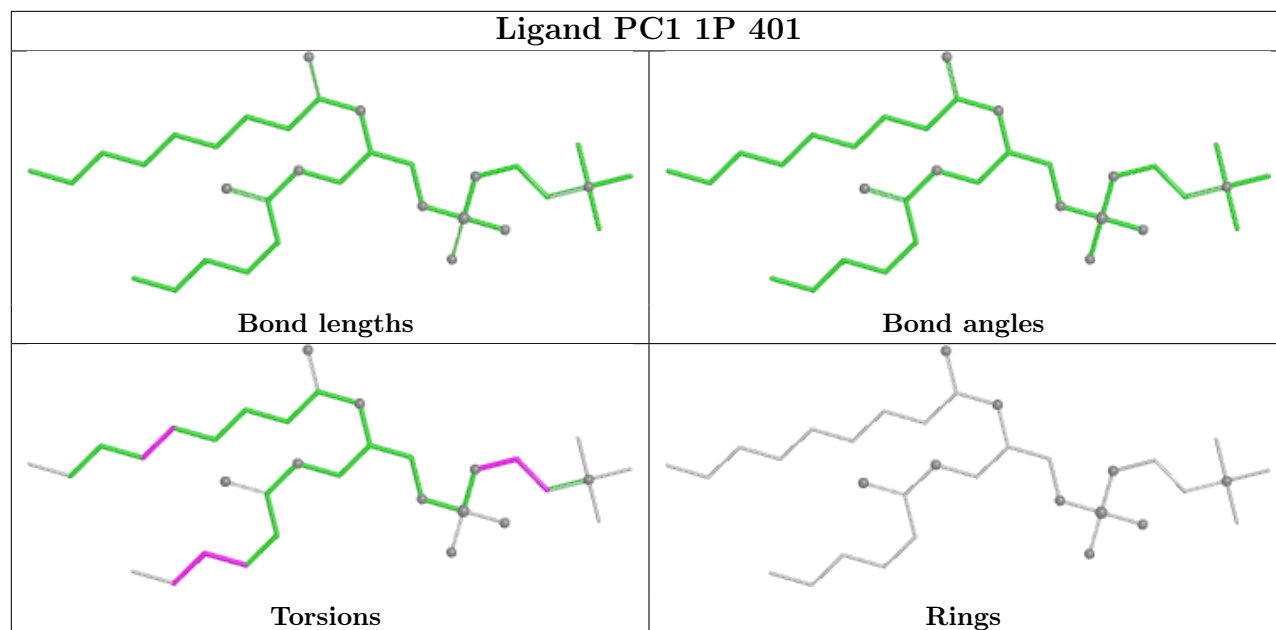


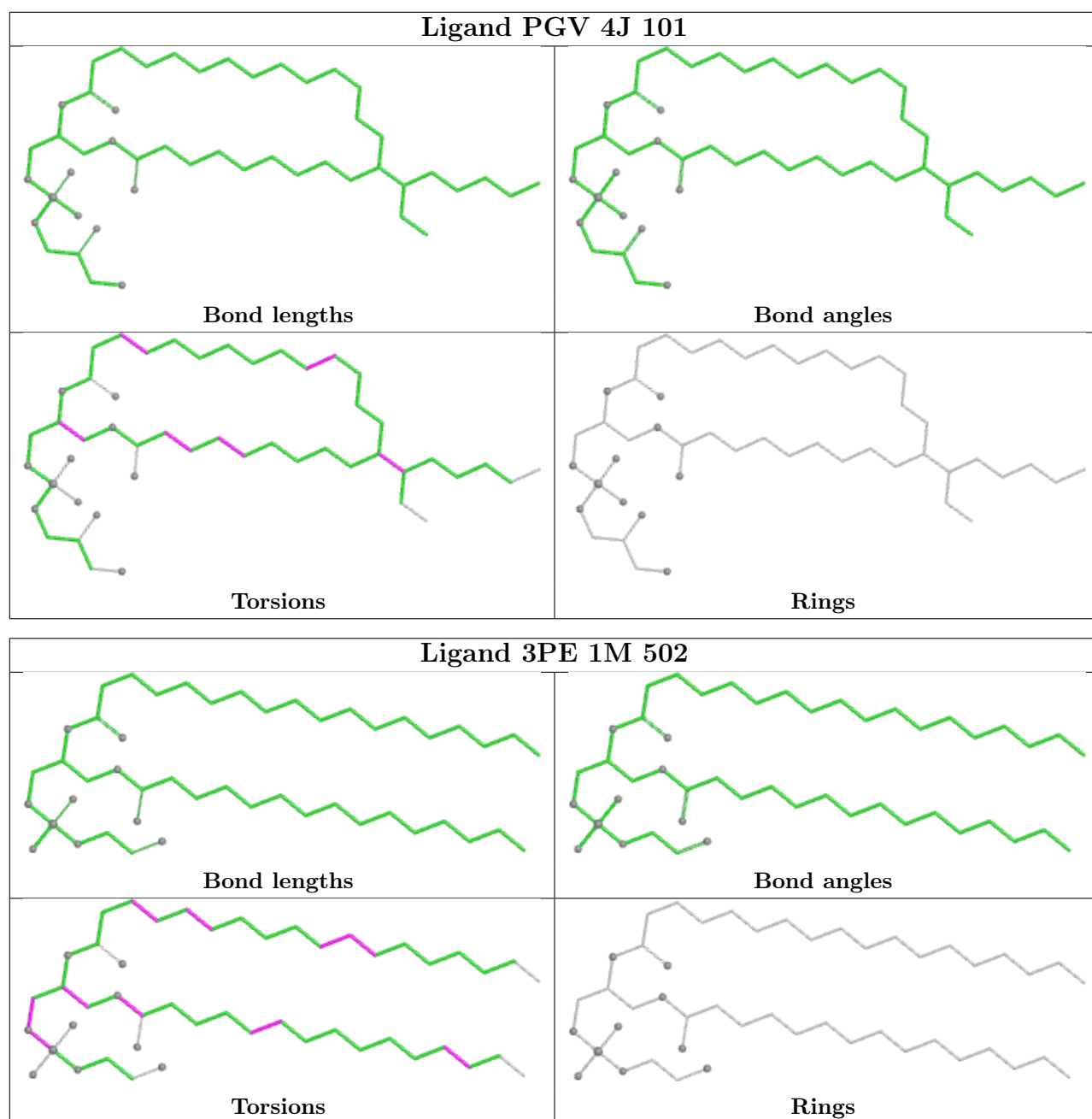


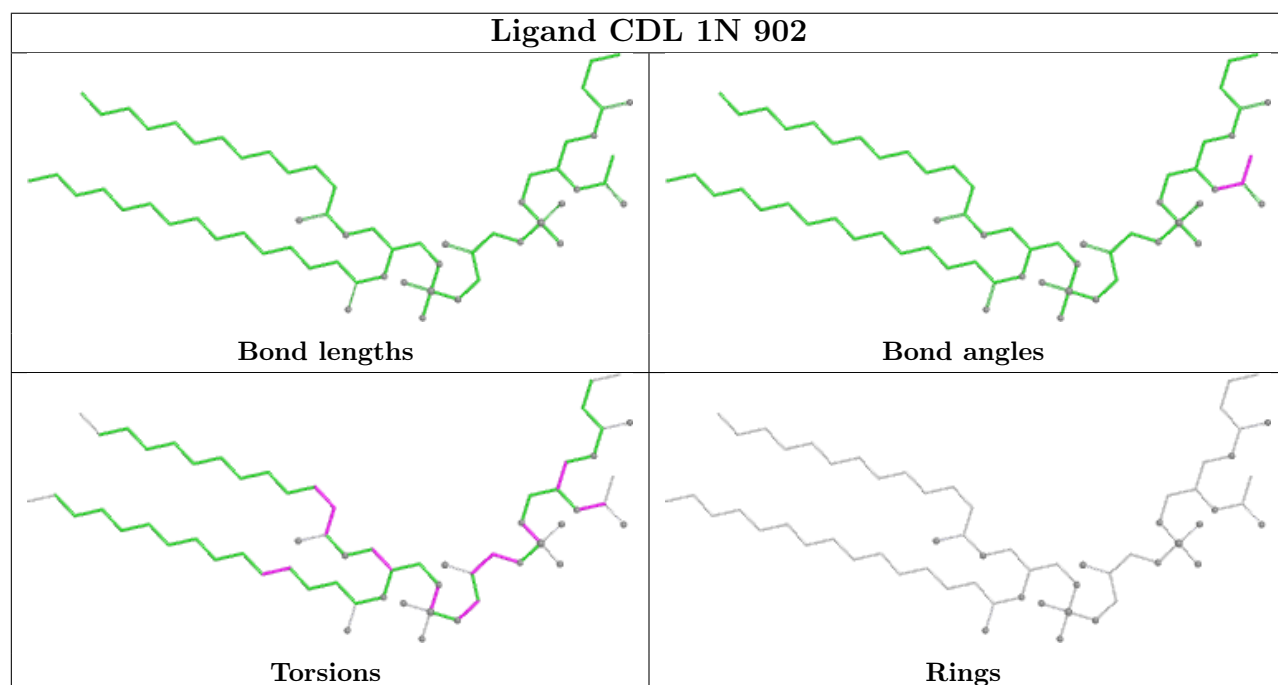
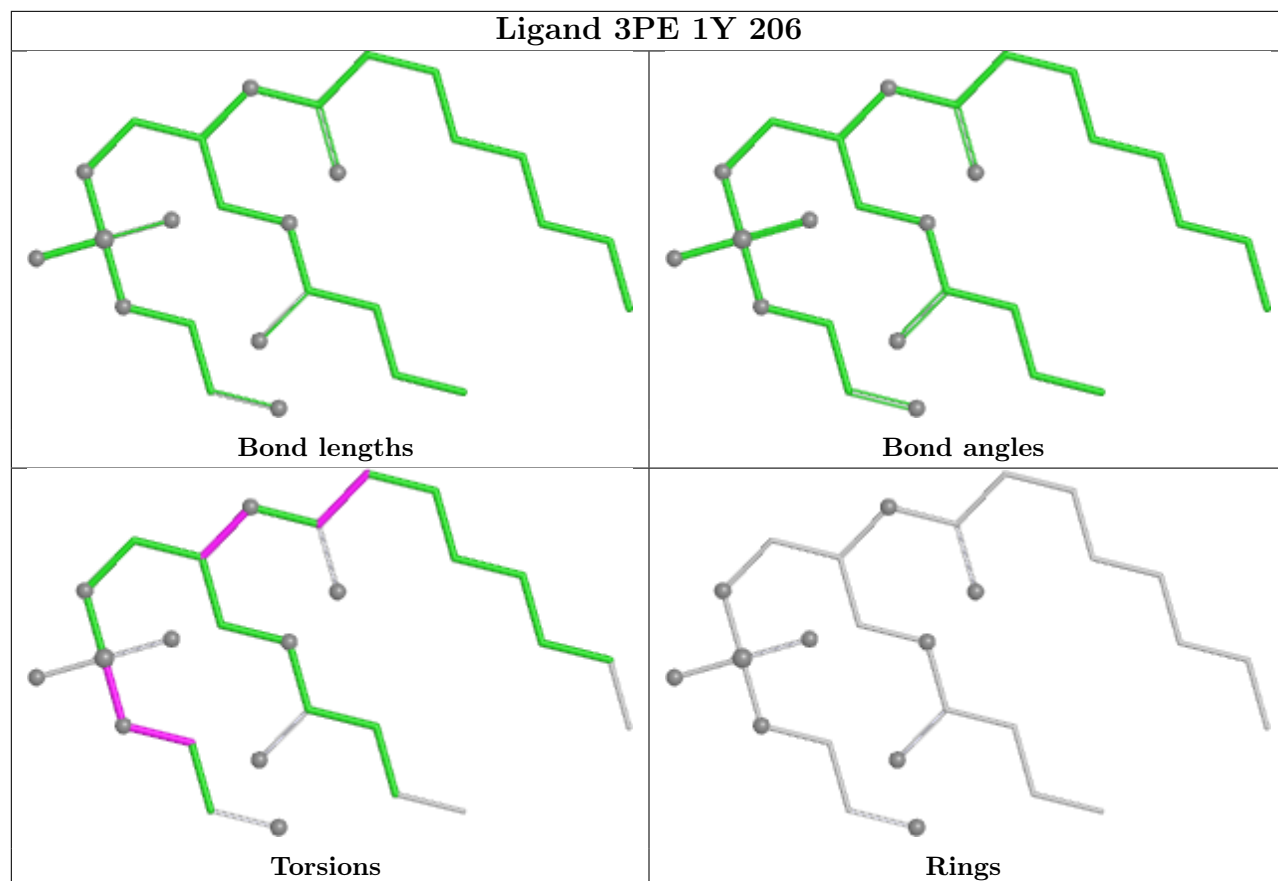


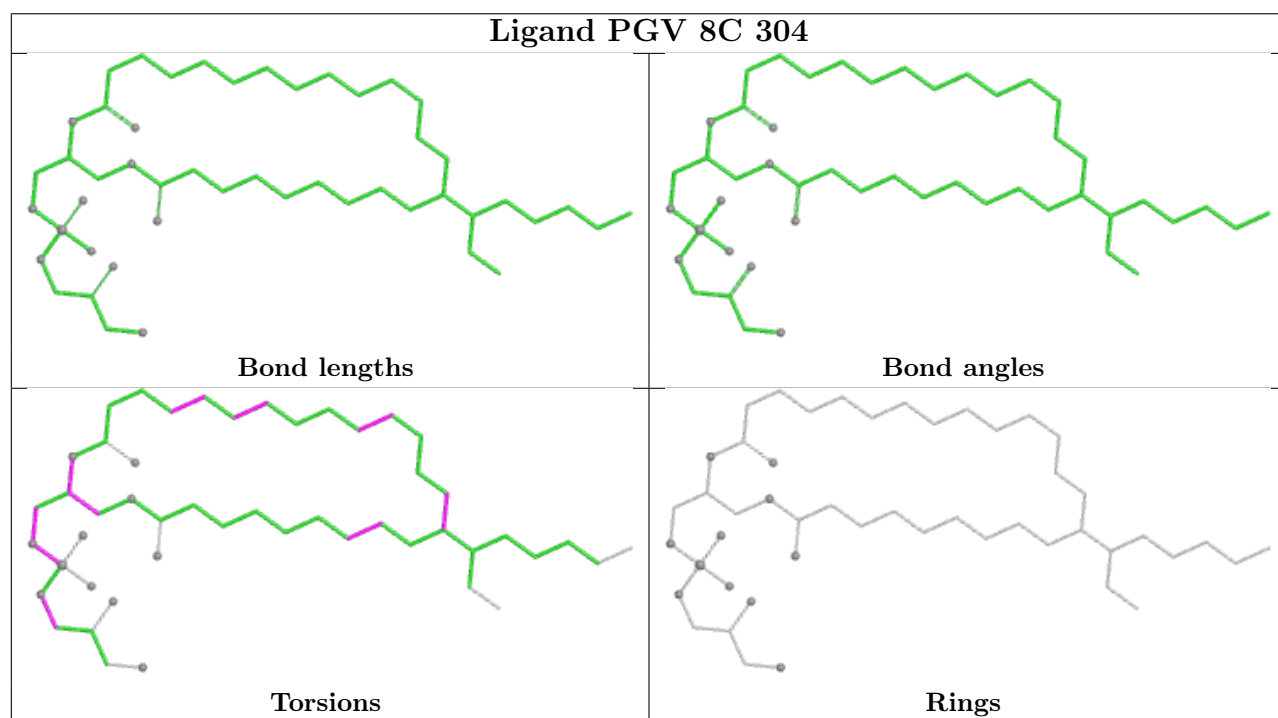
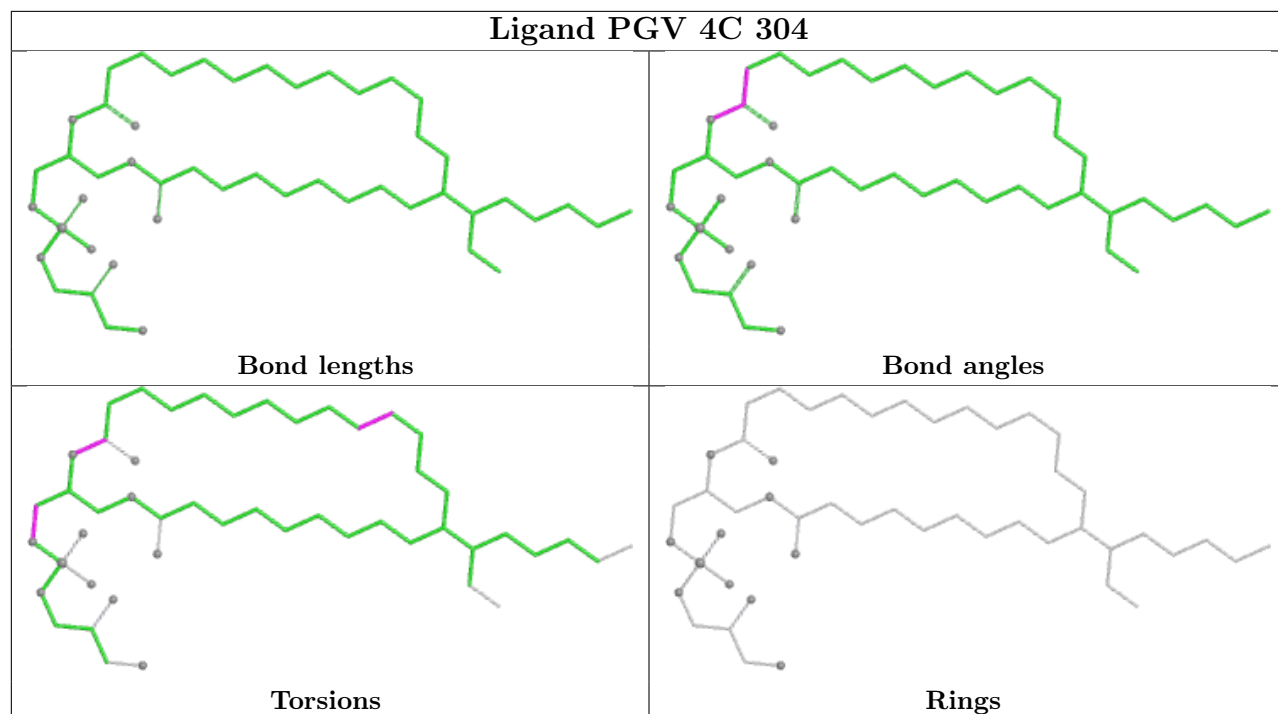


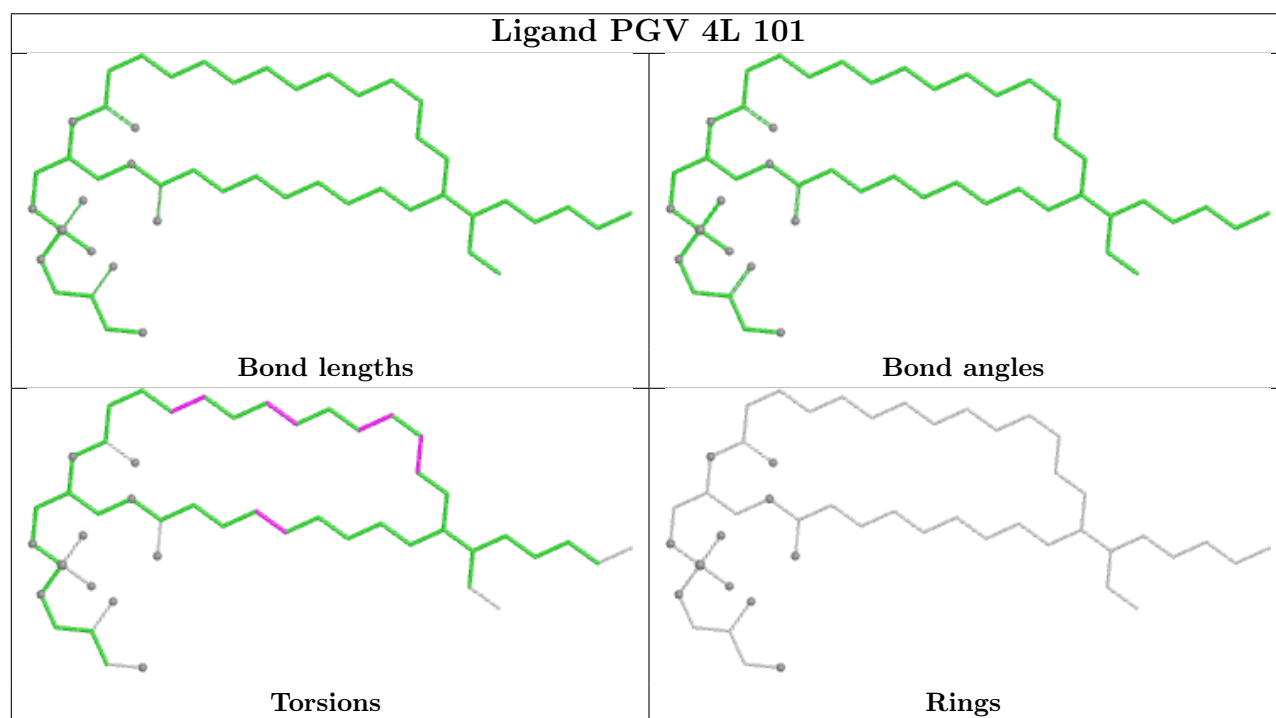
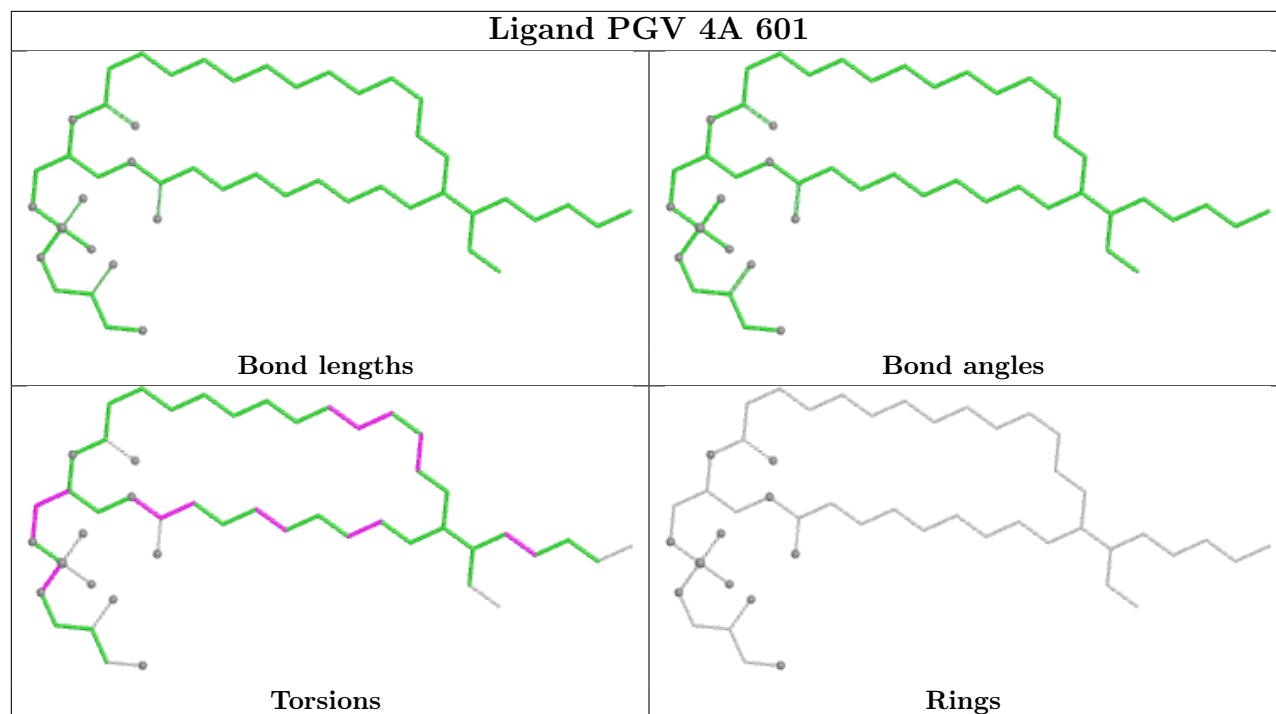


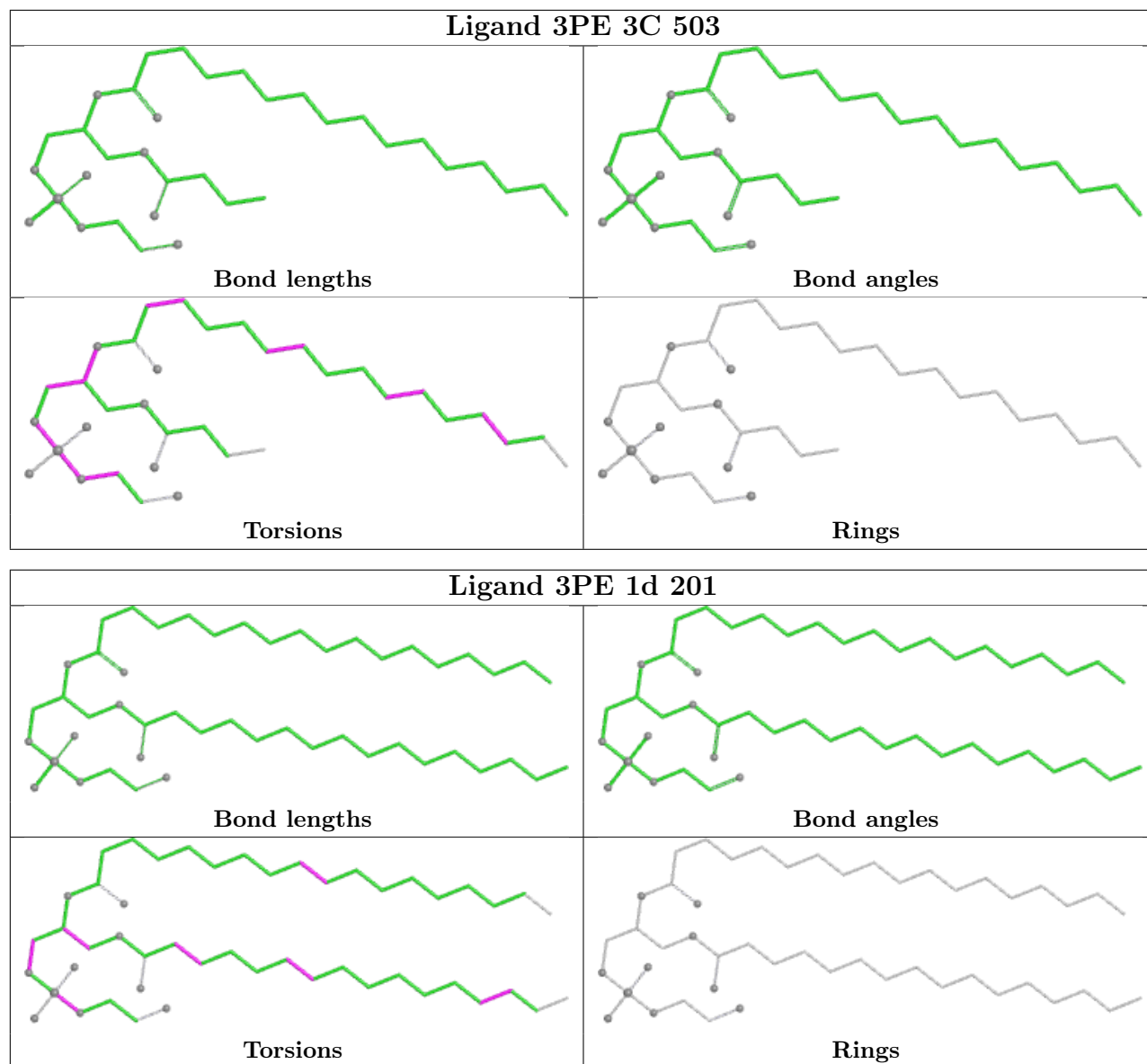


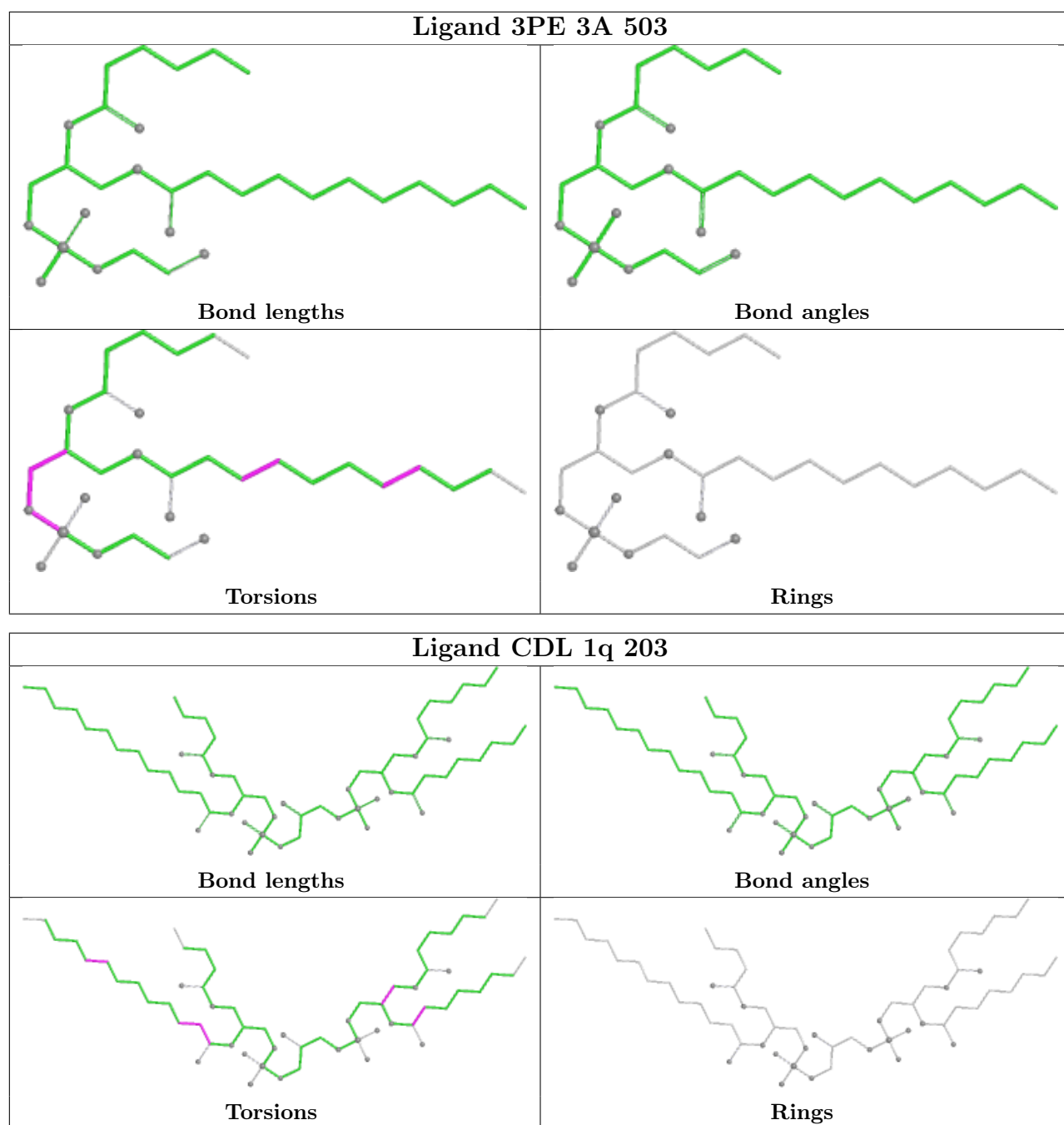


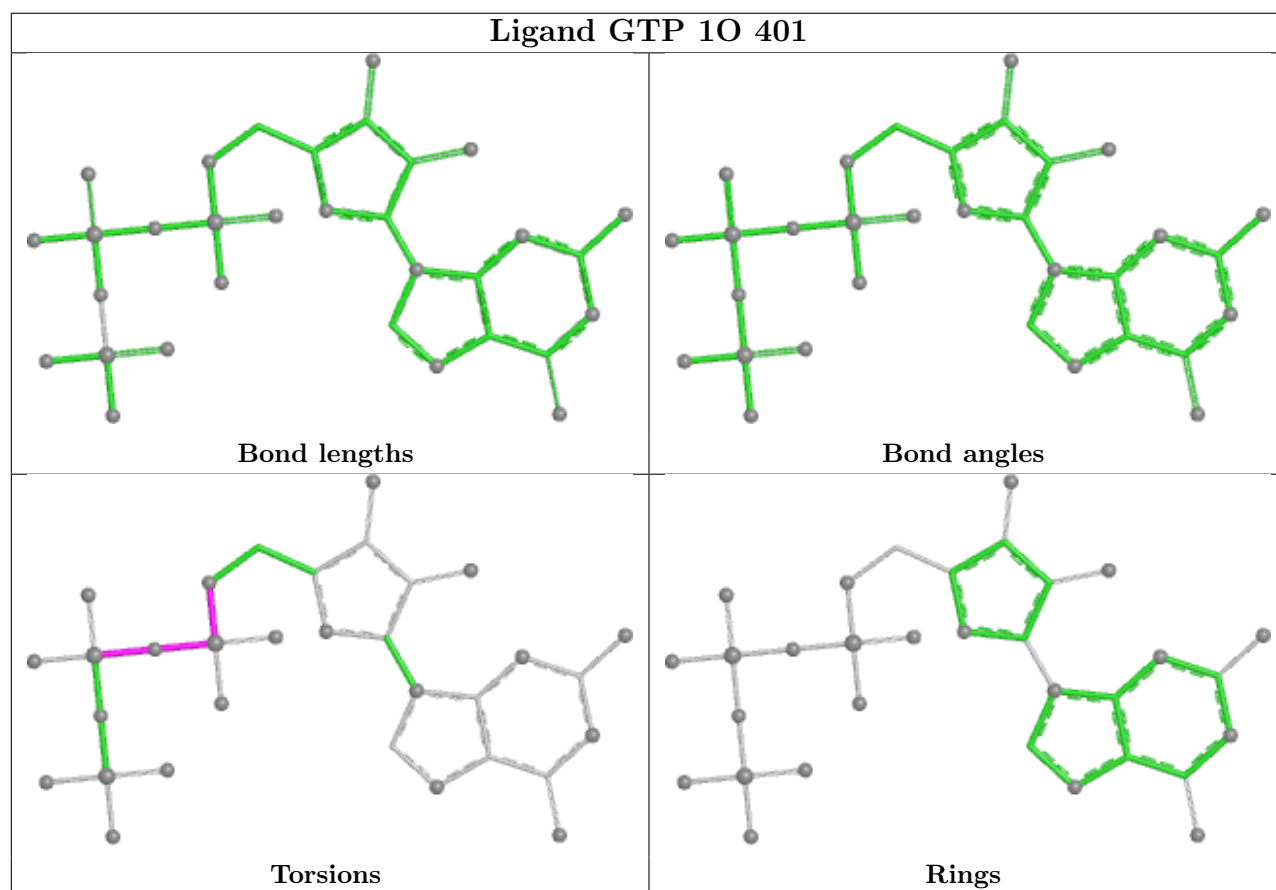
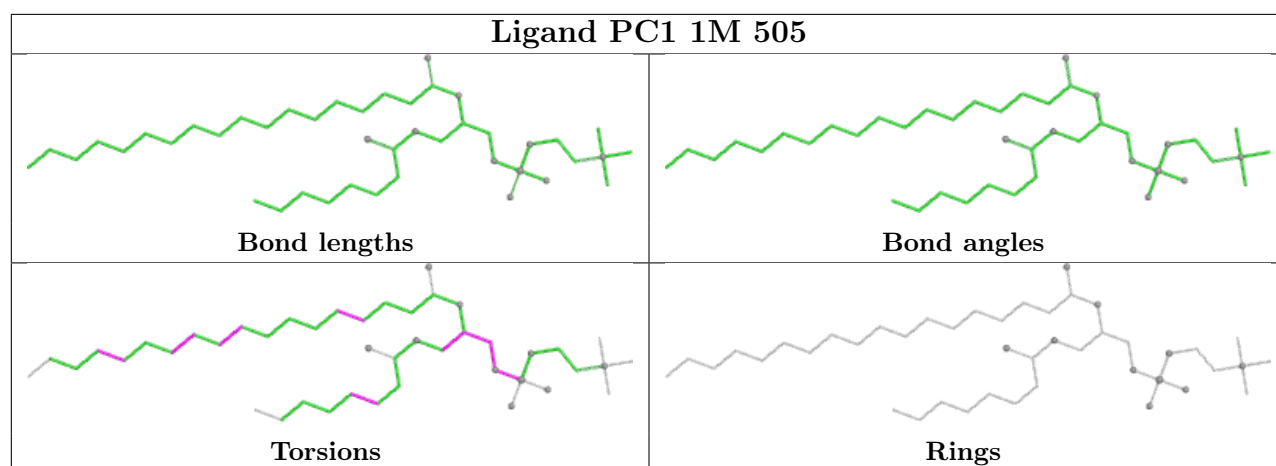


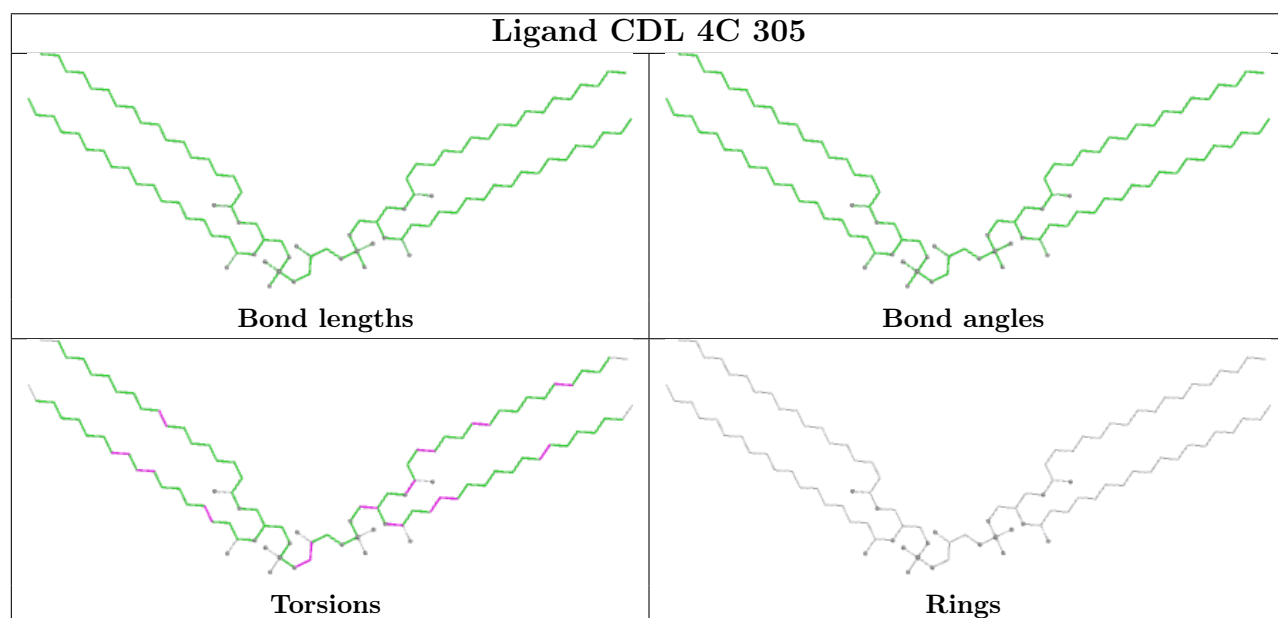
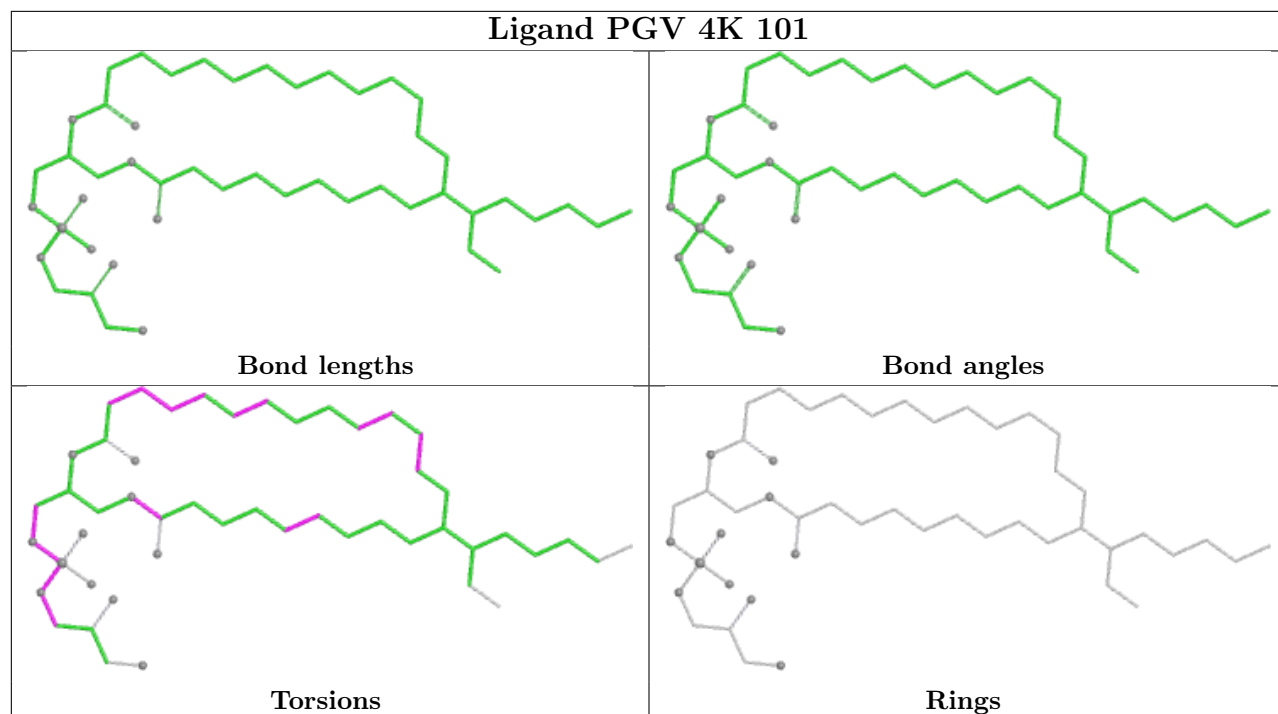


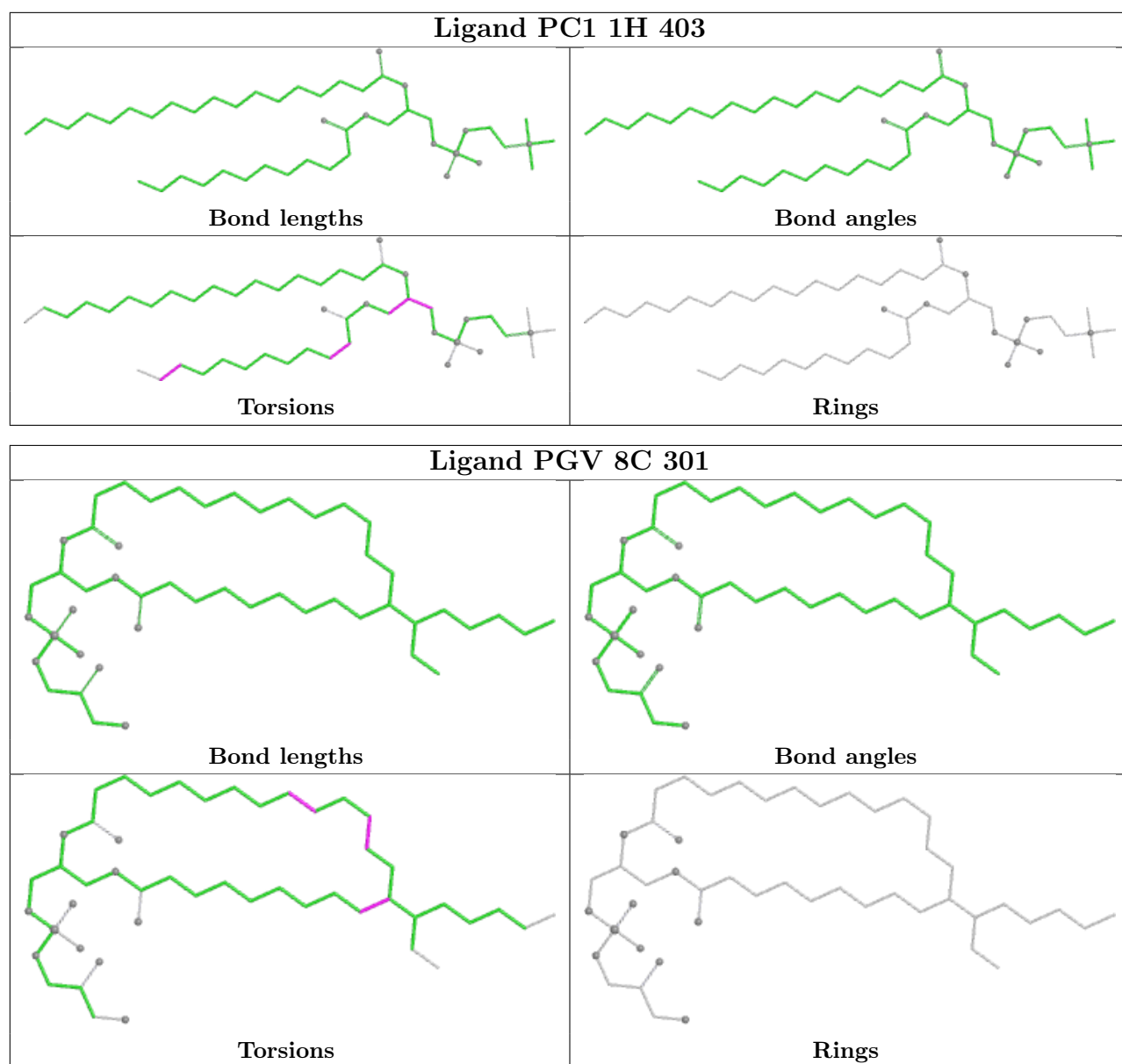




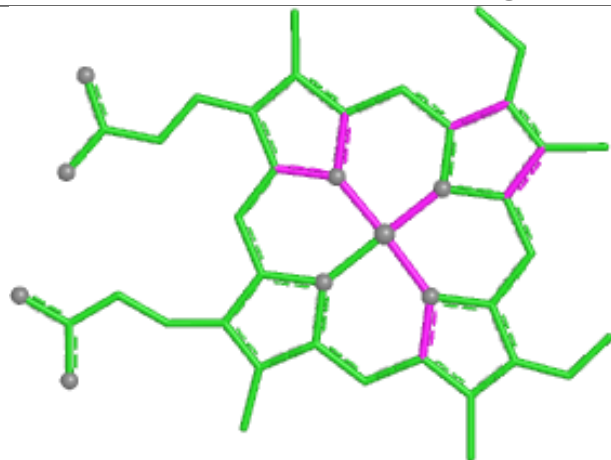




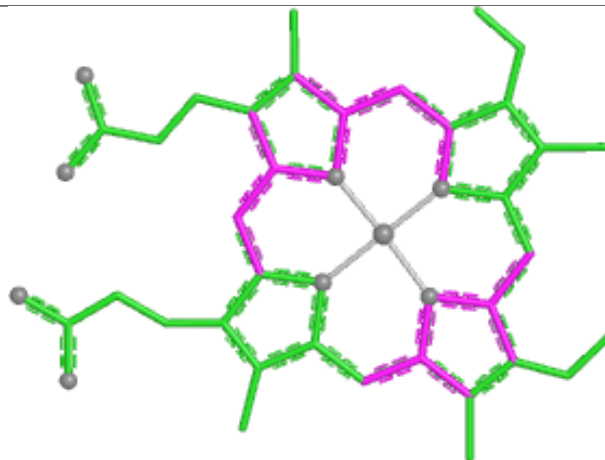




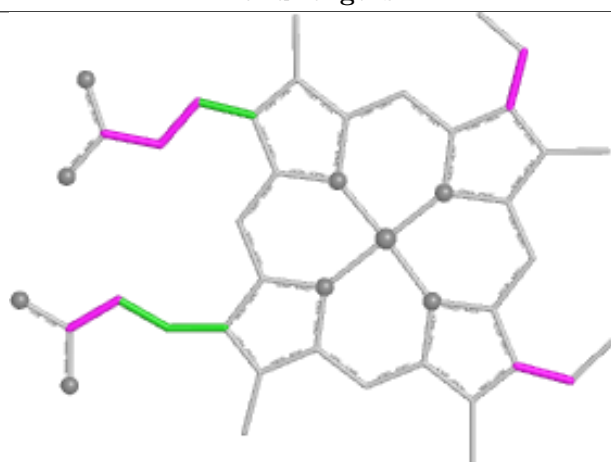
## Ligand HEM 3P 501



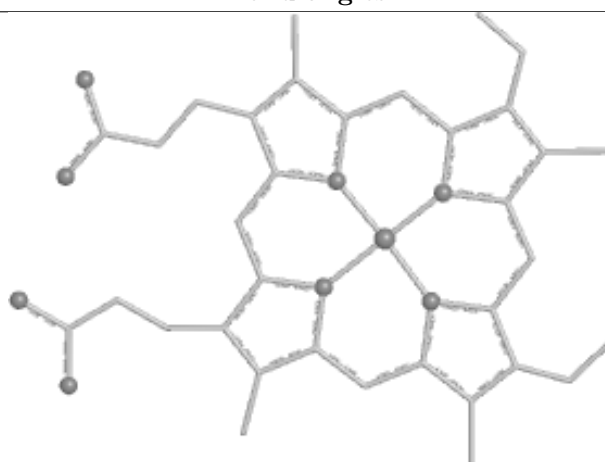
Bond lengths



Bond angles

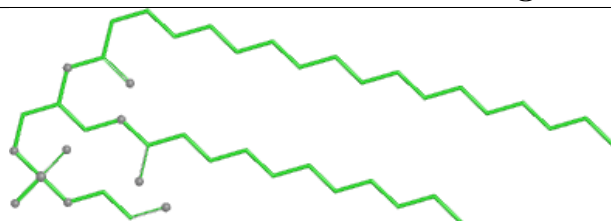


Torsions

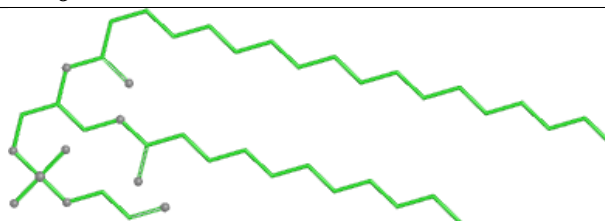


Rings

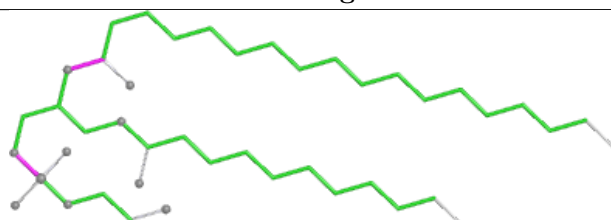
## Ligand 3PE 1j 101



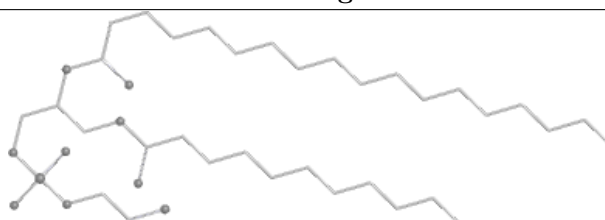
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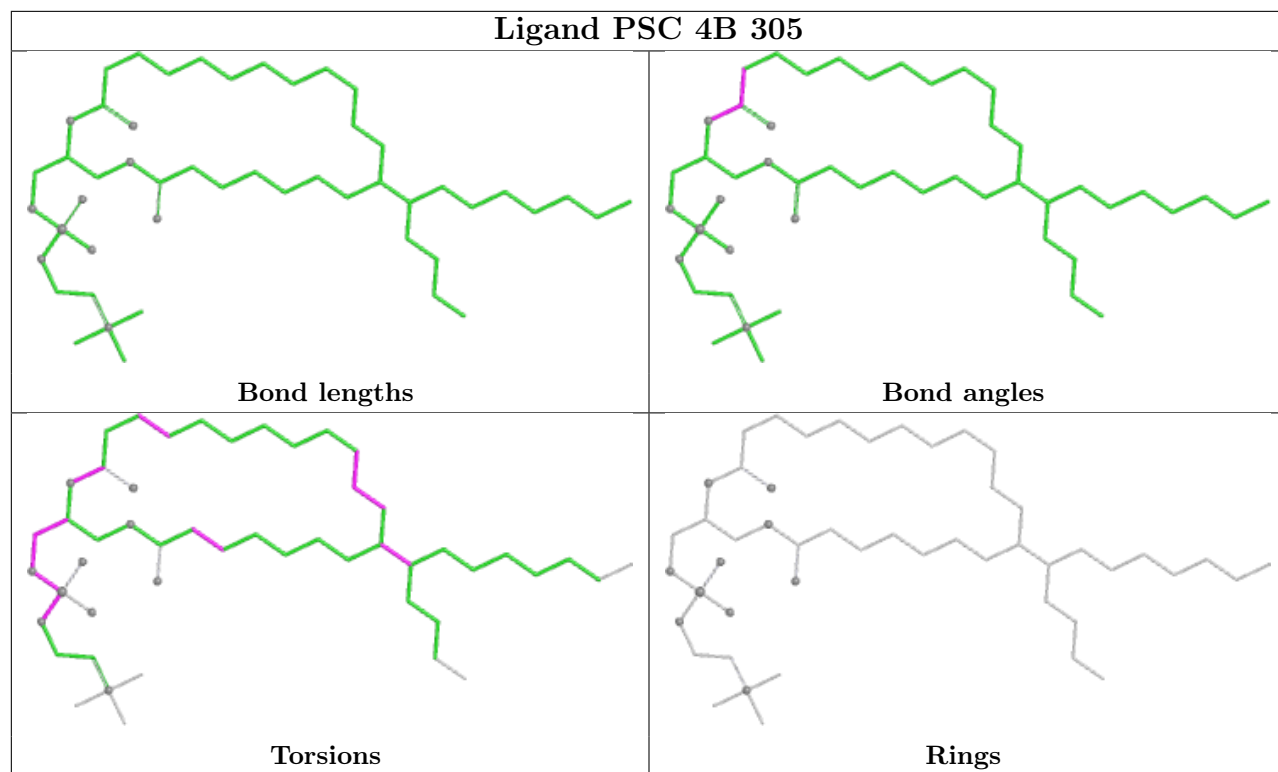
Bond angles



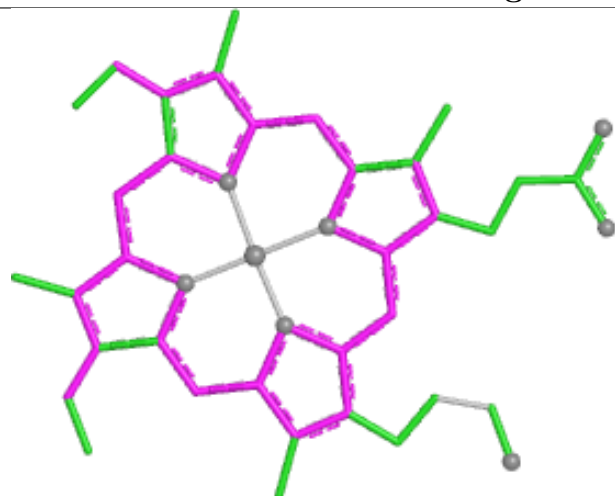
Torsions



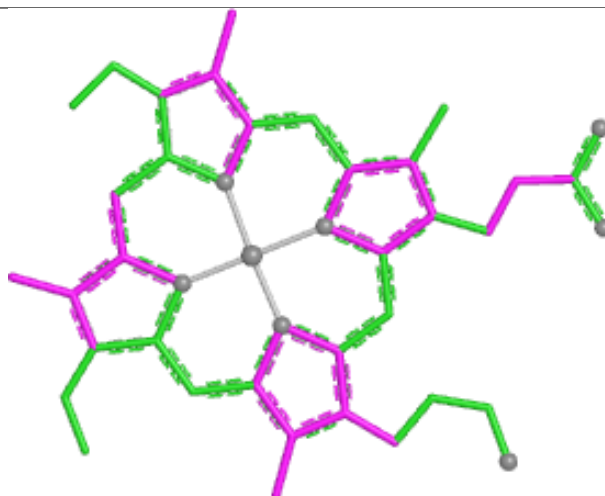
Rings



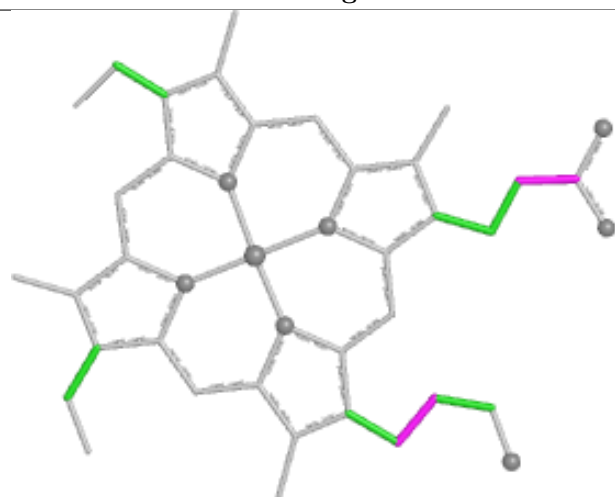
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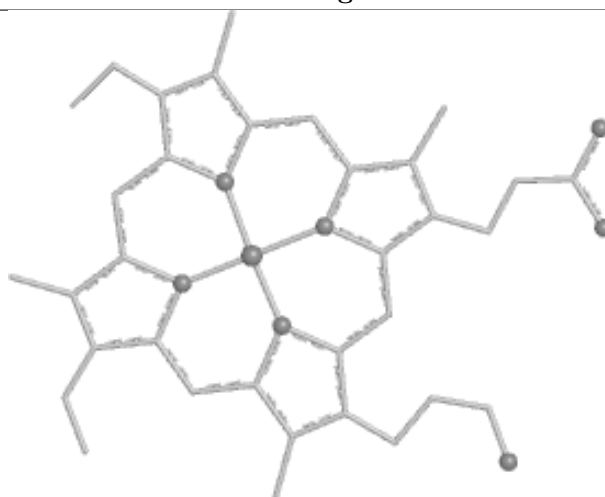
Bond lengths



Bond angles

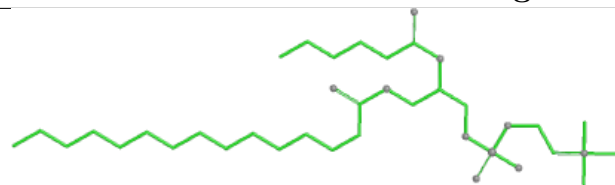


Torsions

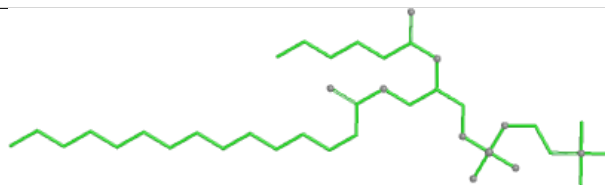


Rings

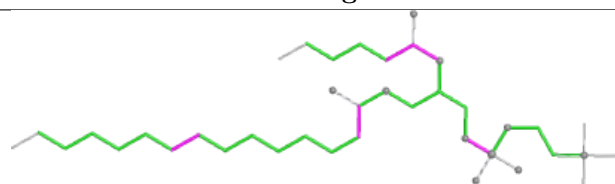
## Ligand PC1 1d 202



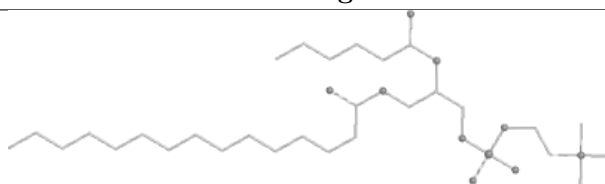
Bond lengths



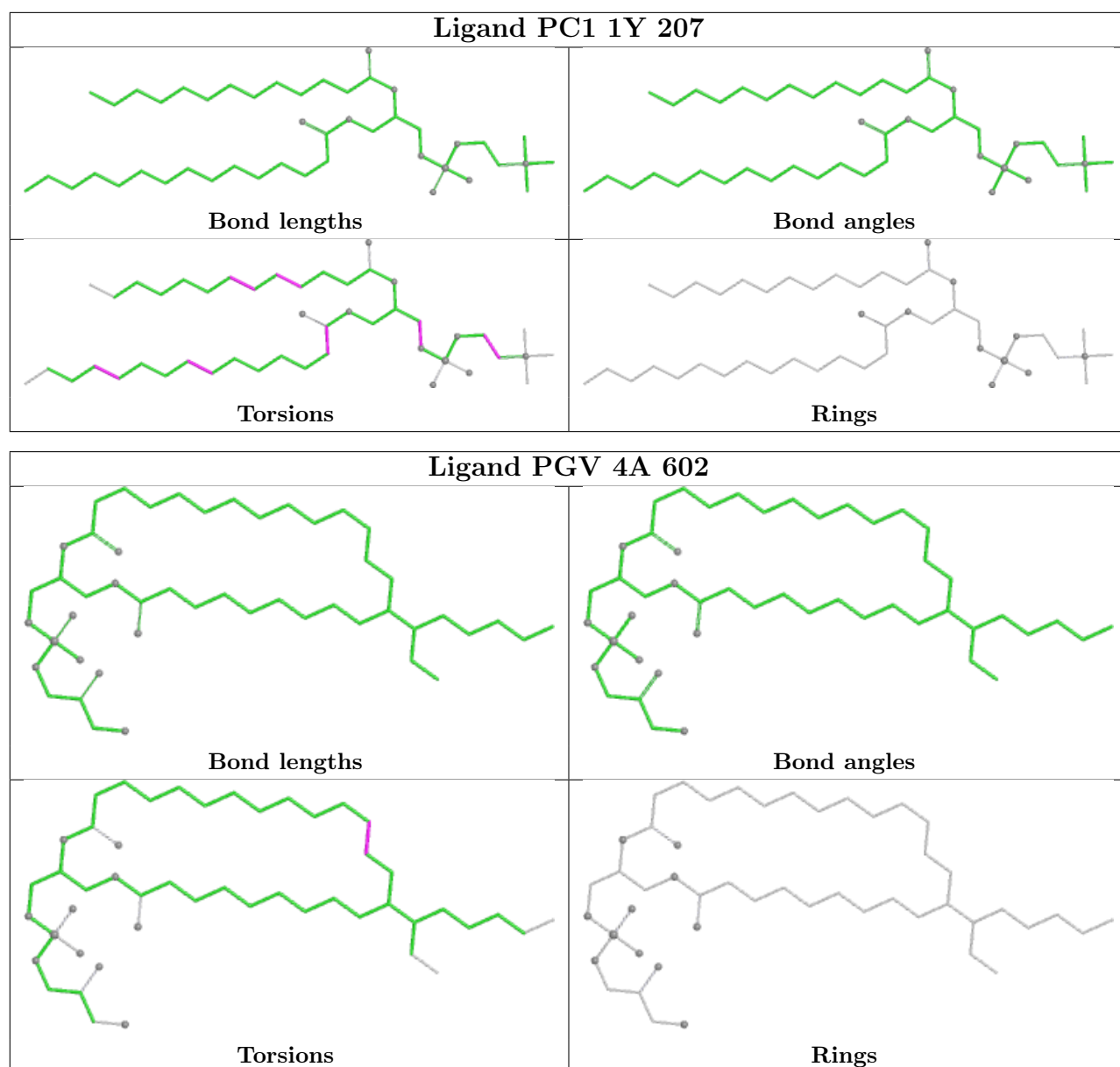
Bond angles

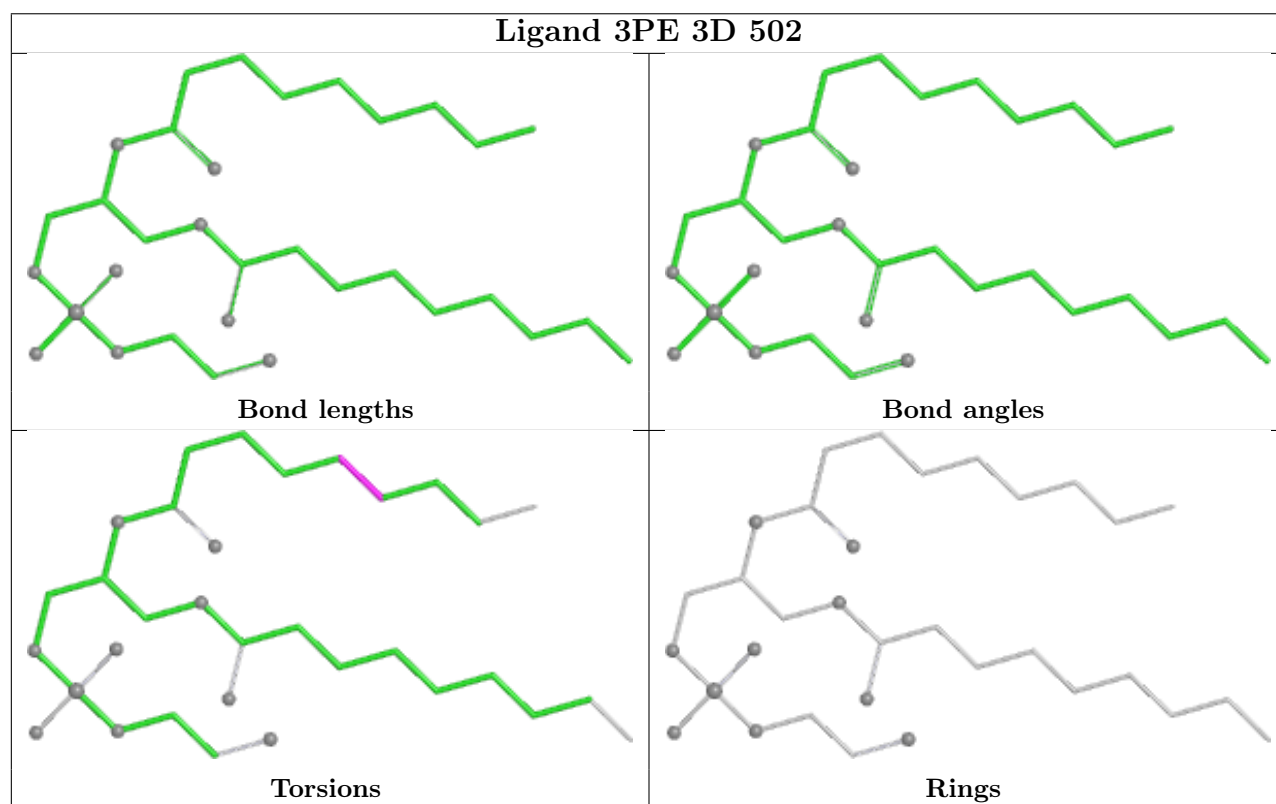
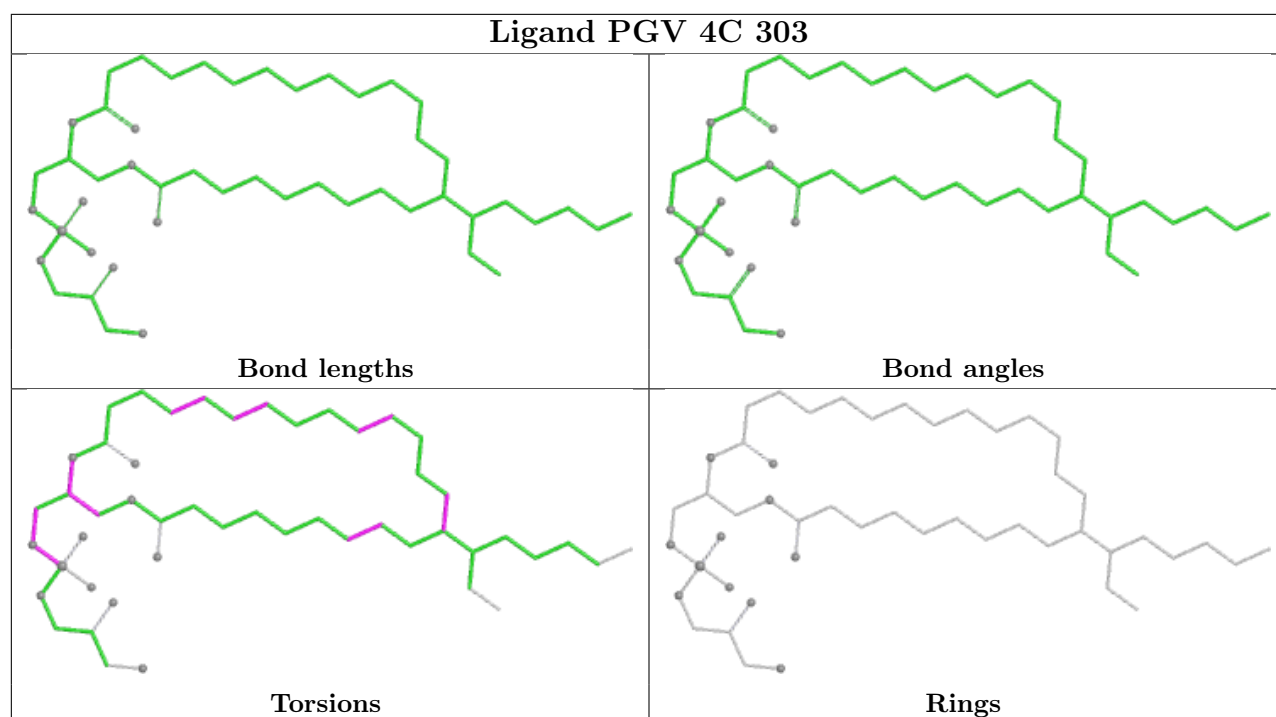


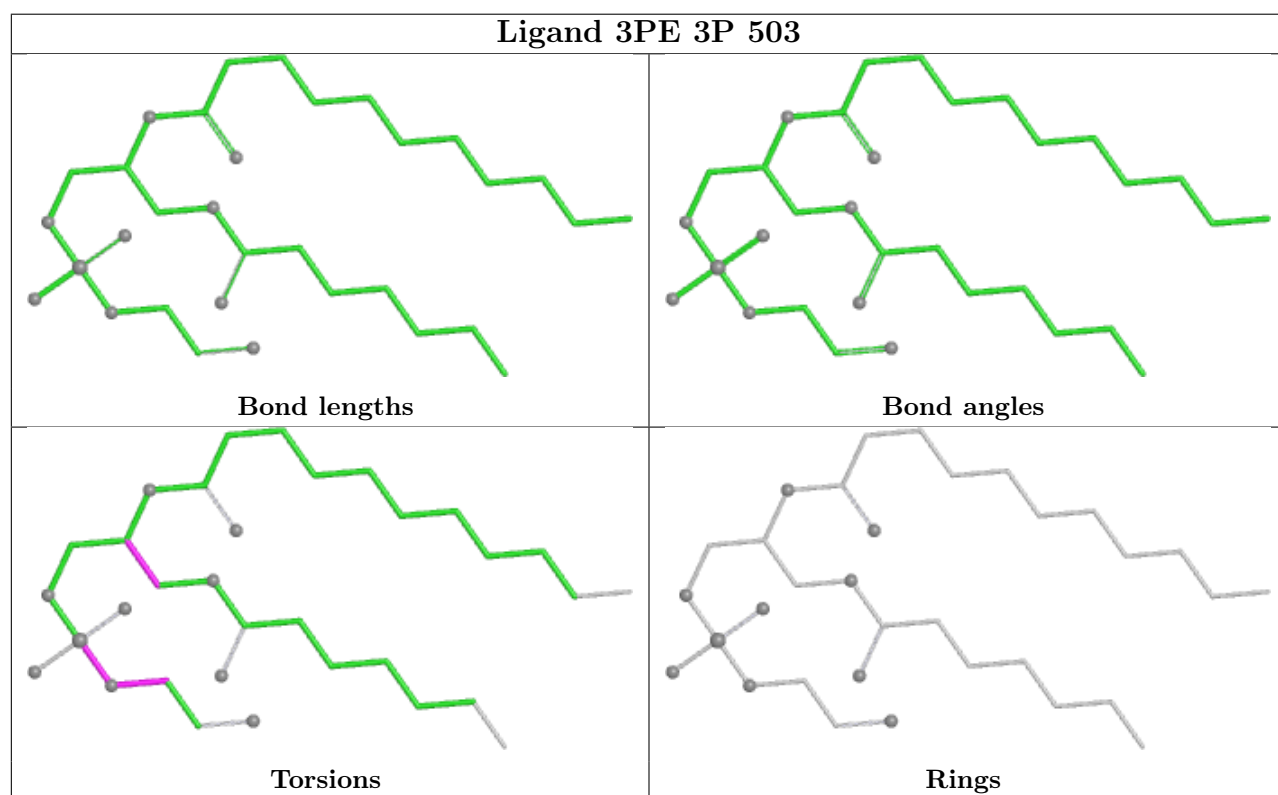
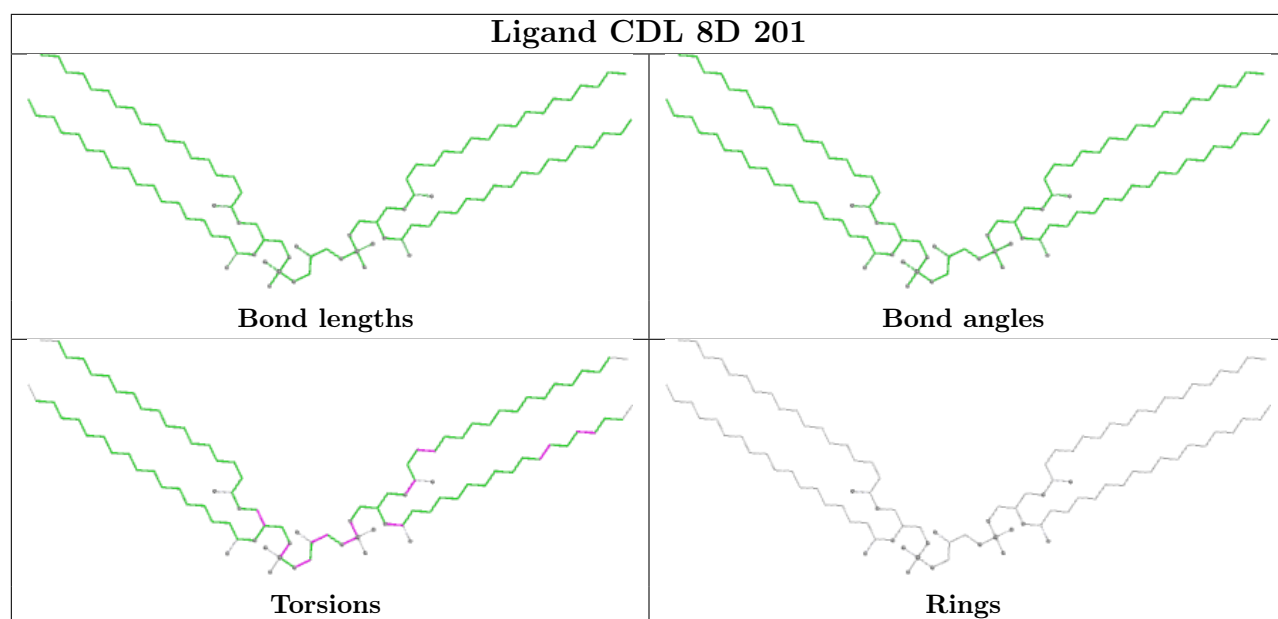
Torsions

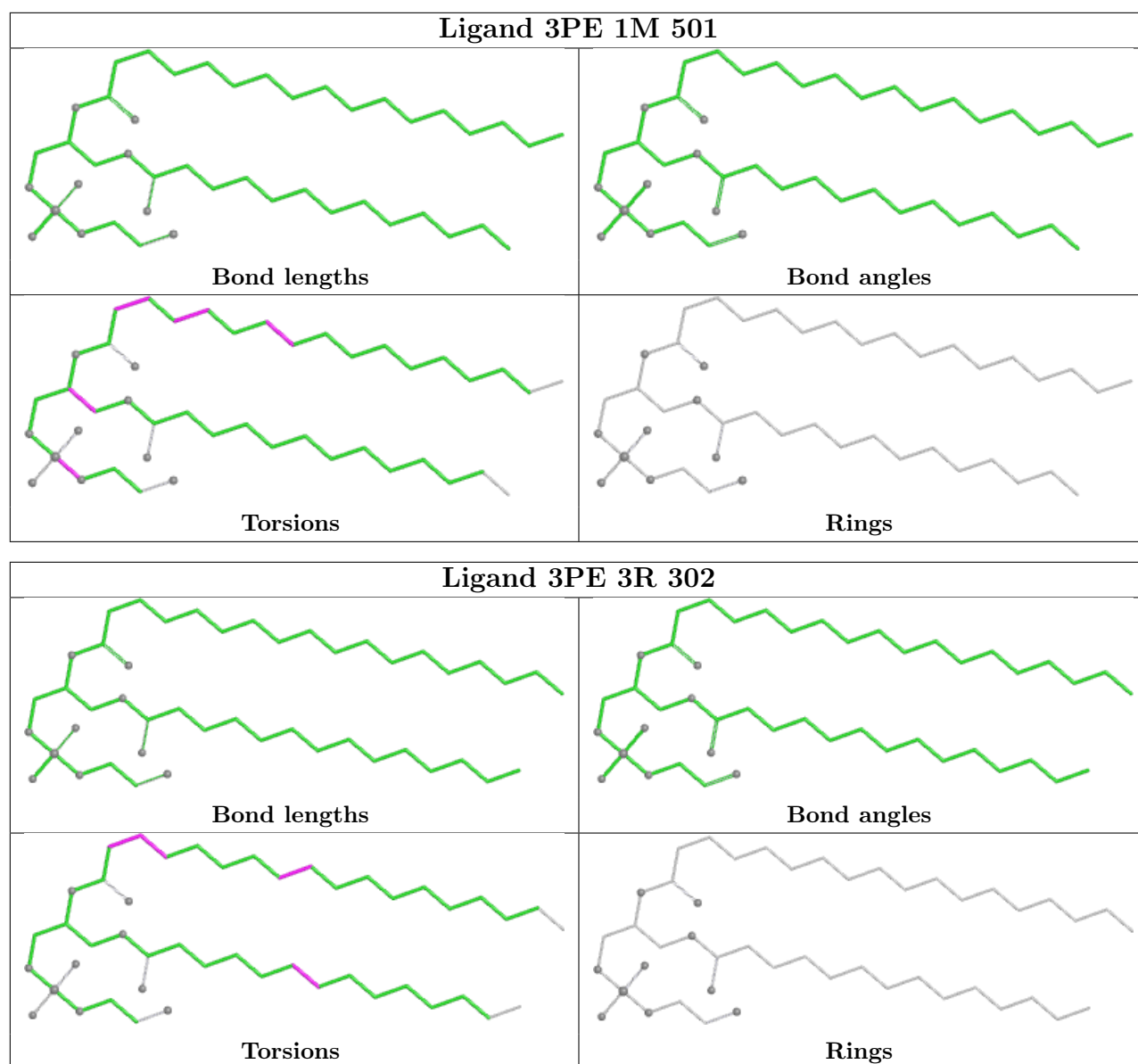


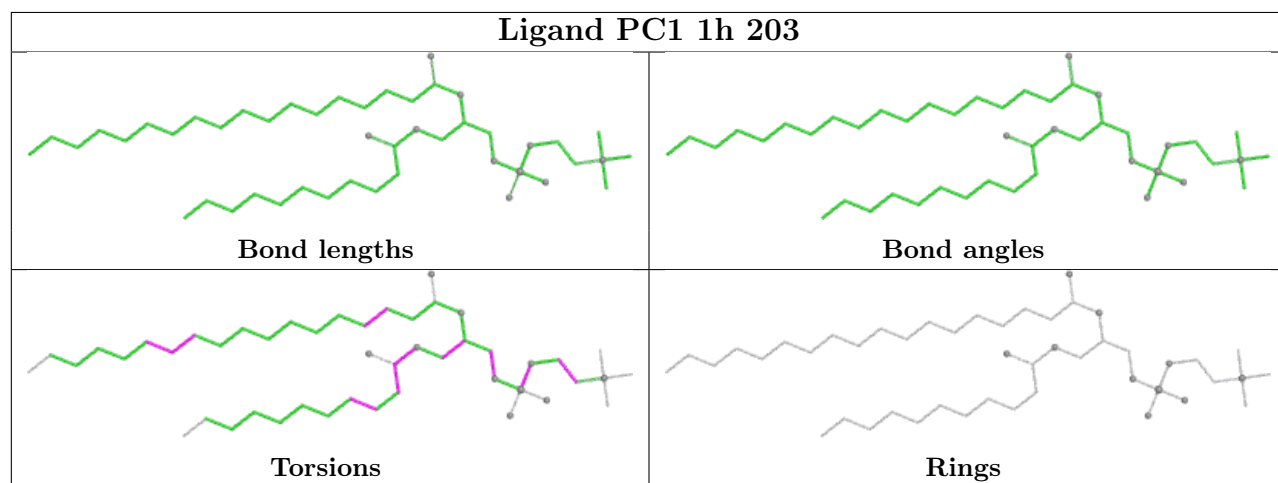
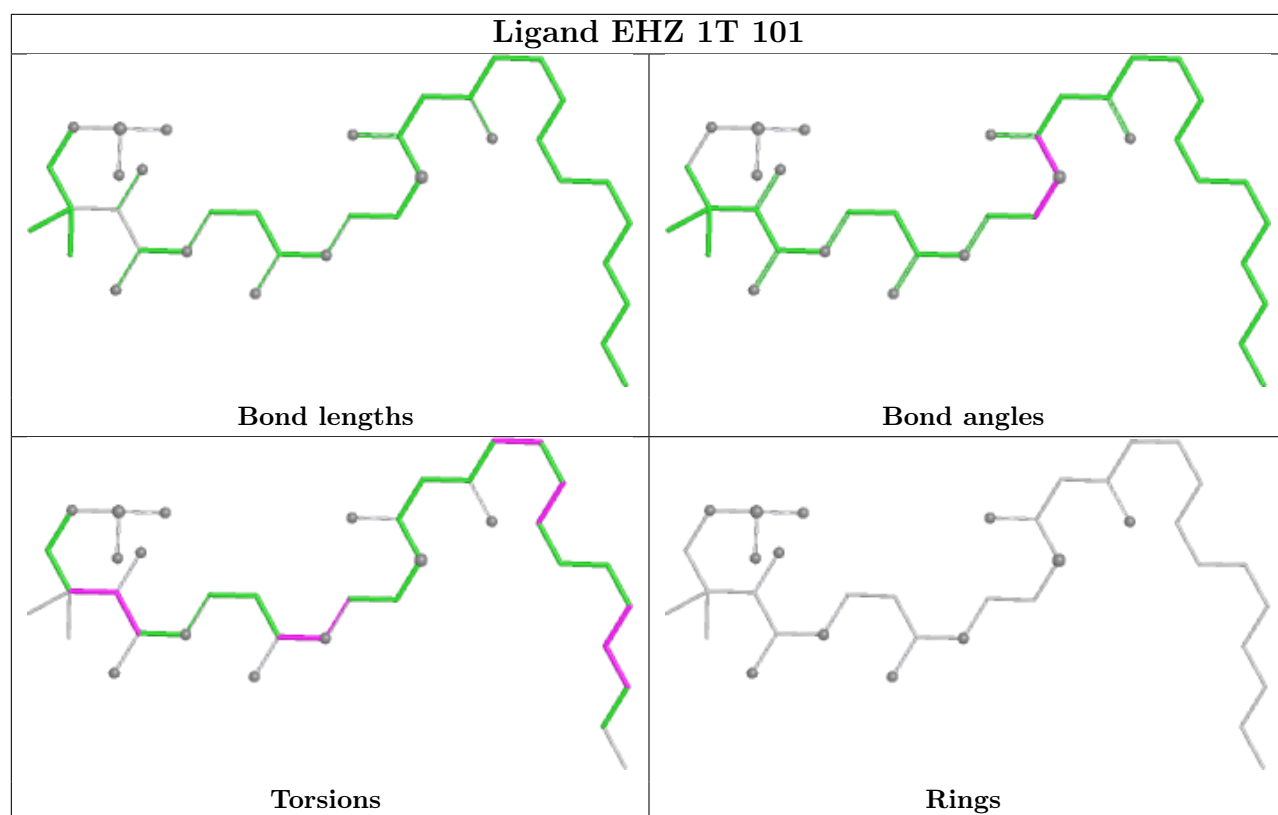
Rings

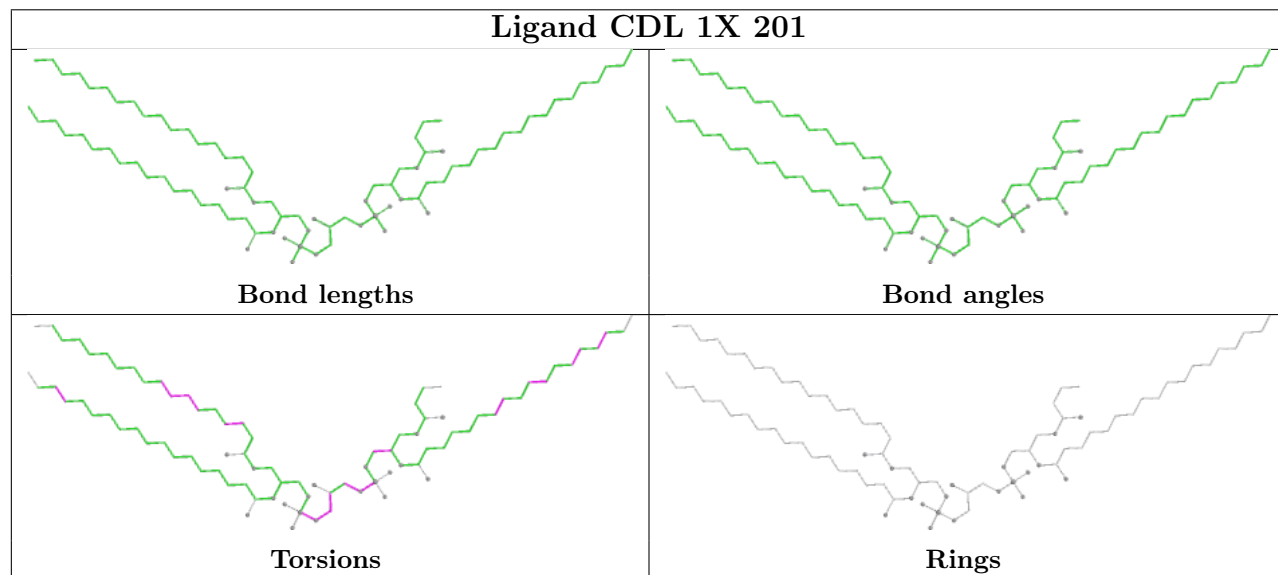
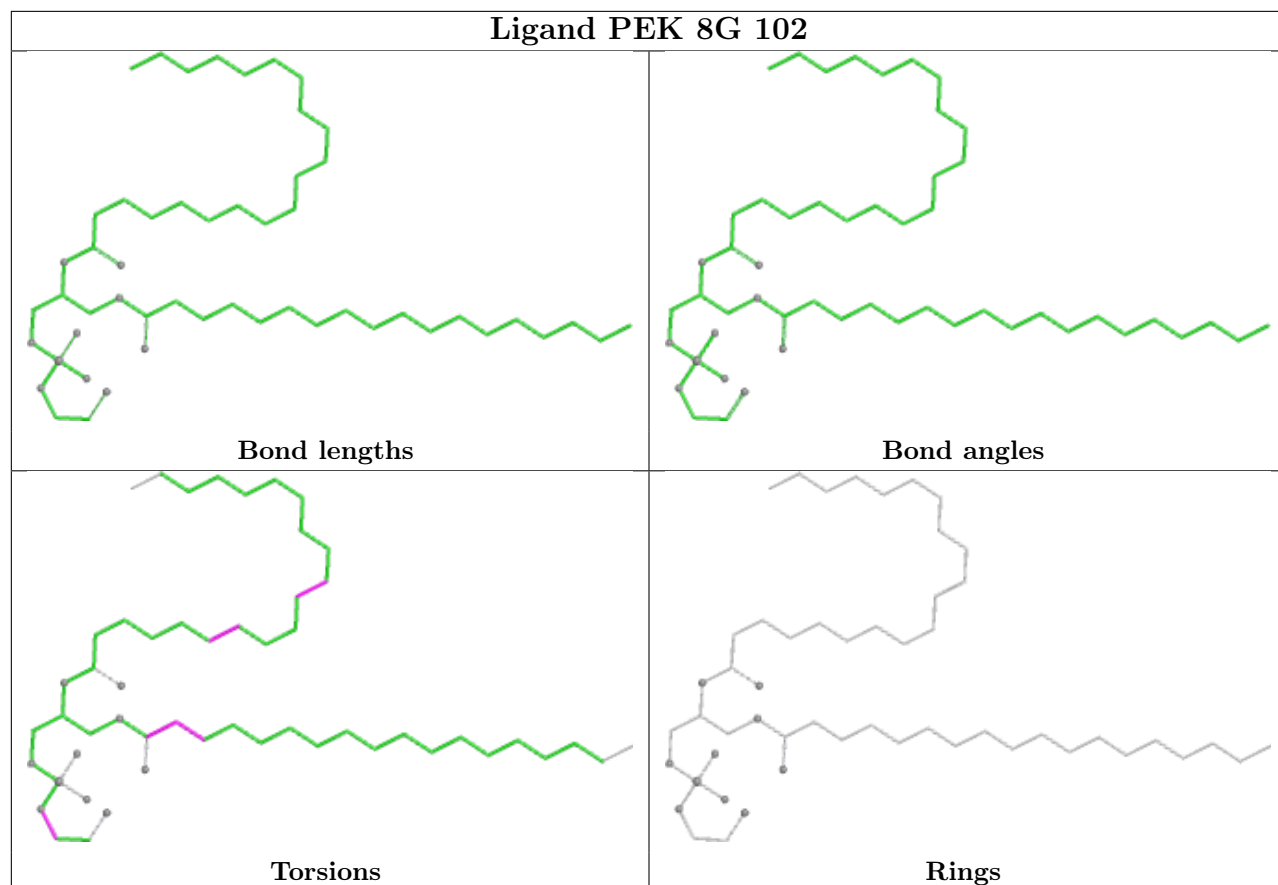




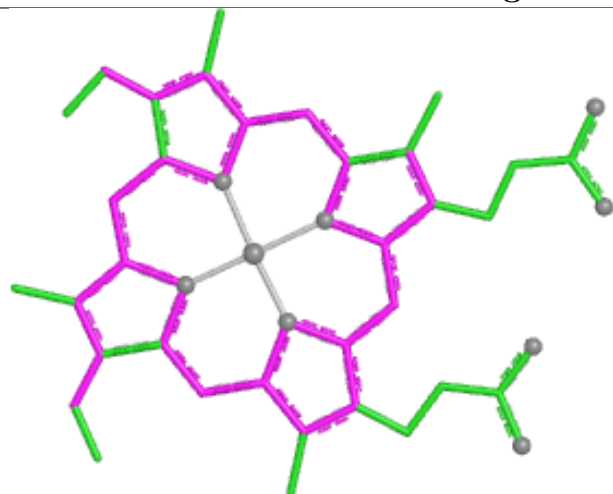




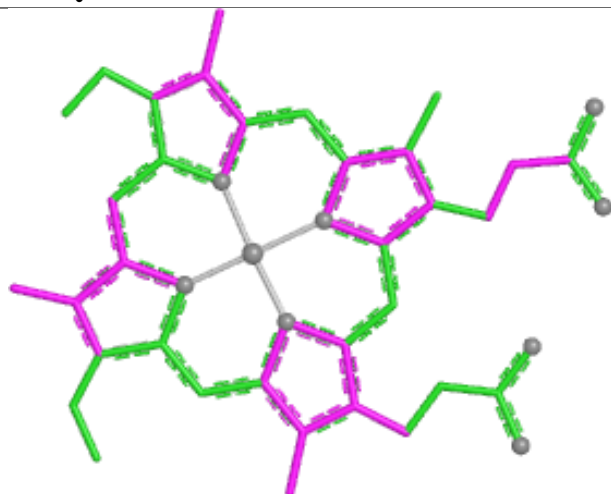




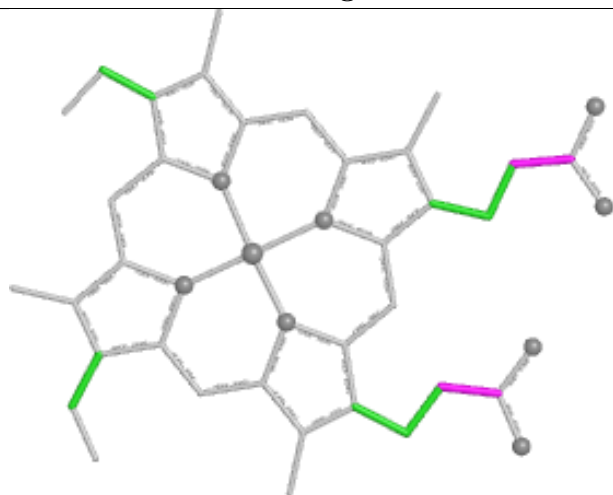
## Ligand HEC 3Q 501



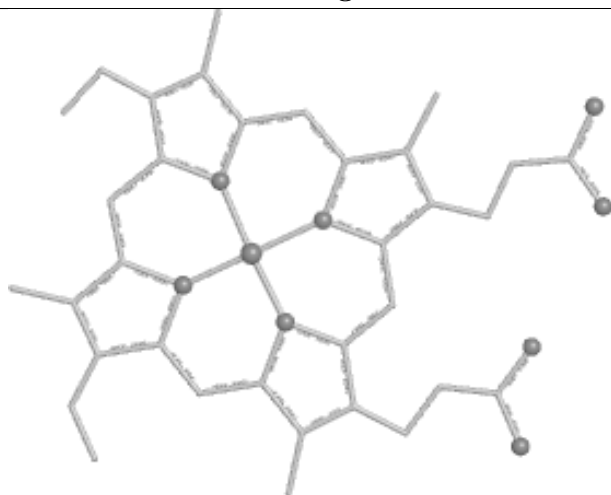
Bond lengths



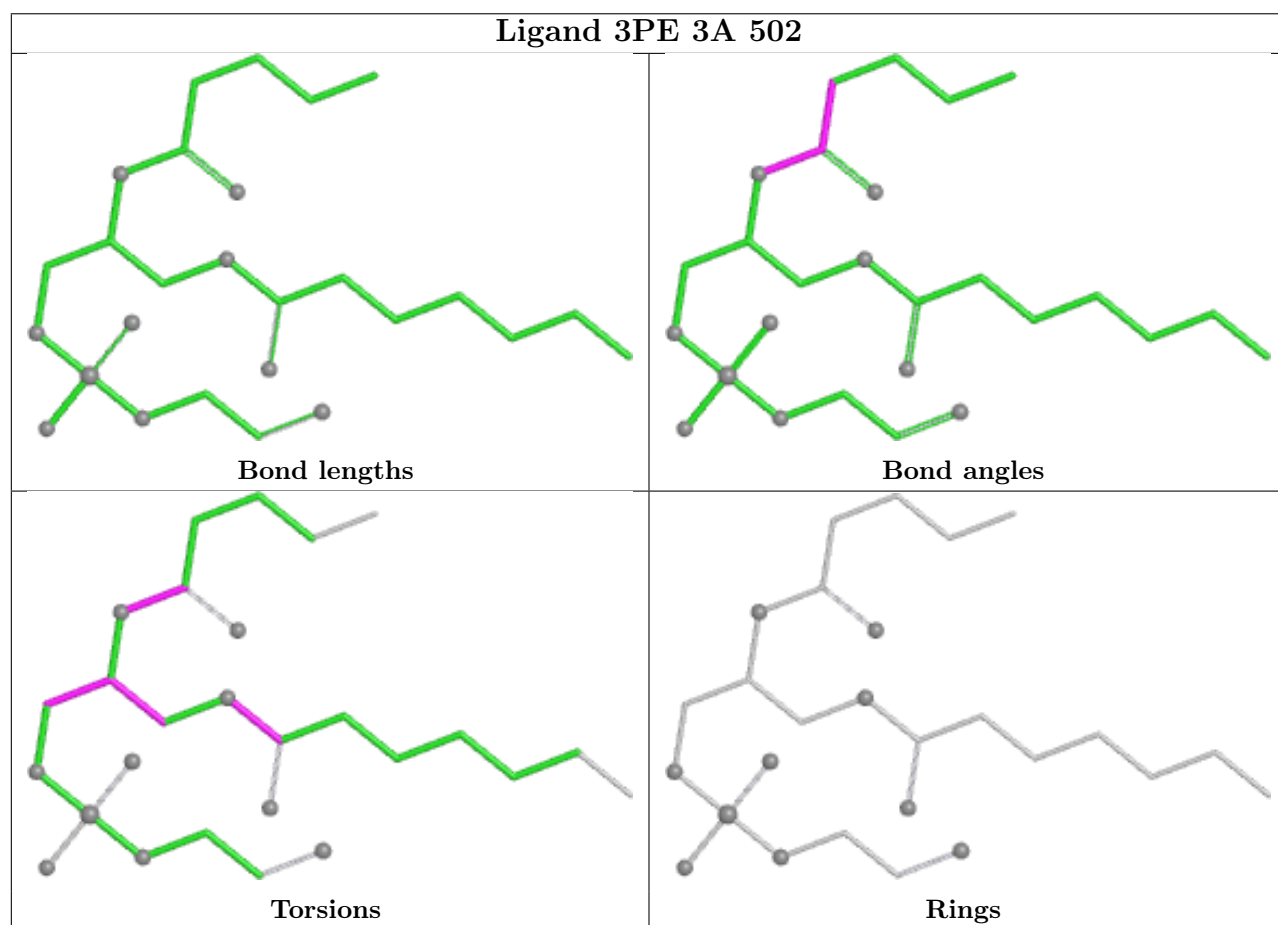
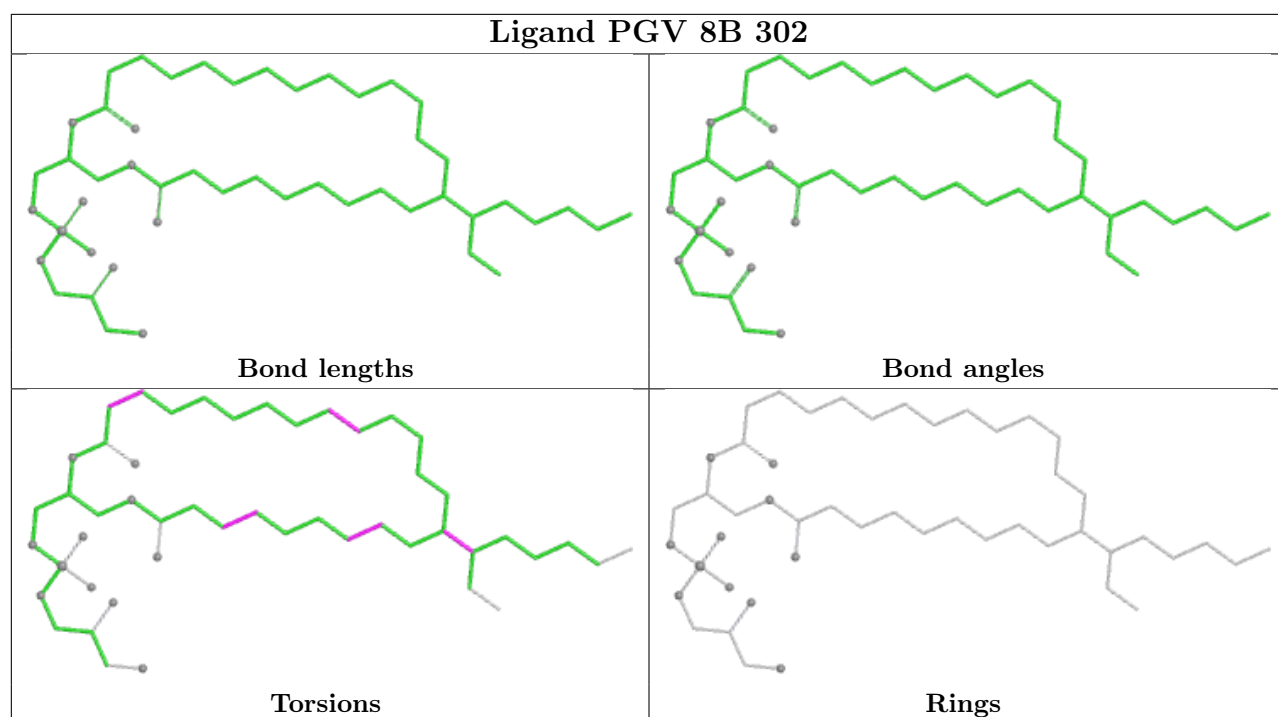
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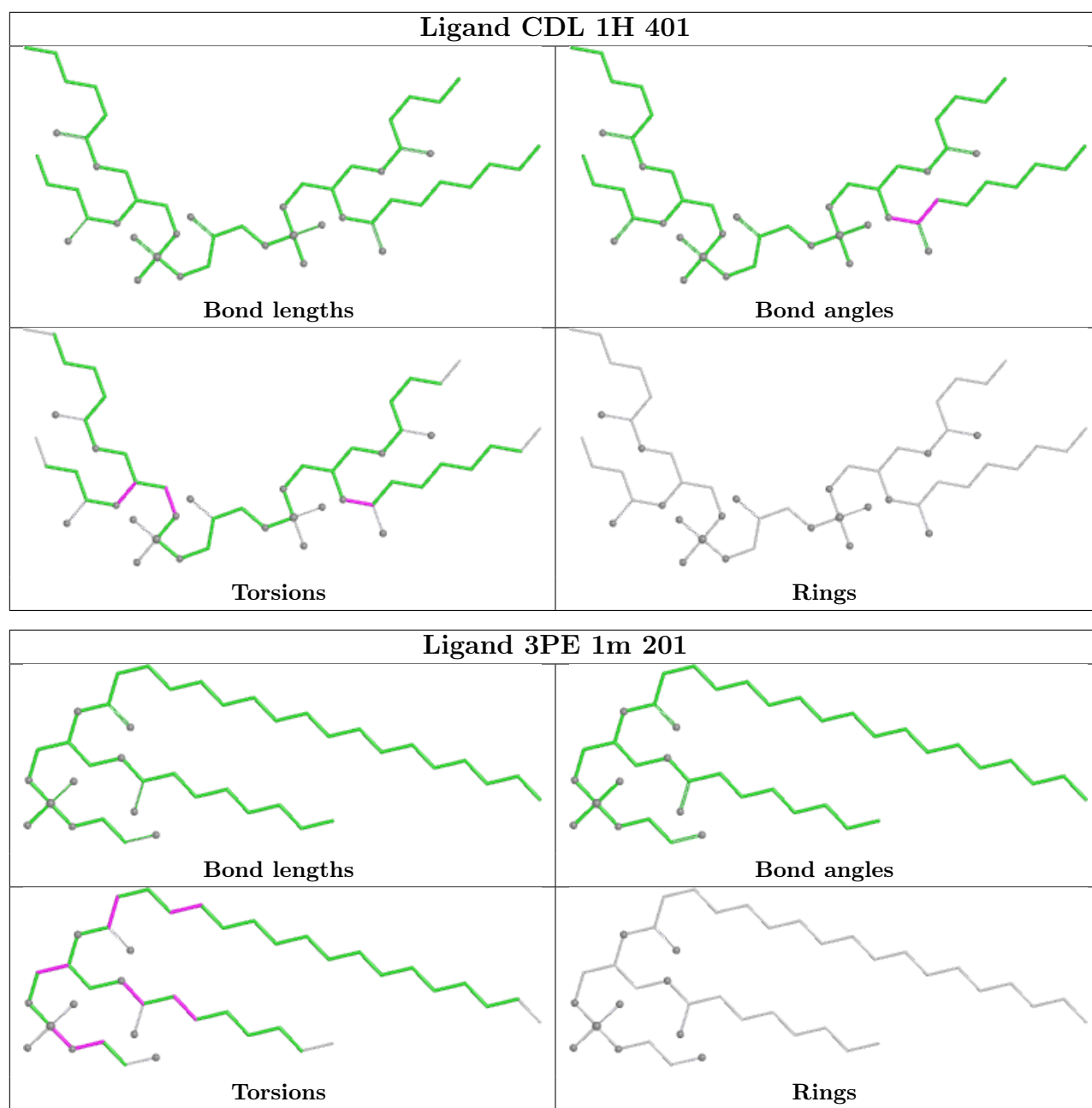


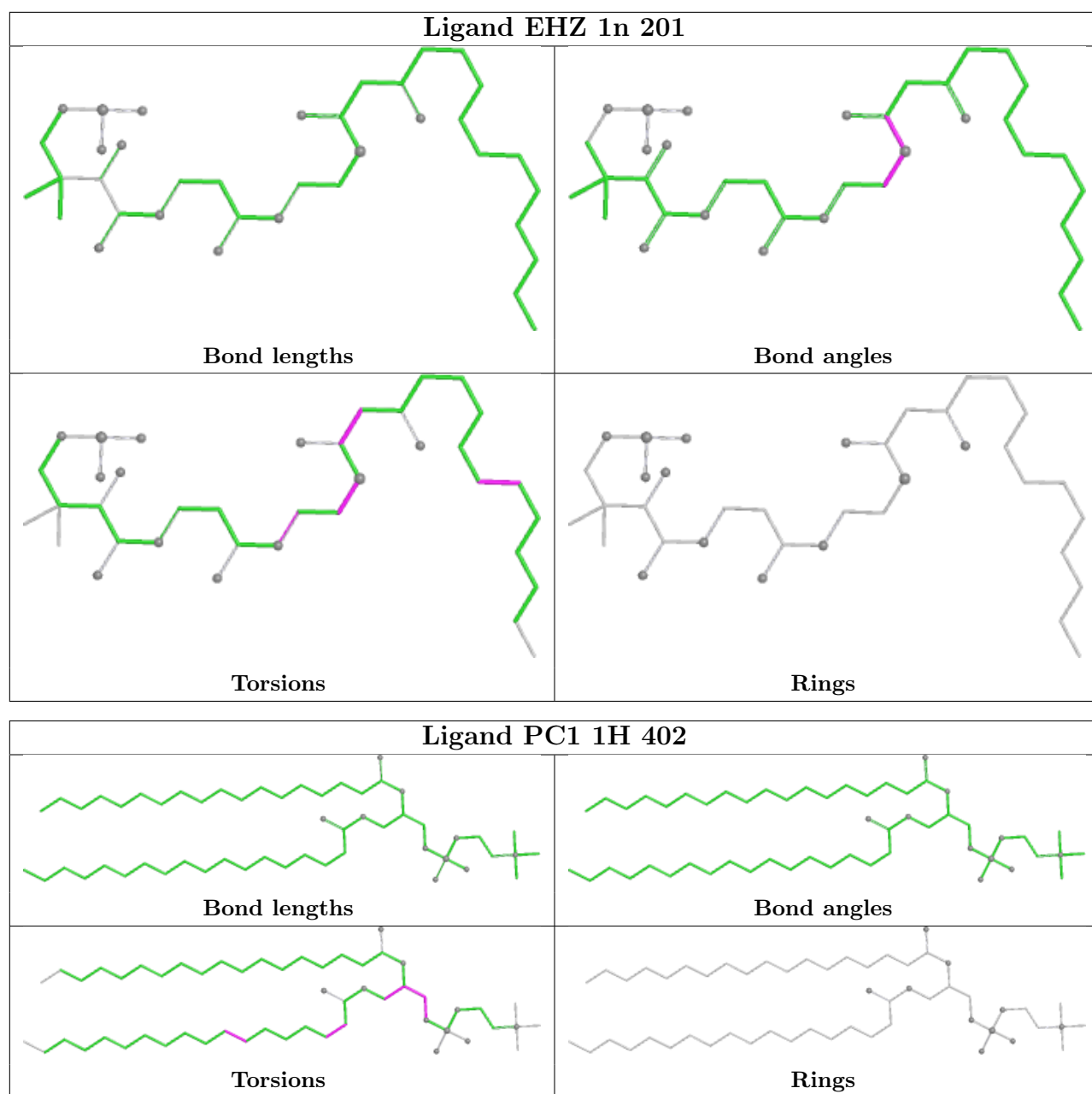
Torsions

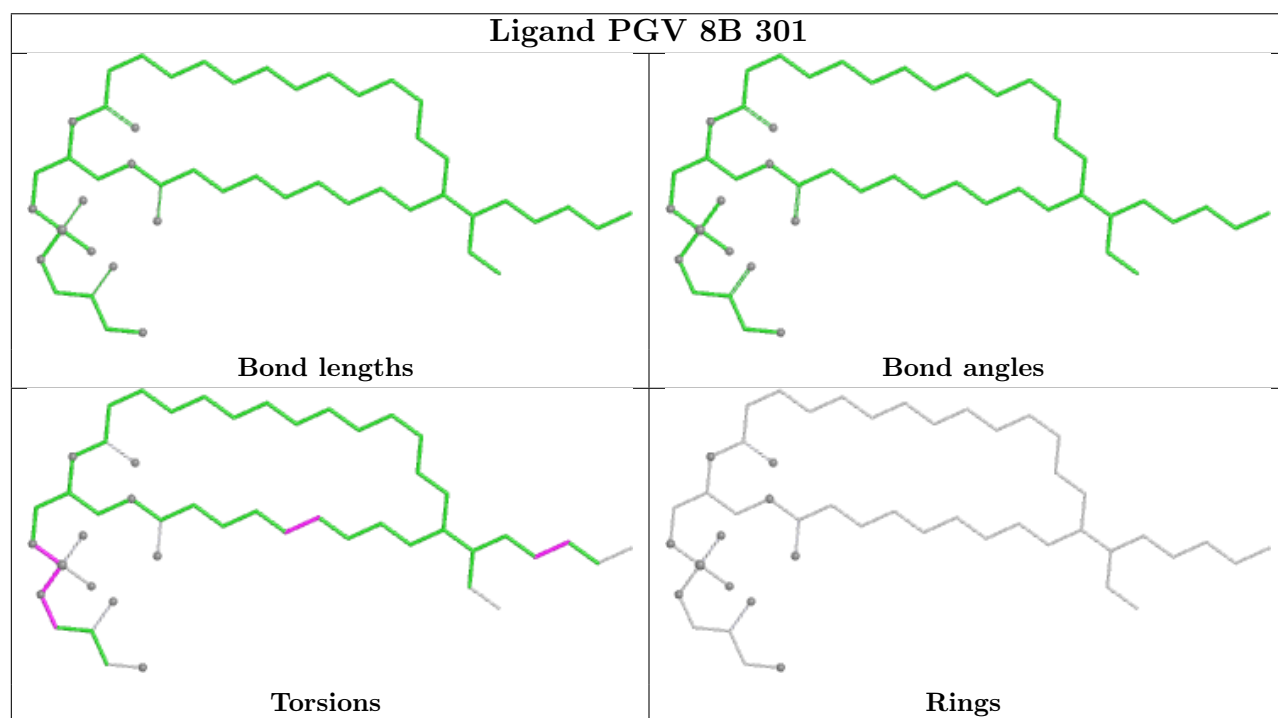
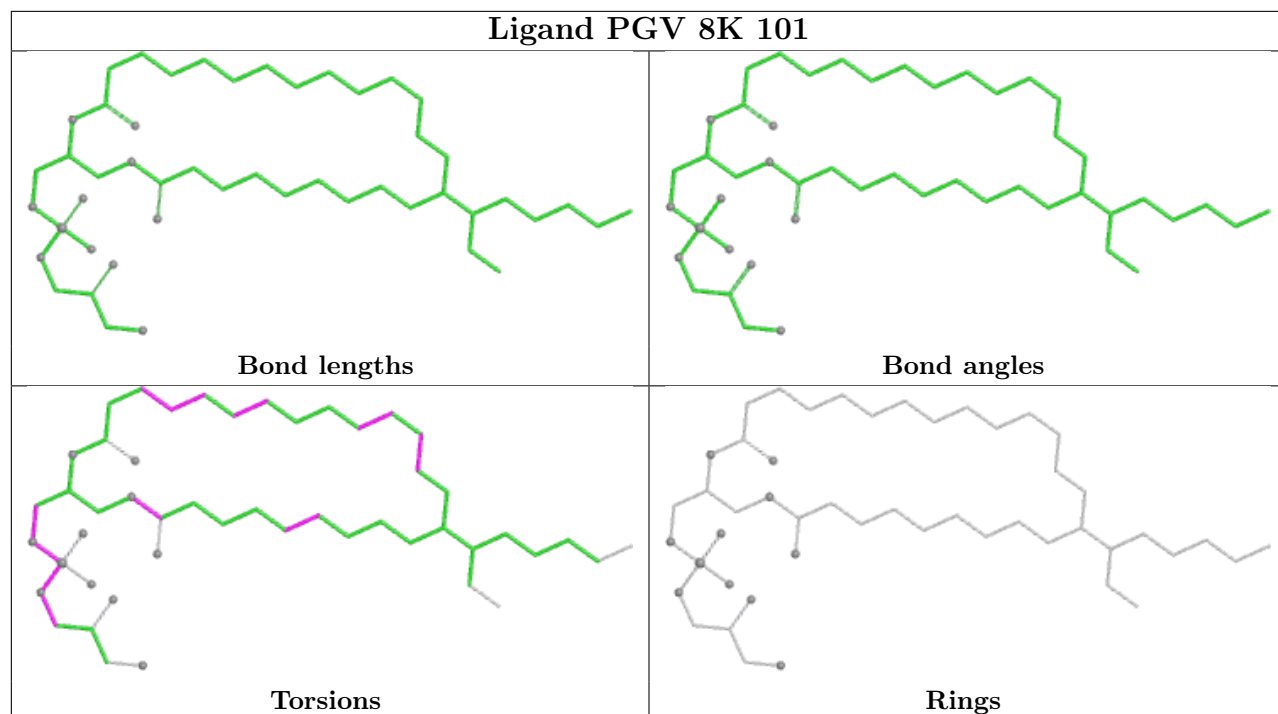


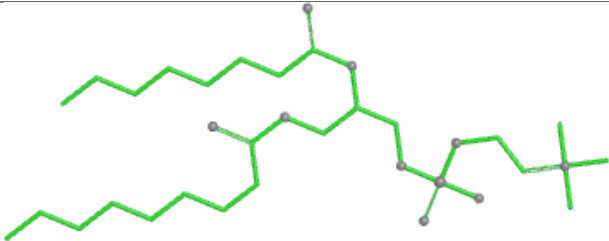
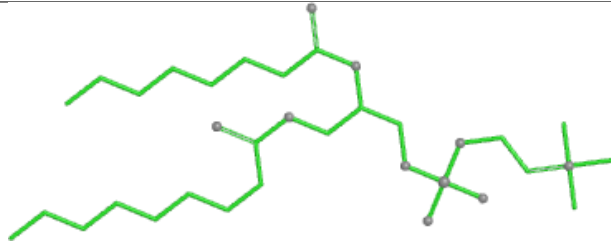
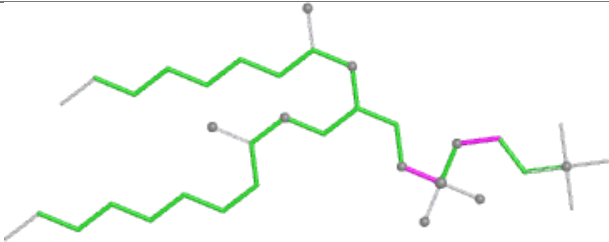
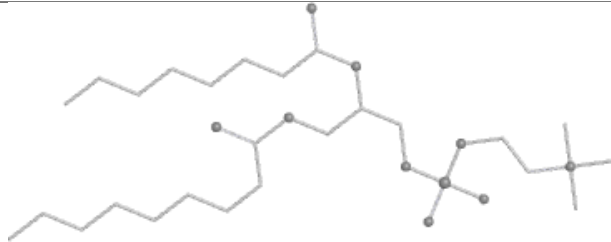
Rings

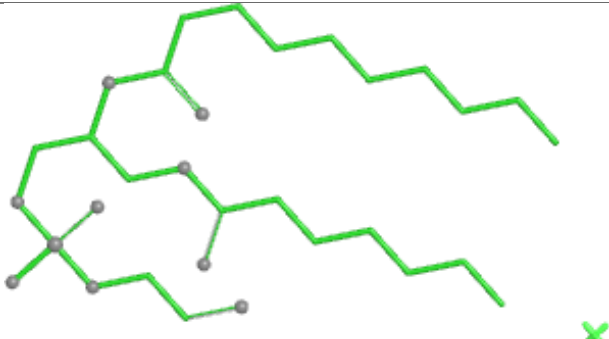
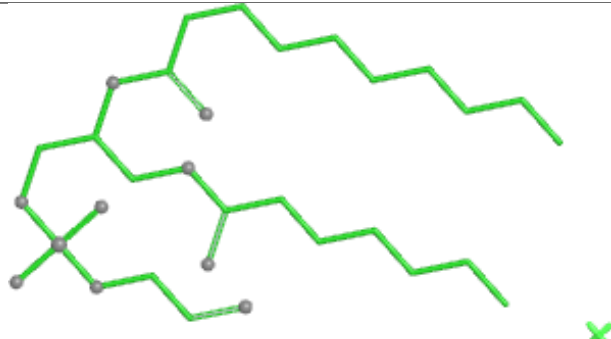
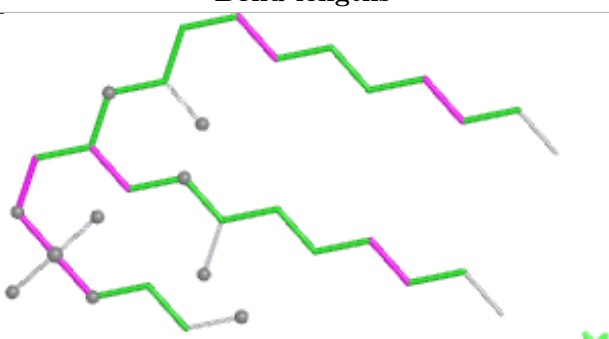


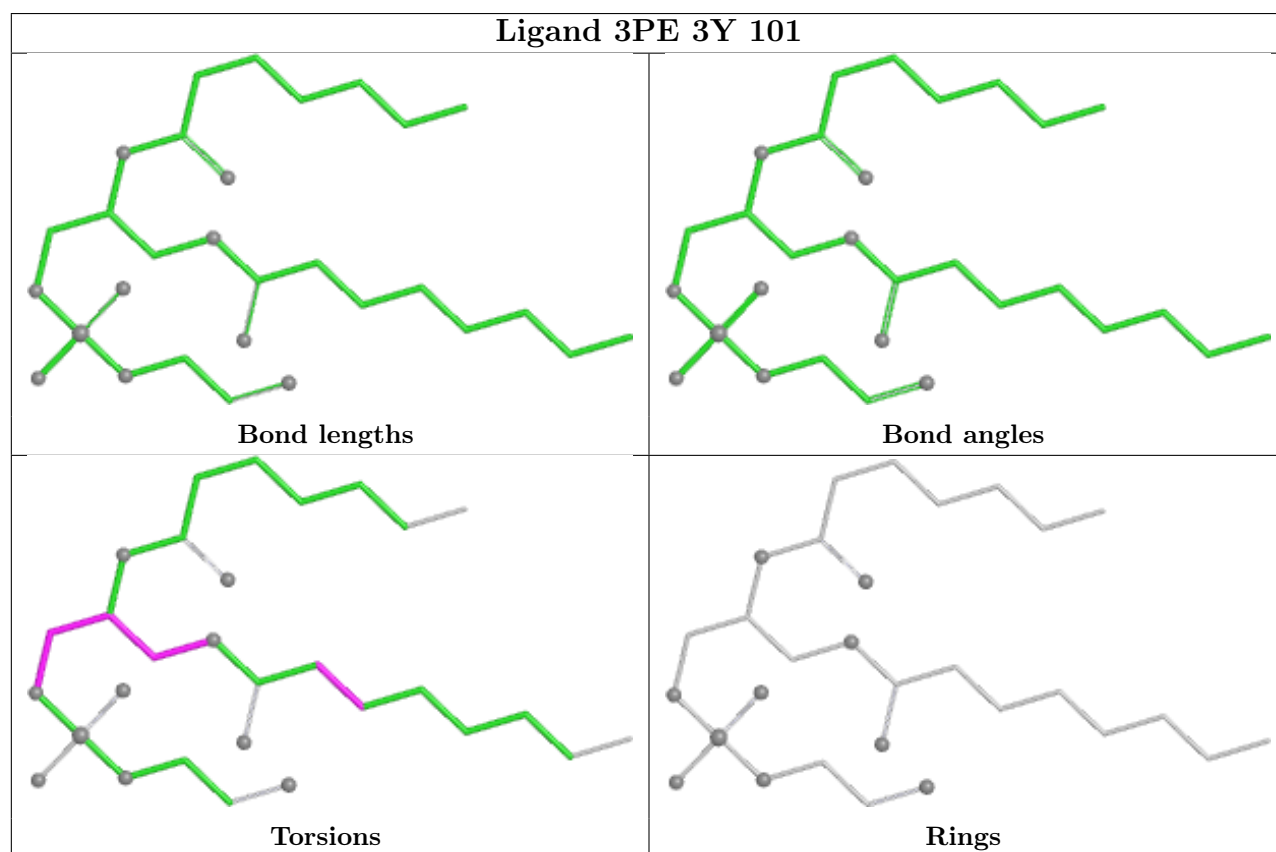
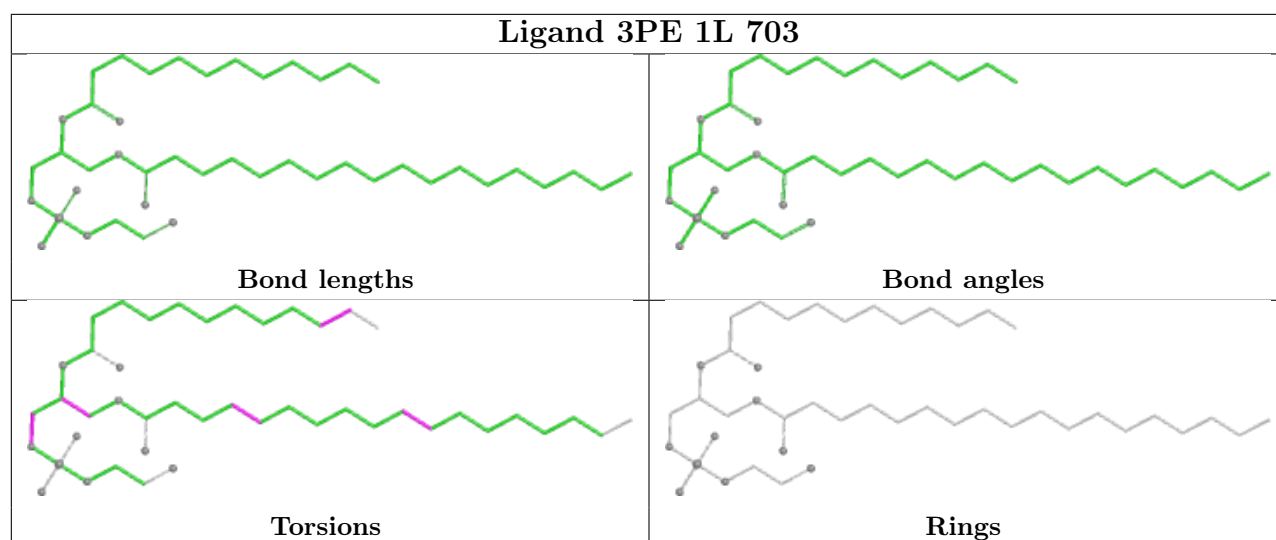


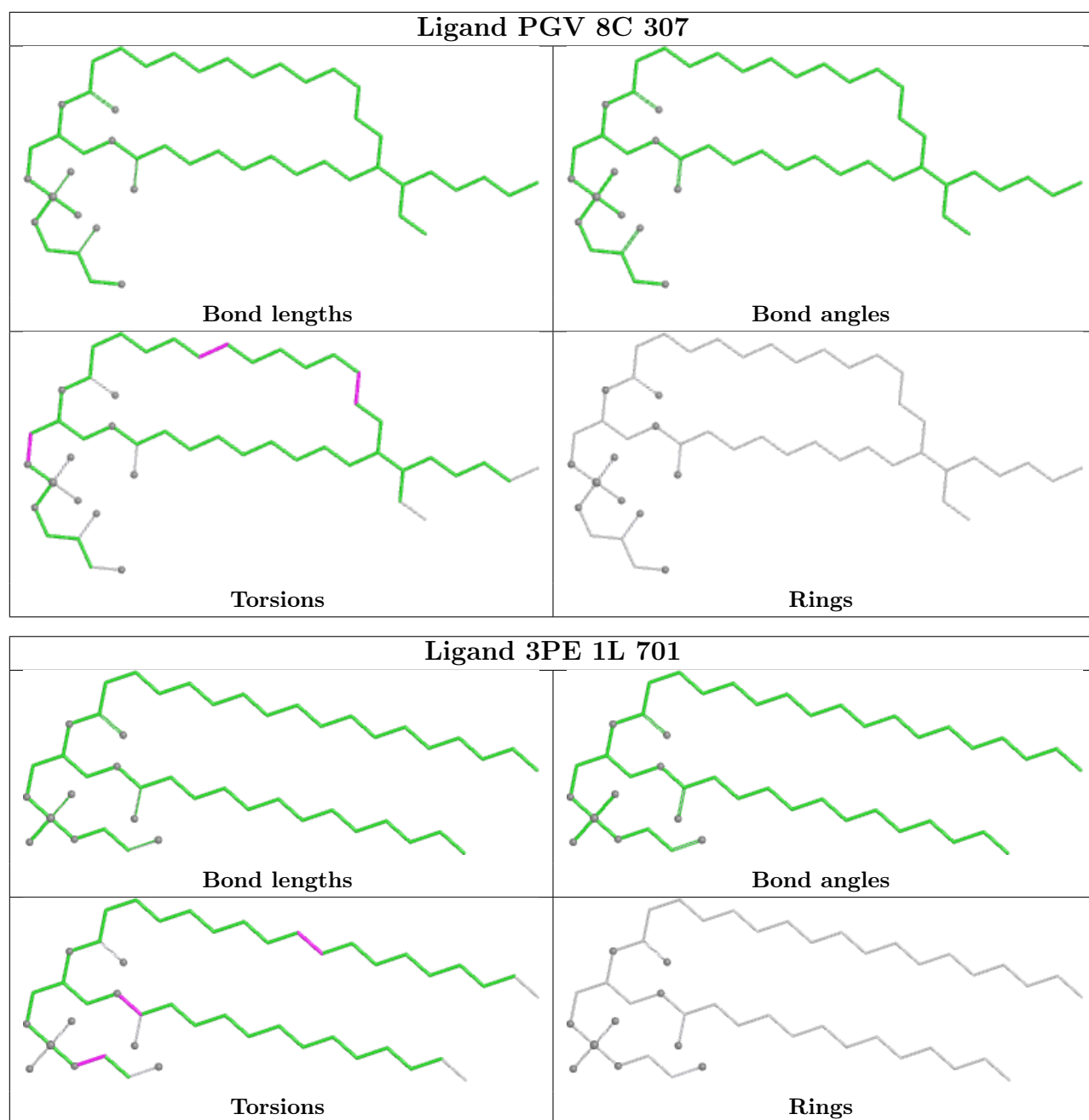


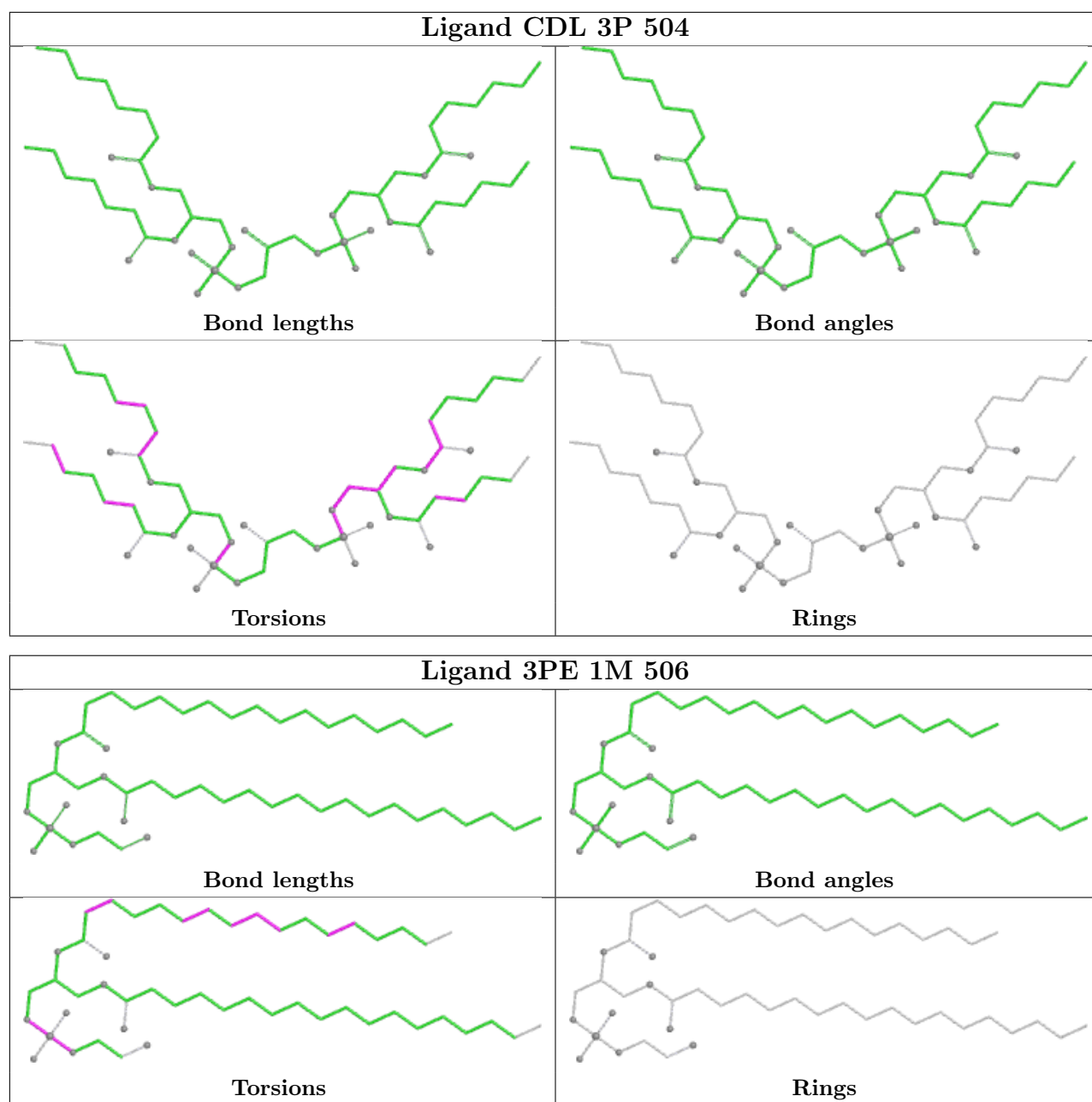


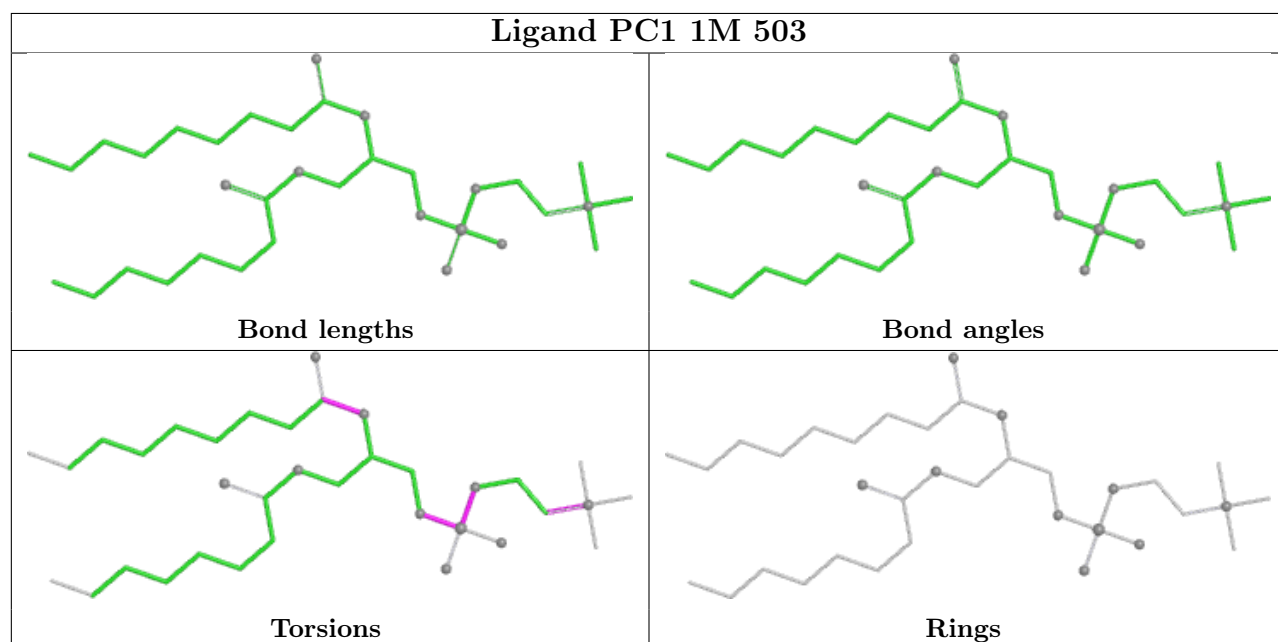
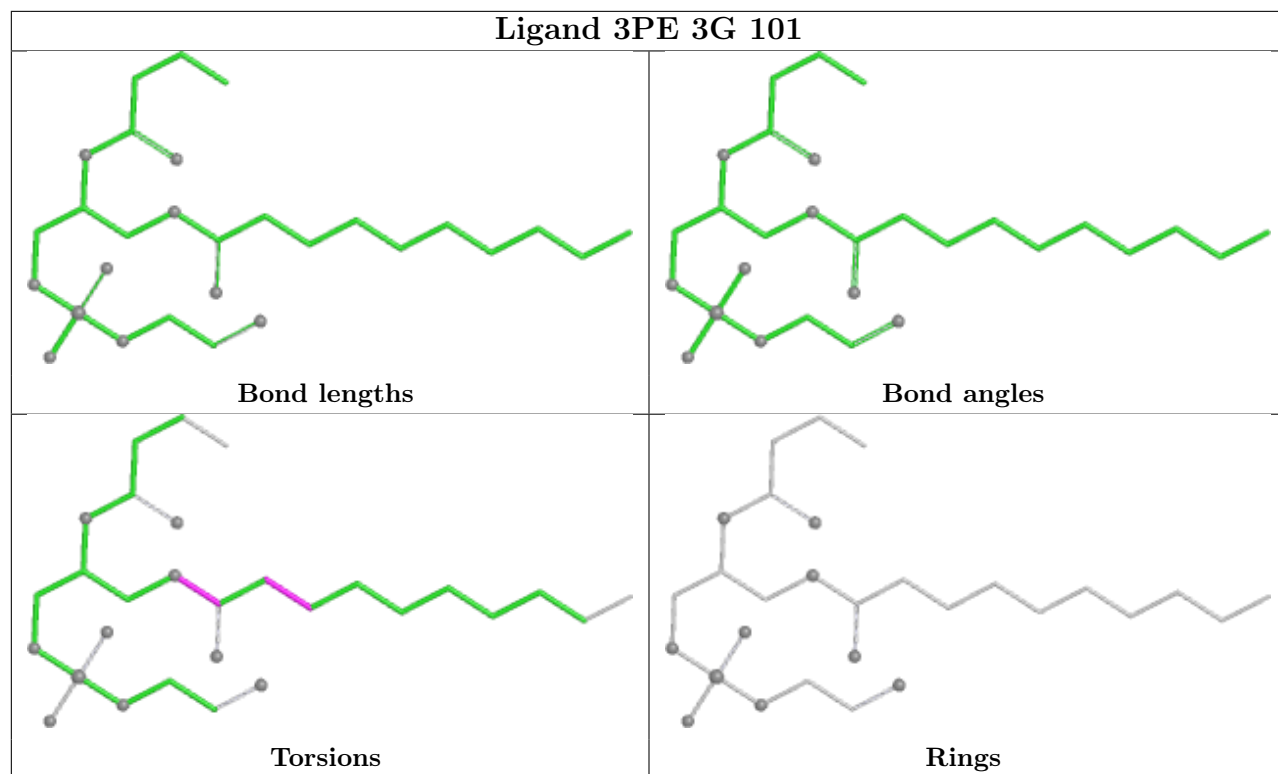
| Ligand PC1 1A 203                                                                 |                                                                                    |
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|  |  |
| Bond lengths                                                                      | Bond angles                                                                        |
|  |  |
| Torsions                                                                          | Rings                                                                              |

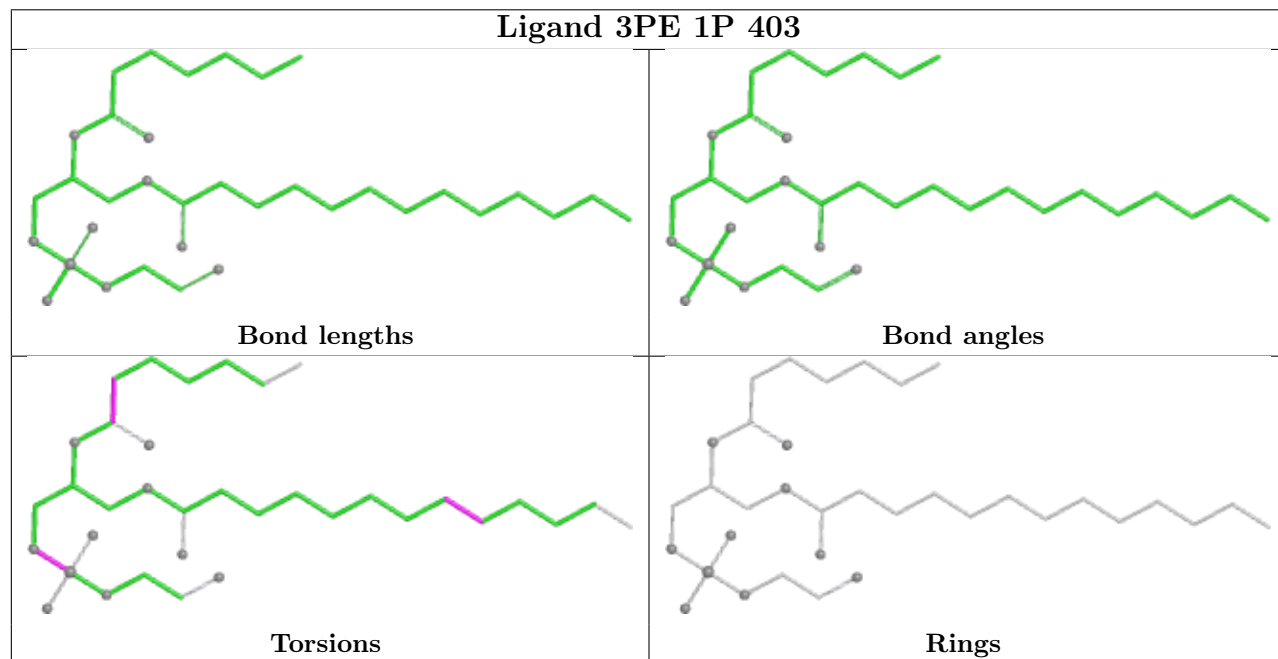
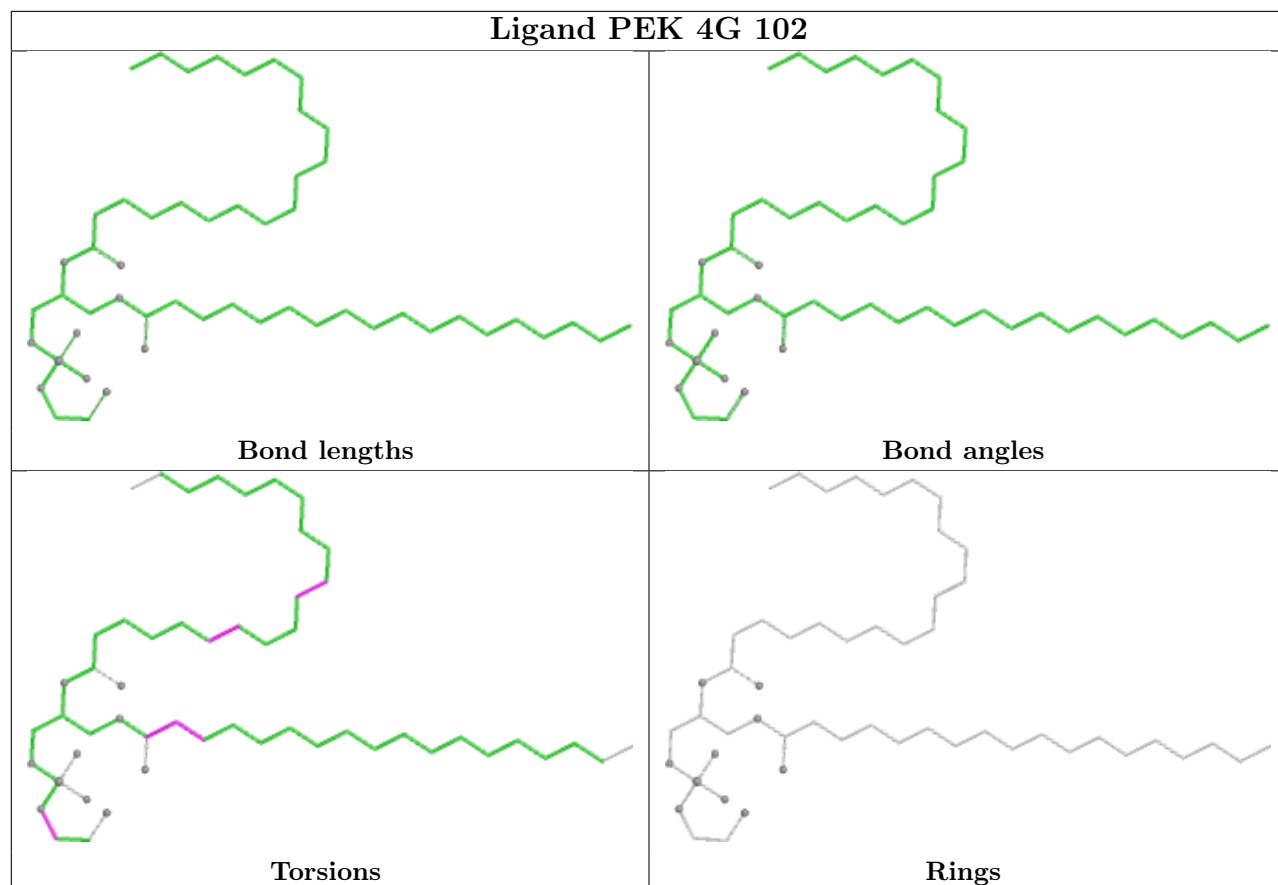
| Ligand 3PE 3N 501                                                                   |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|   |   |
| Bond lengths                                                                        | Bond angles                                                                          |
|  |  |
| Torsions                                                                            | Rings                                                                                |

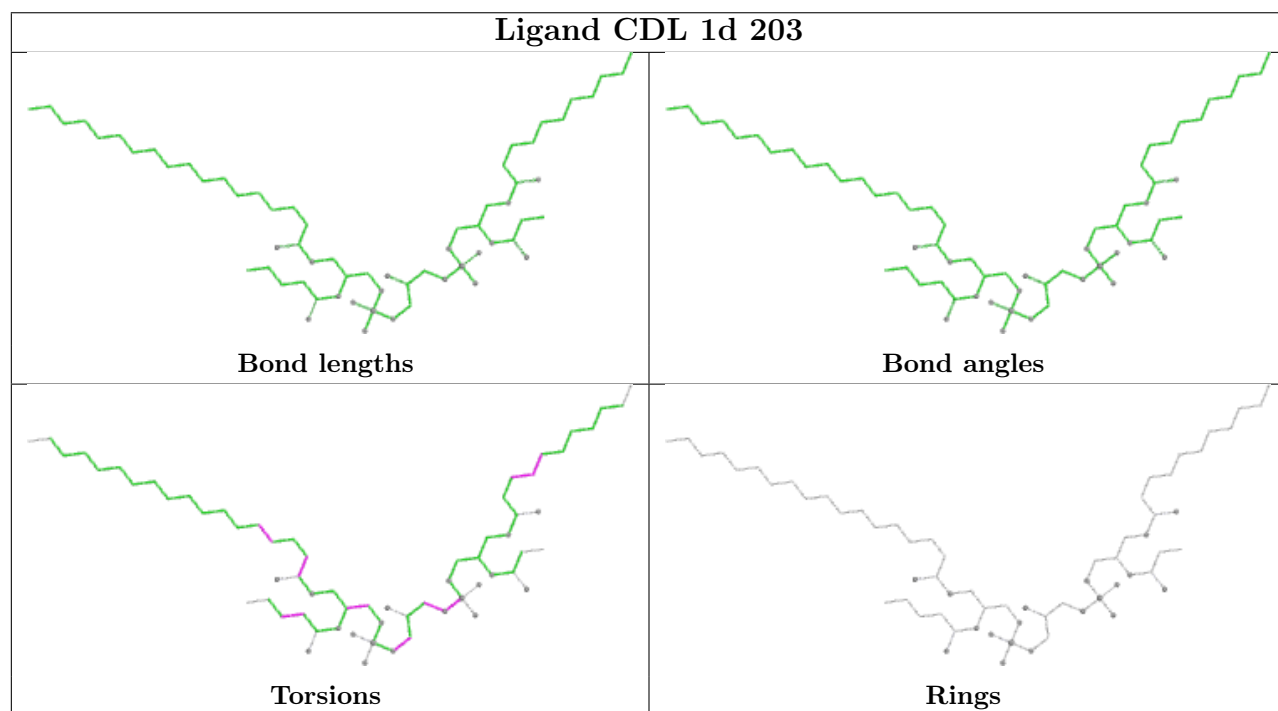
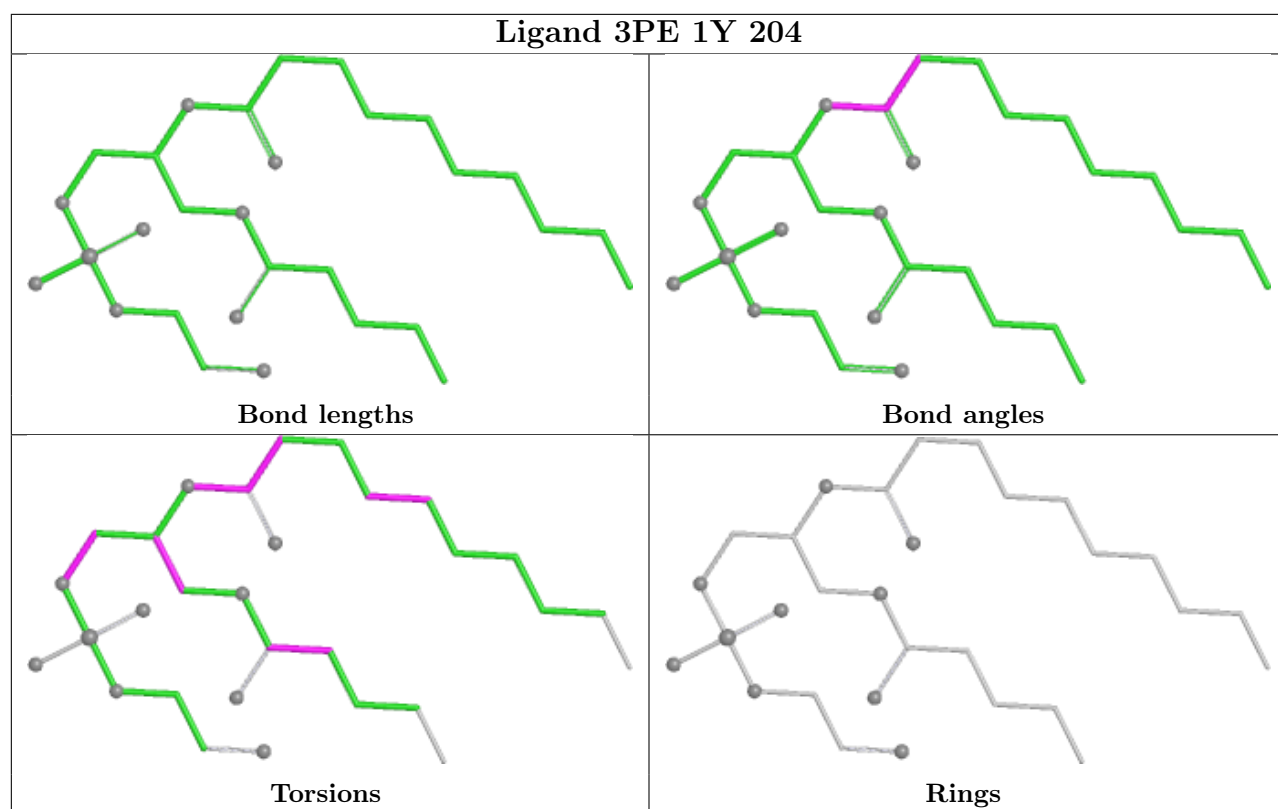


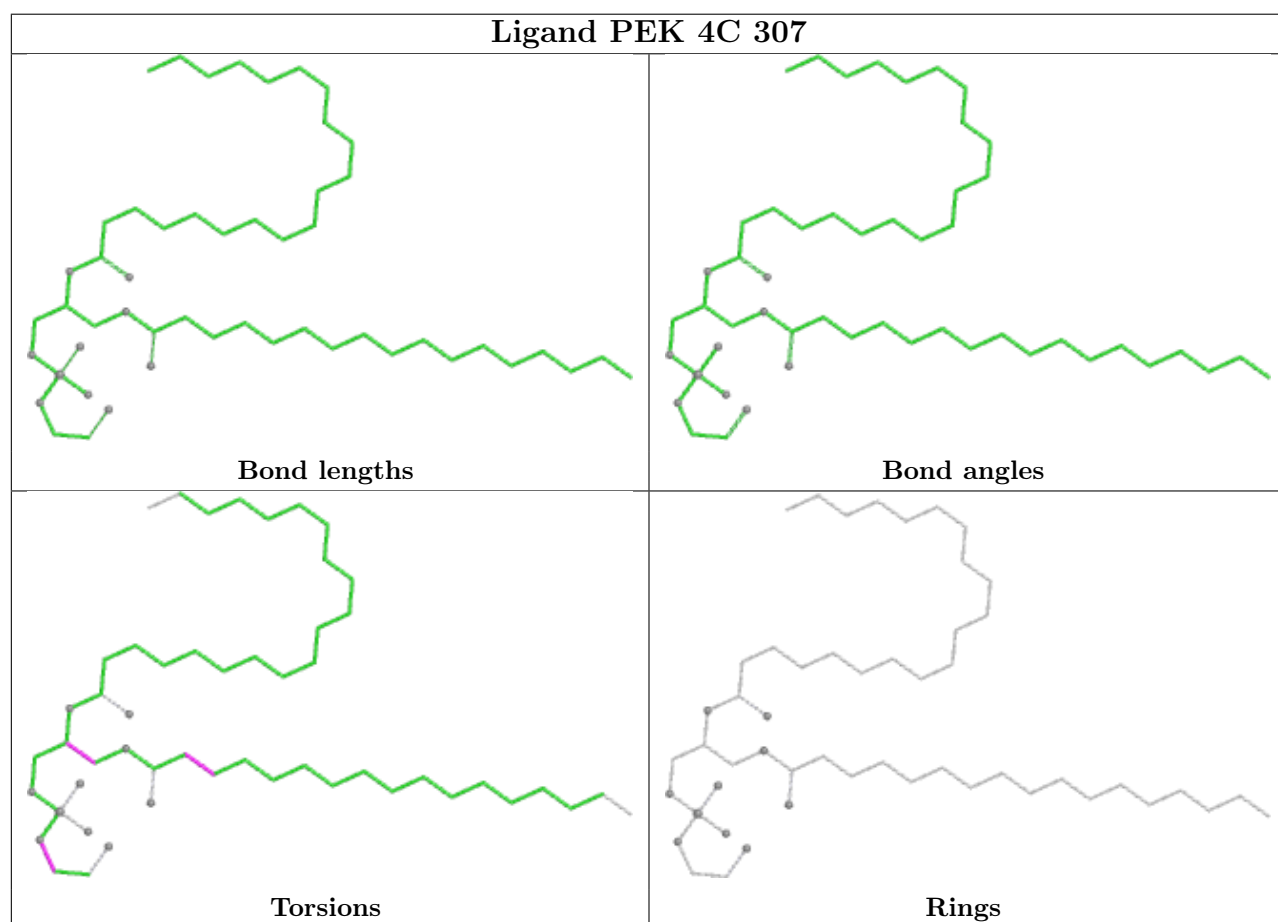
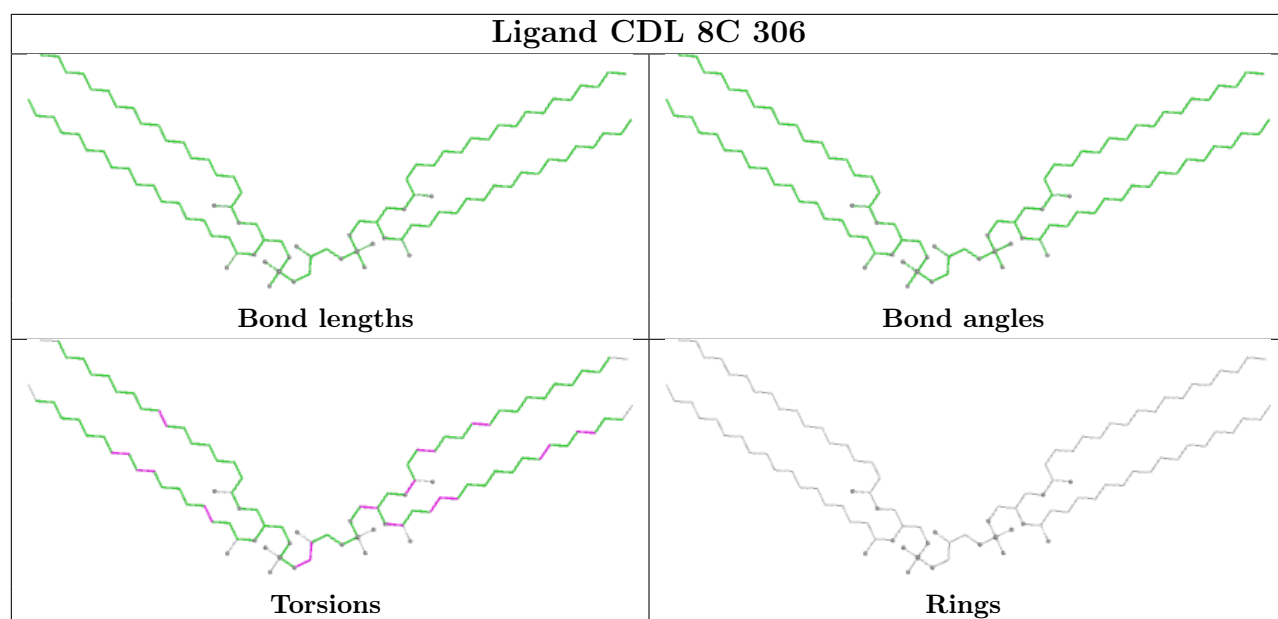


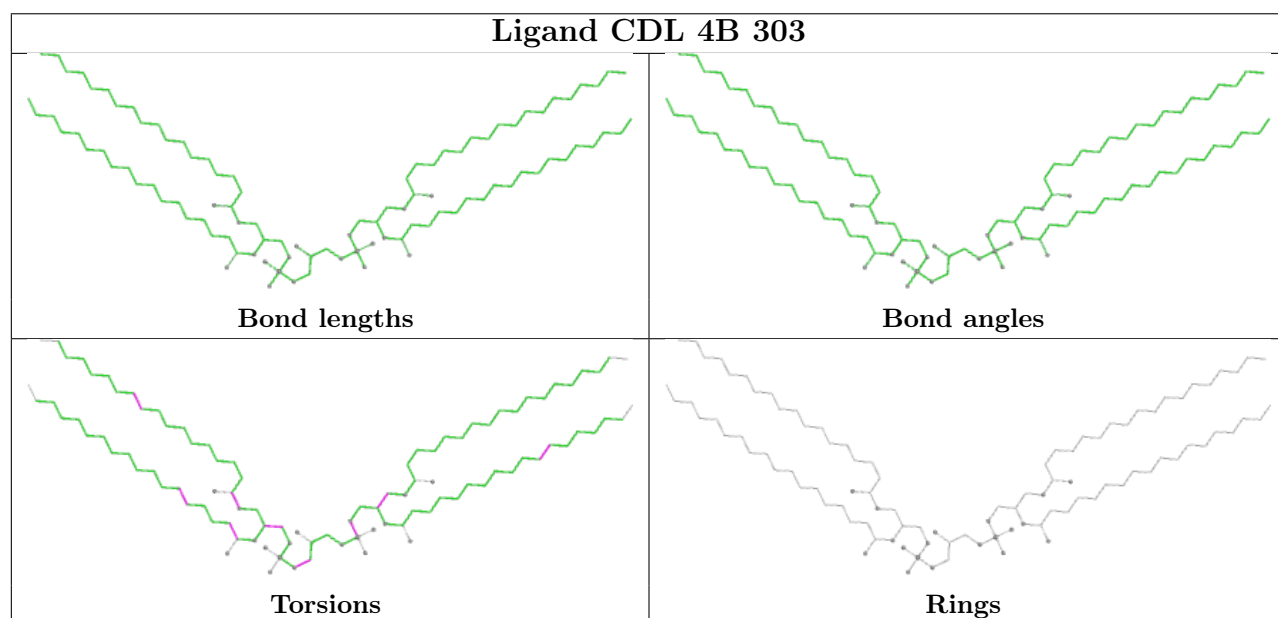
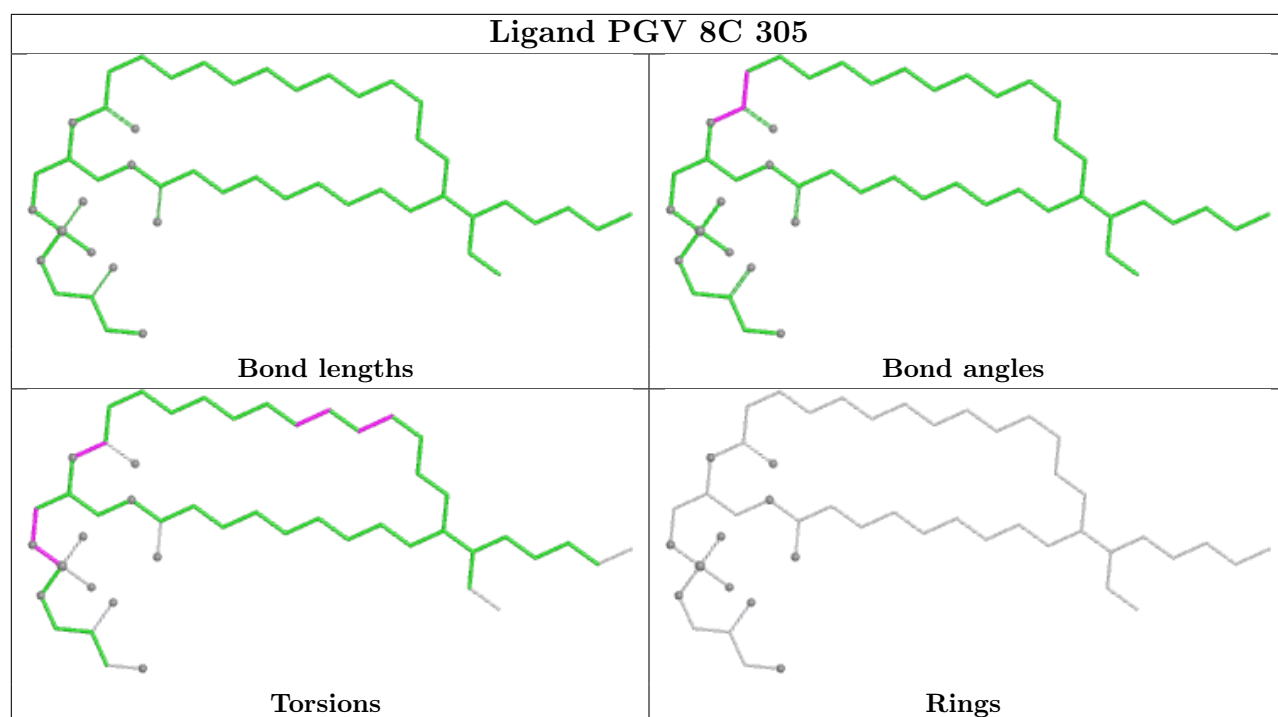


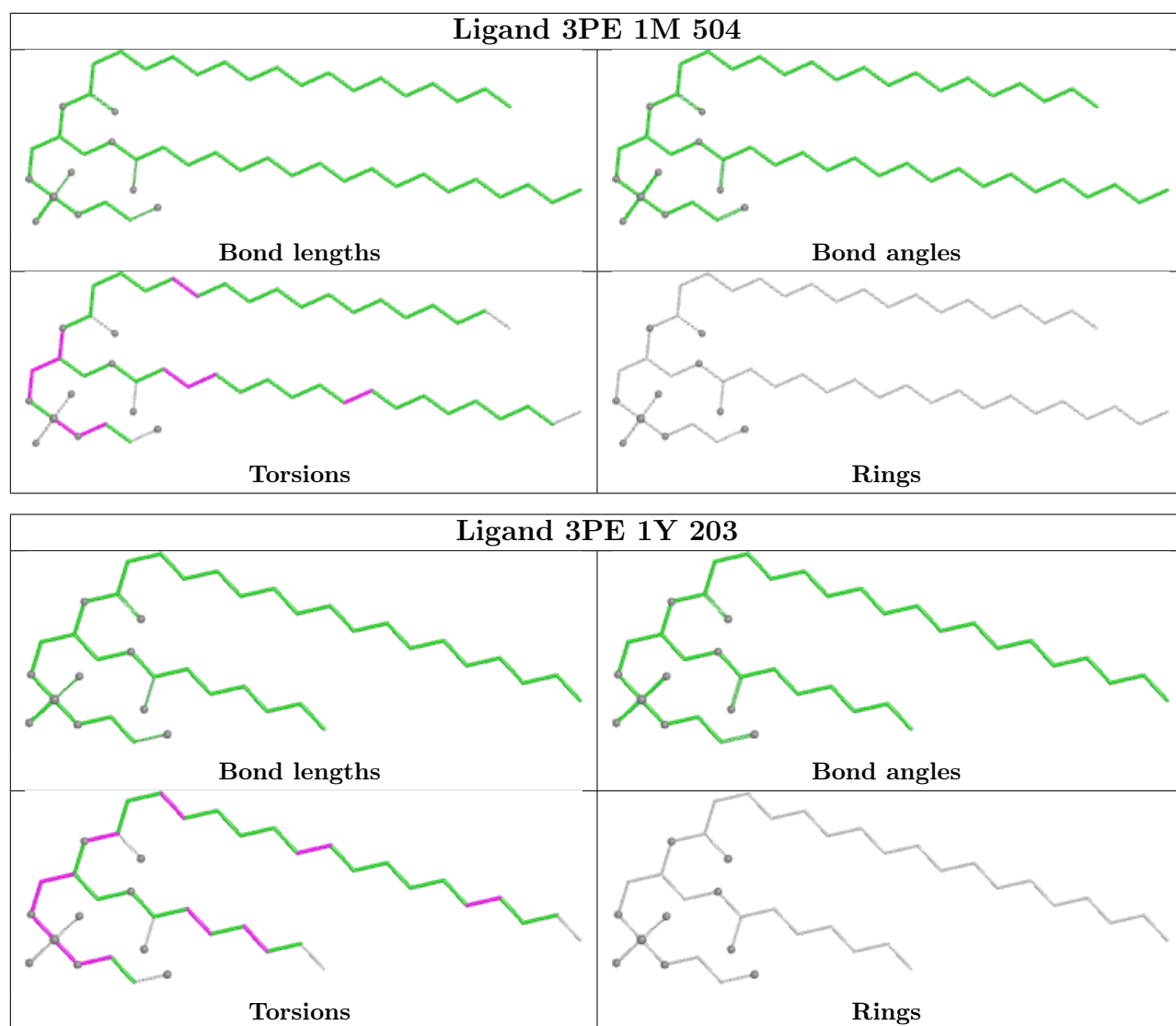


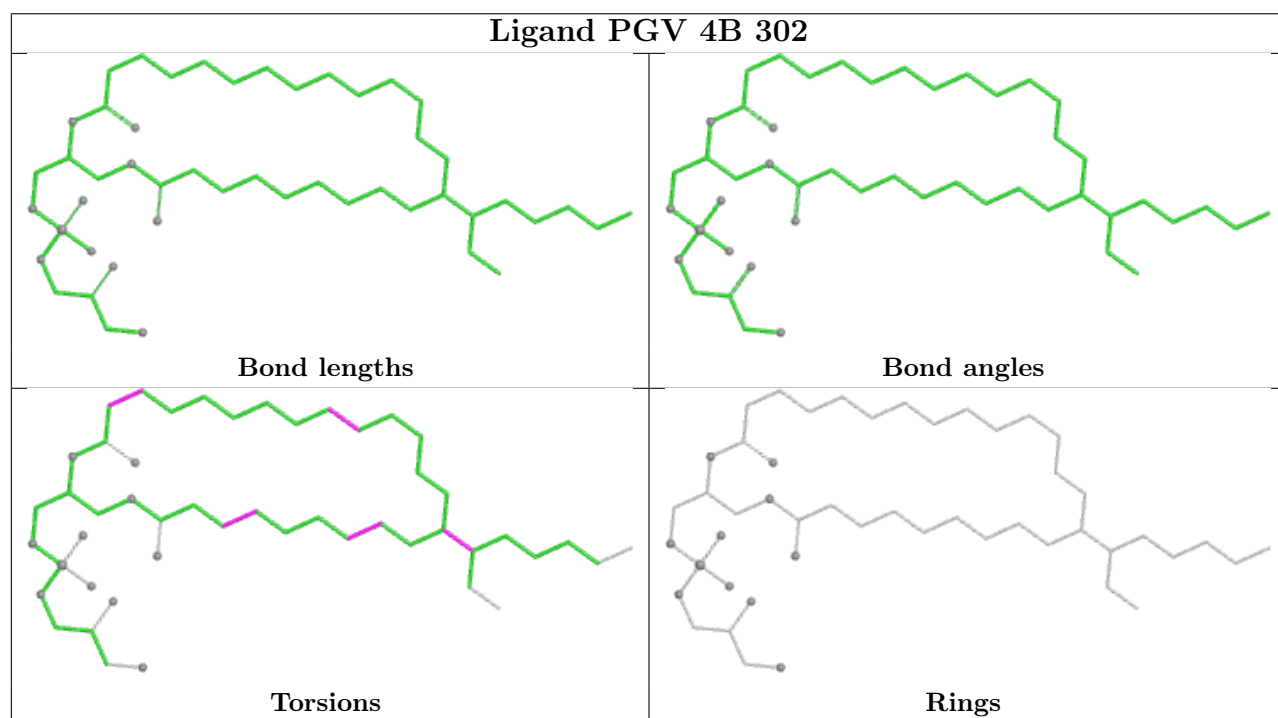
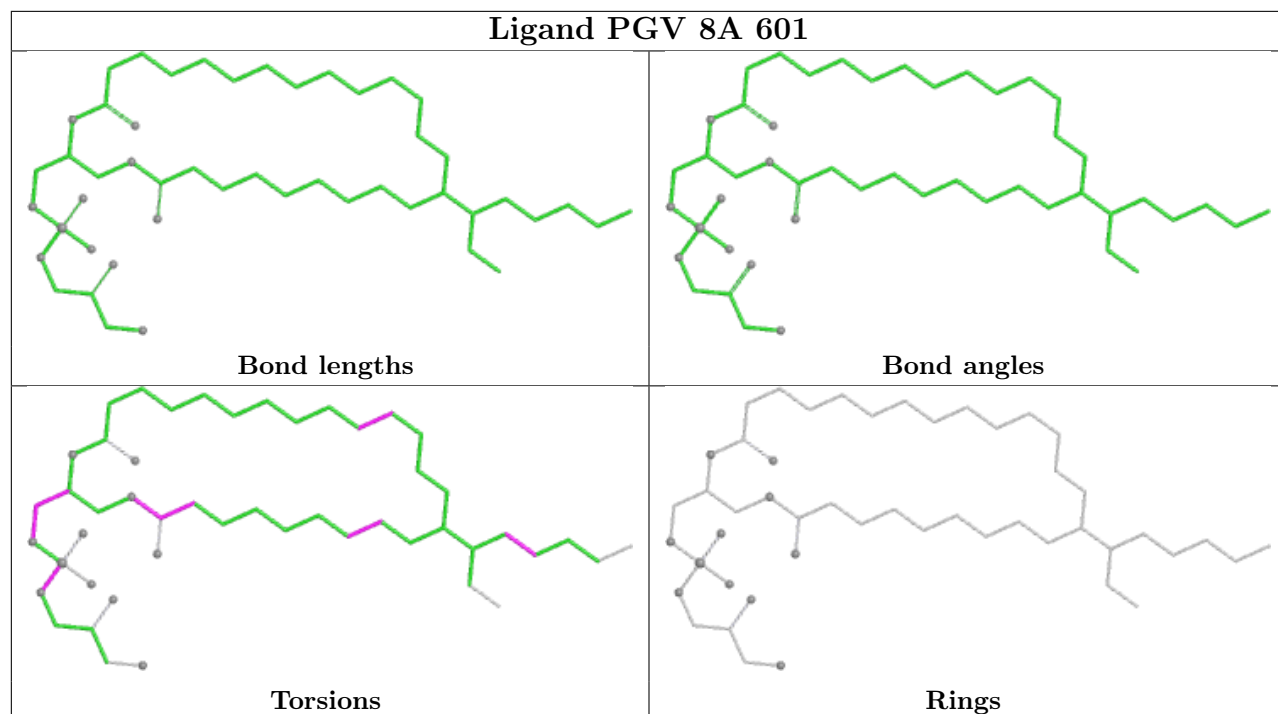


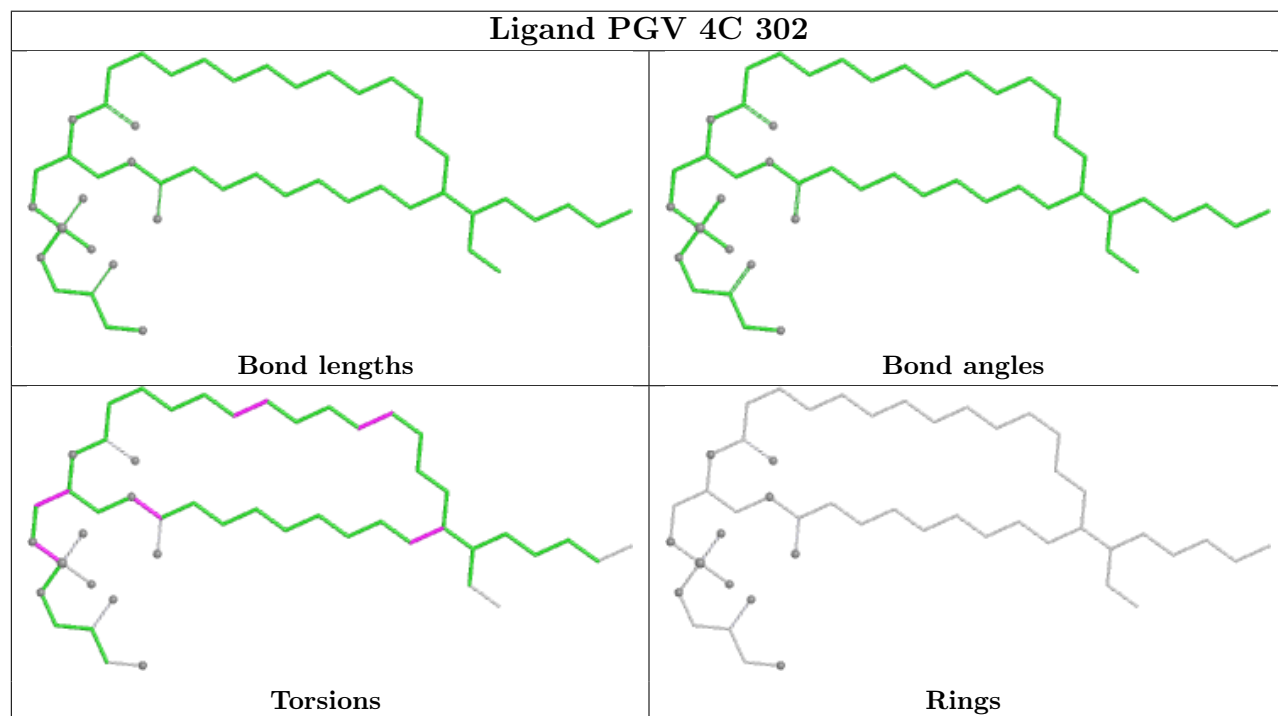
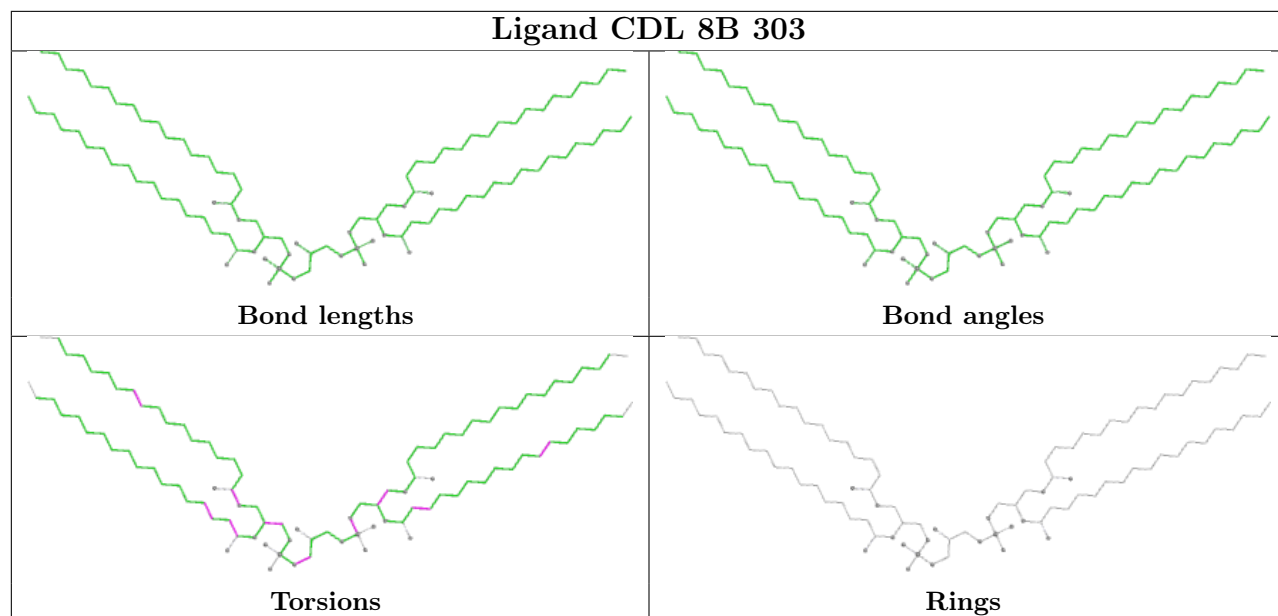


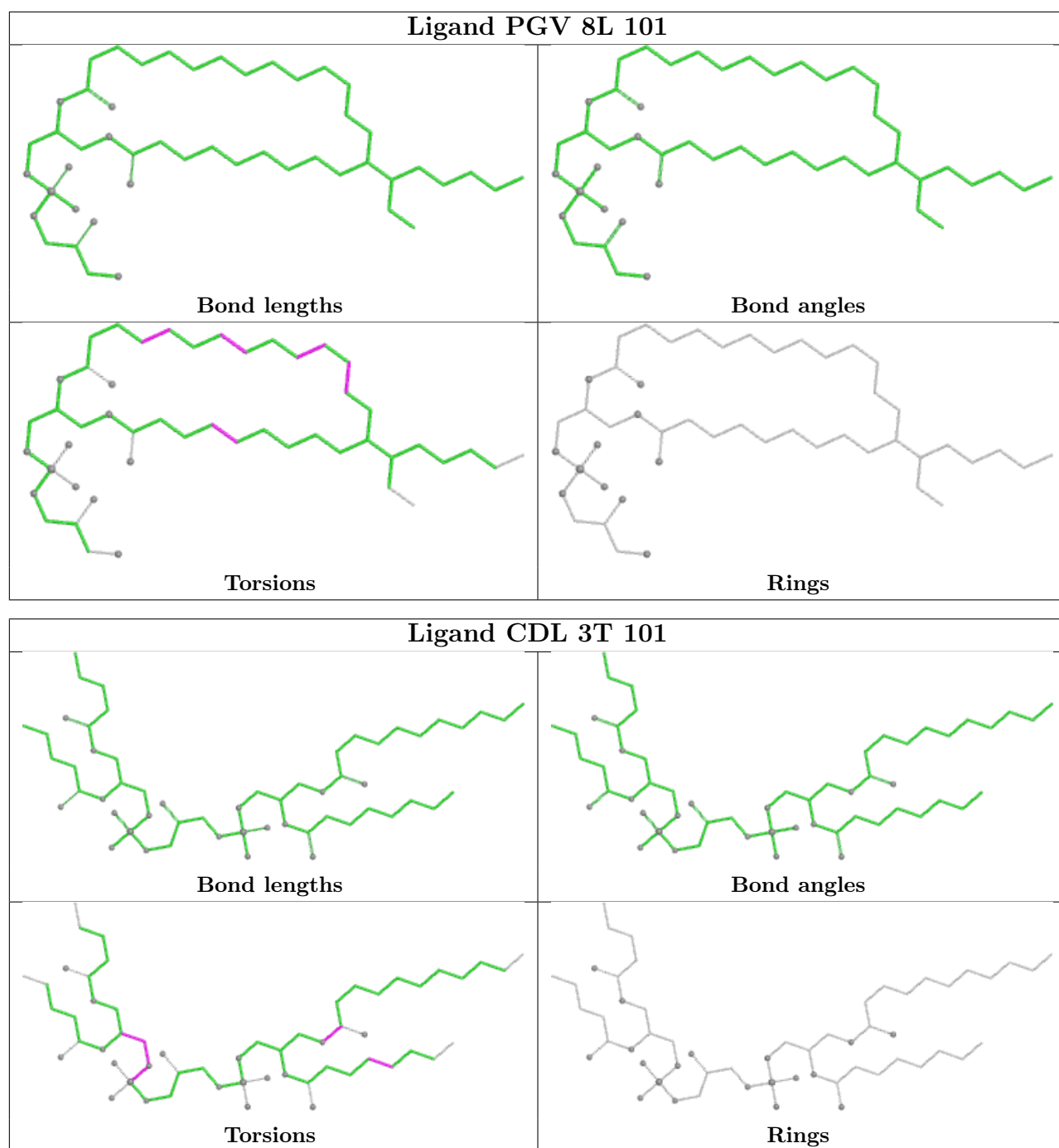


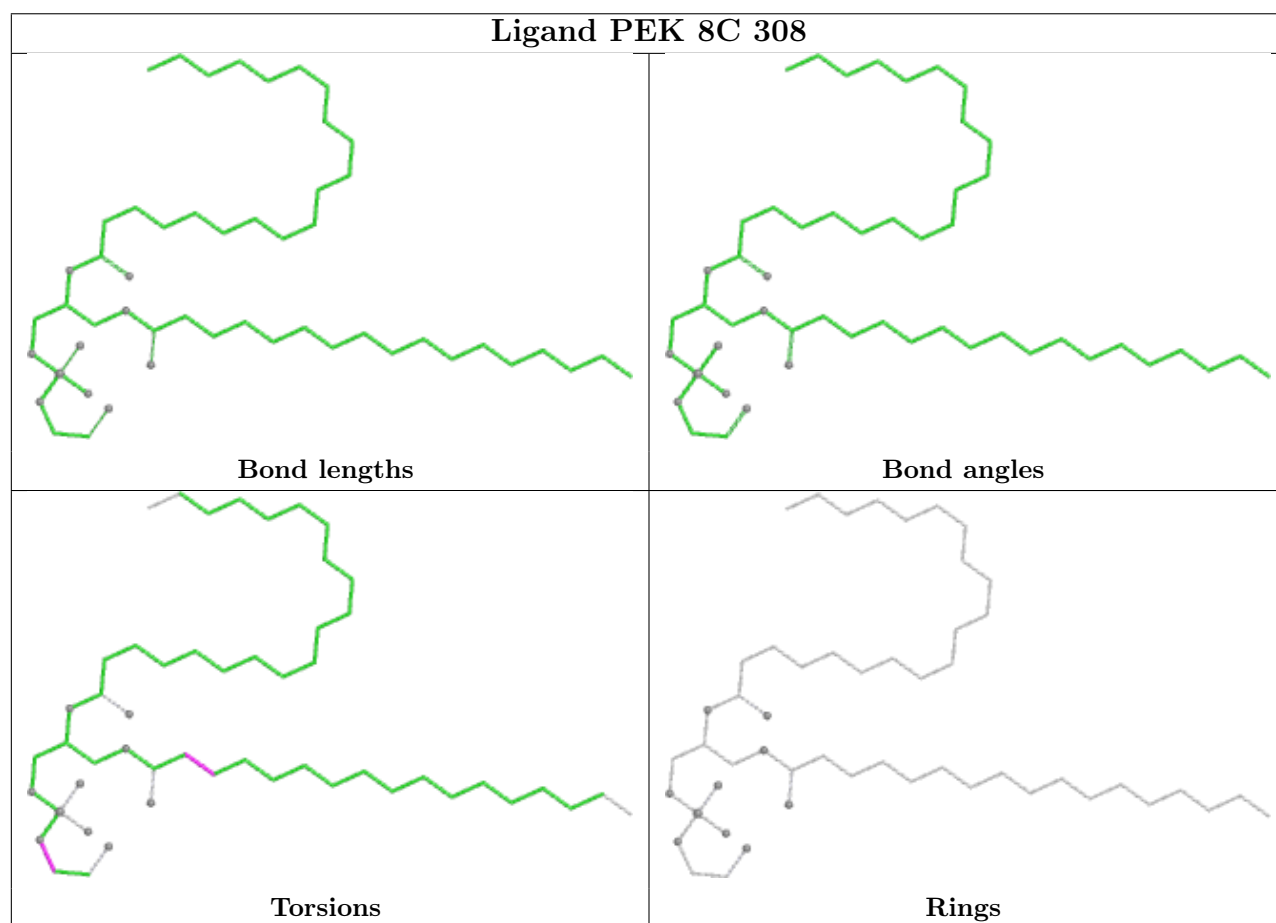
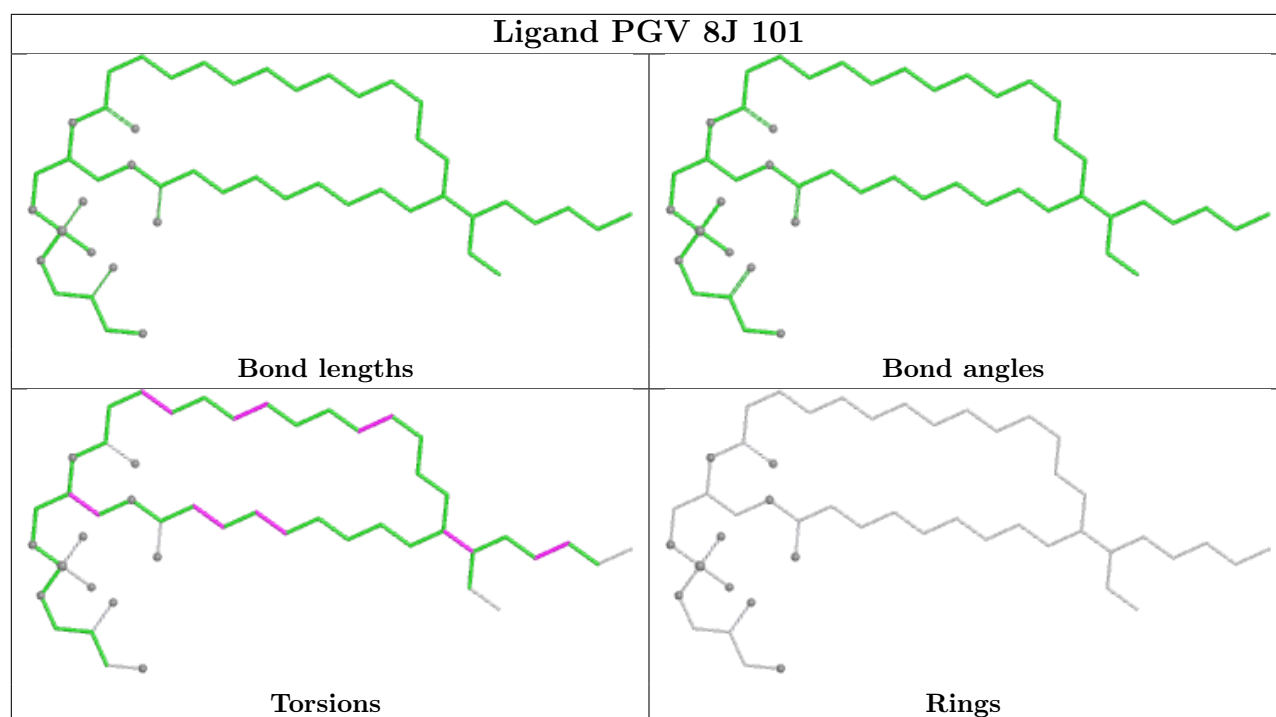


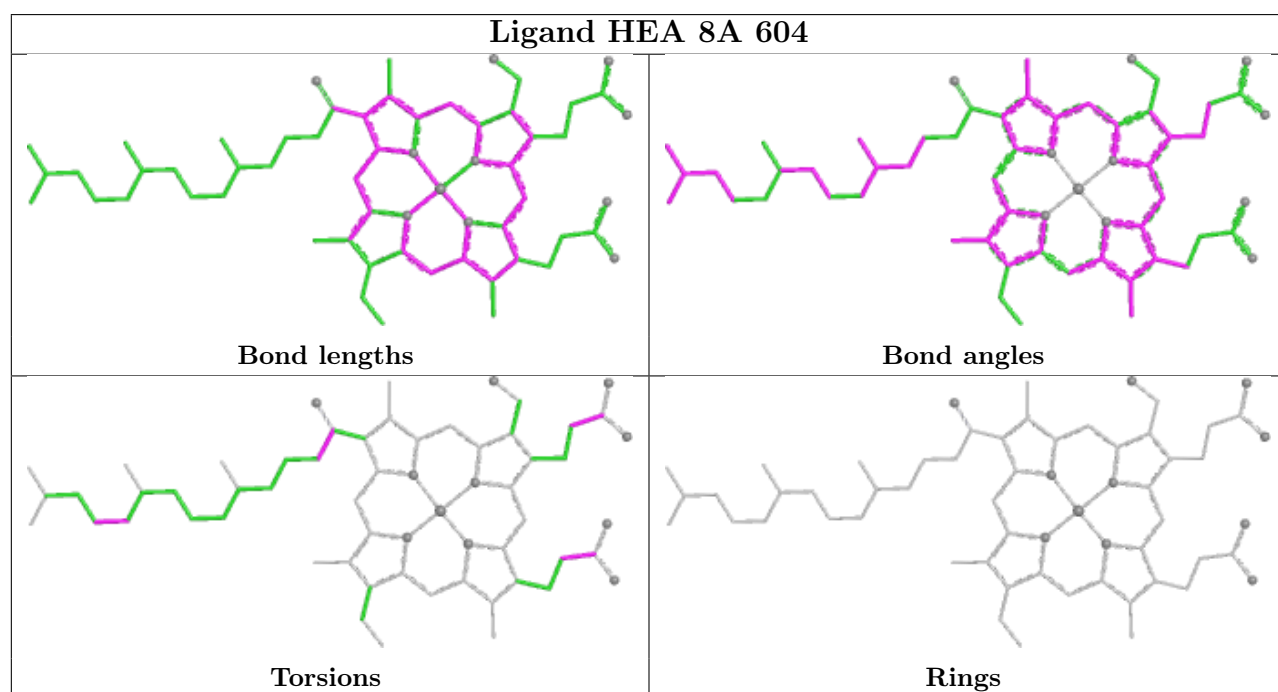
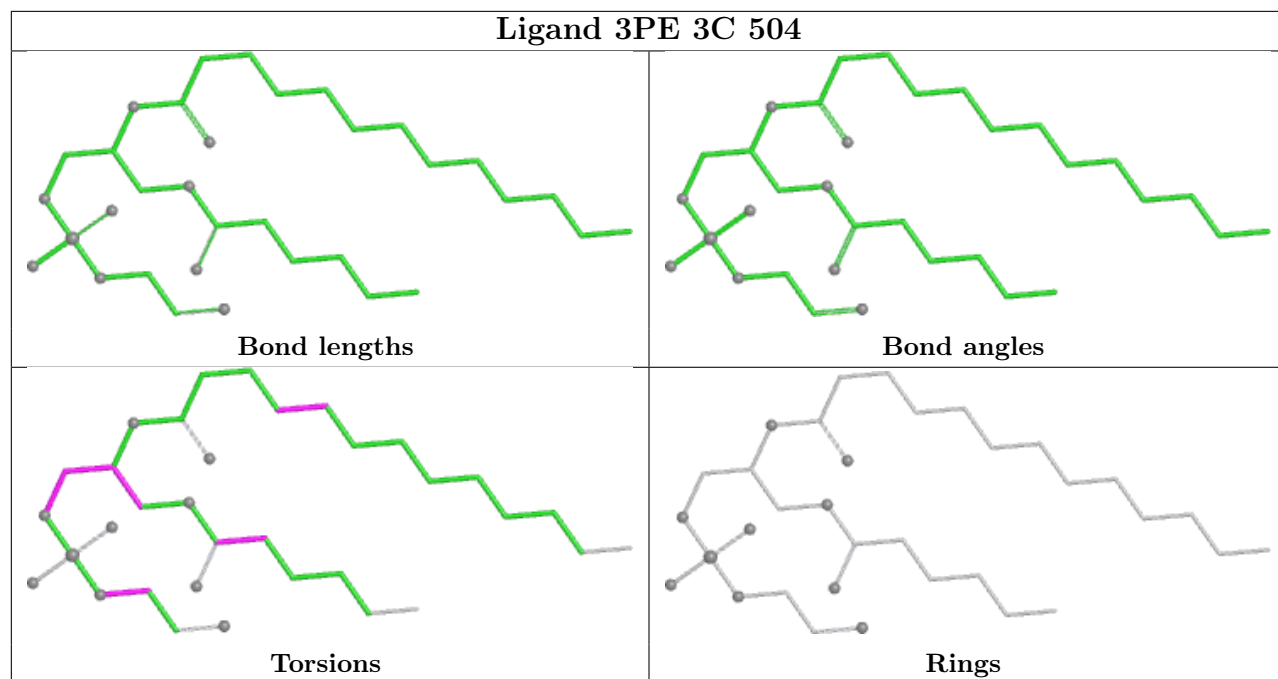


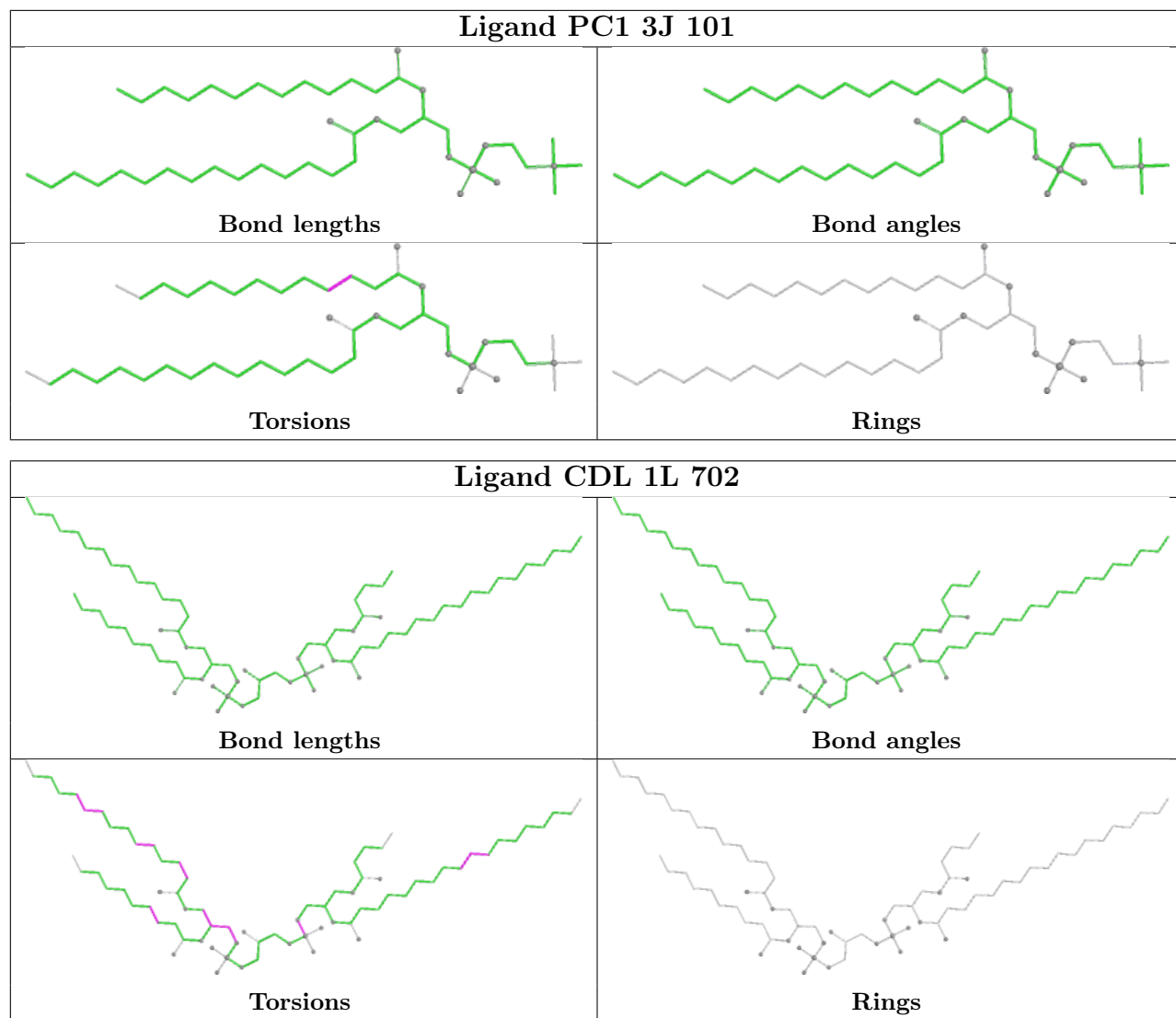


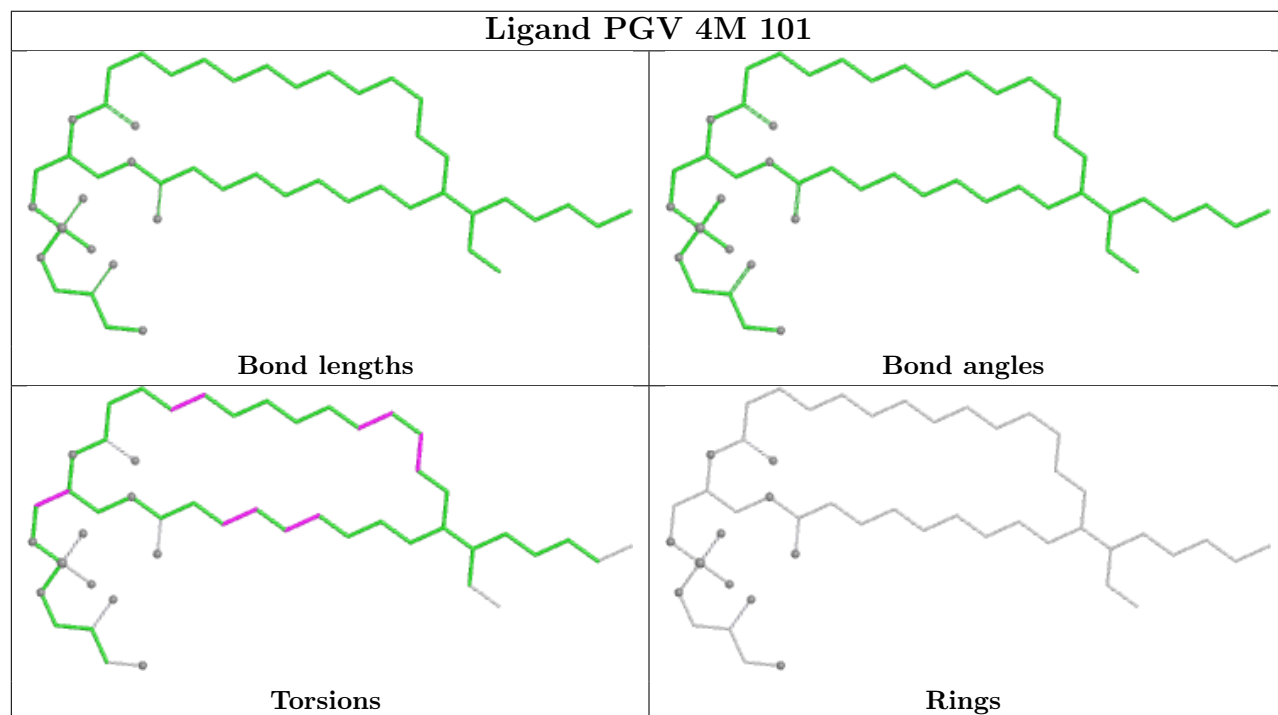
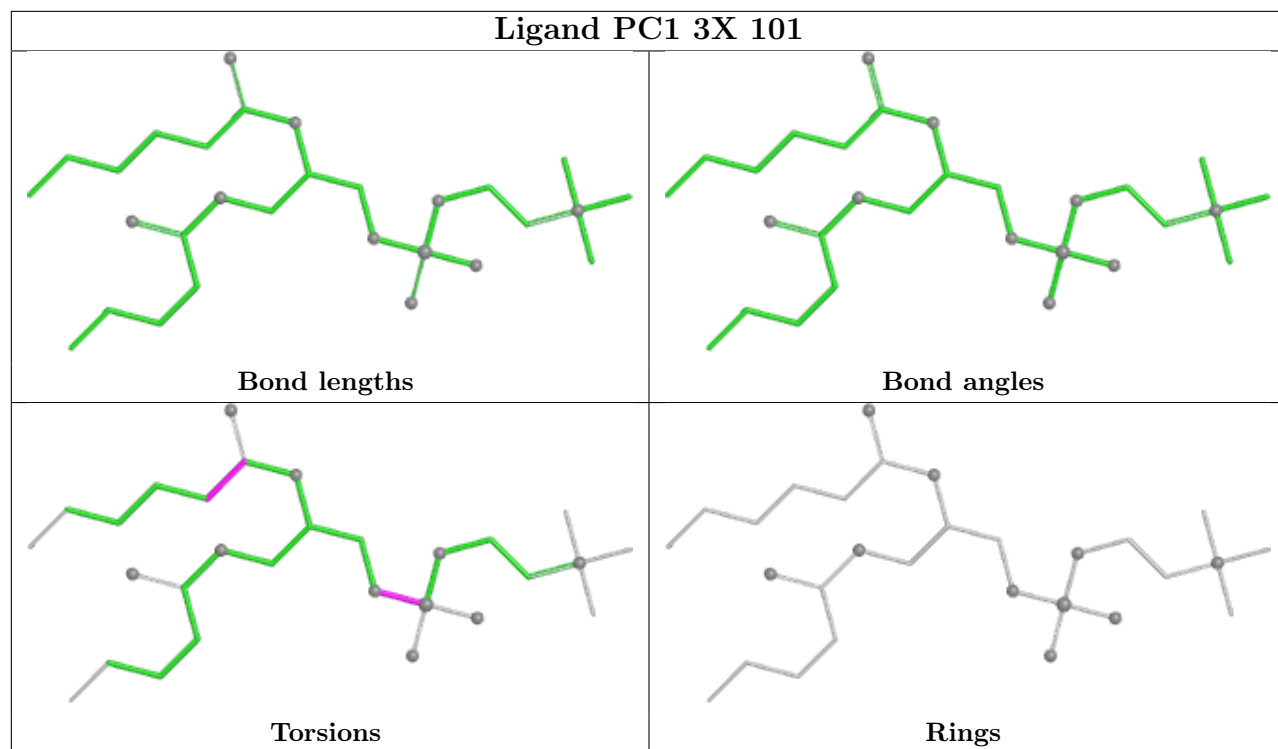


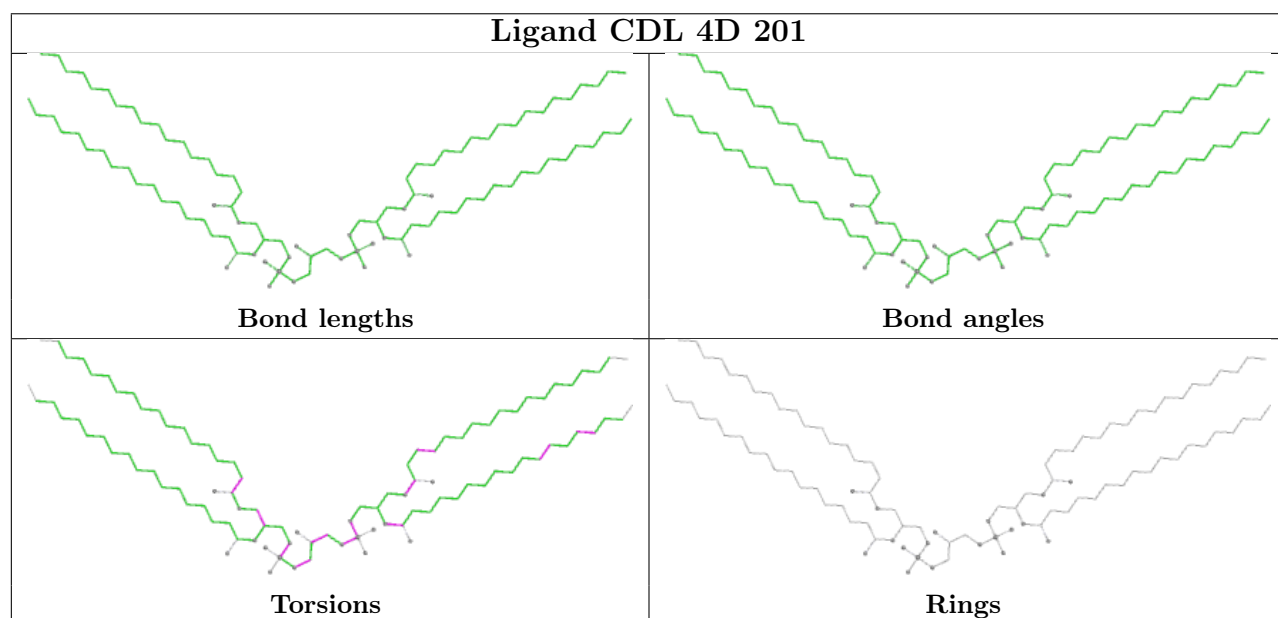
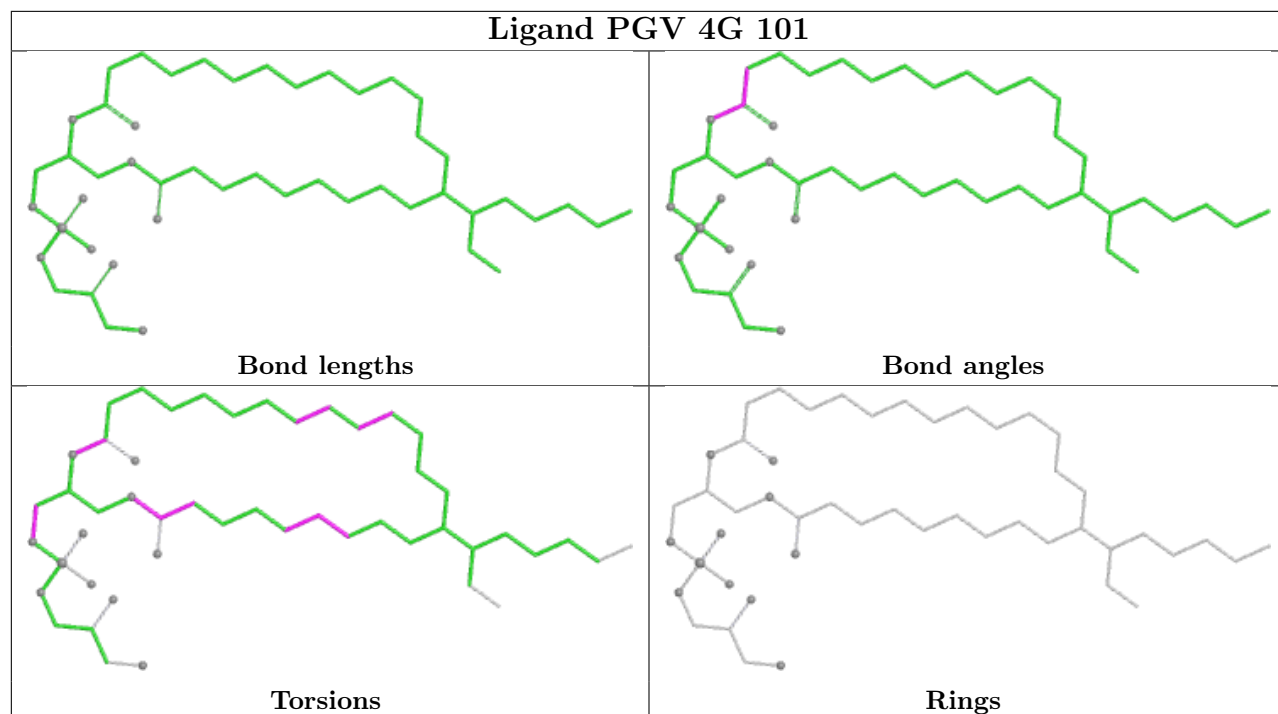


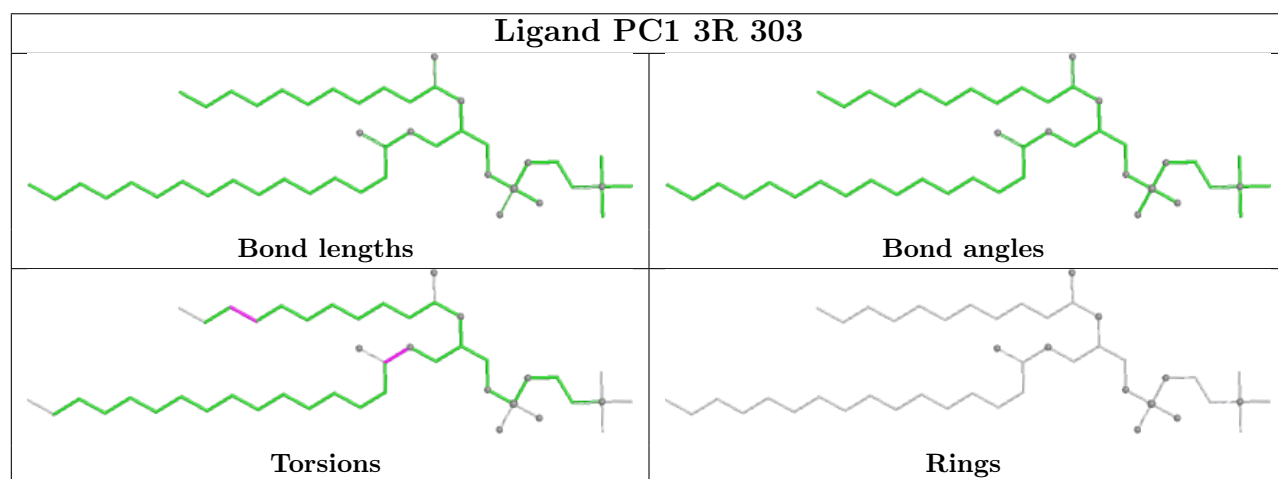
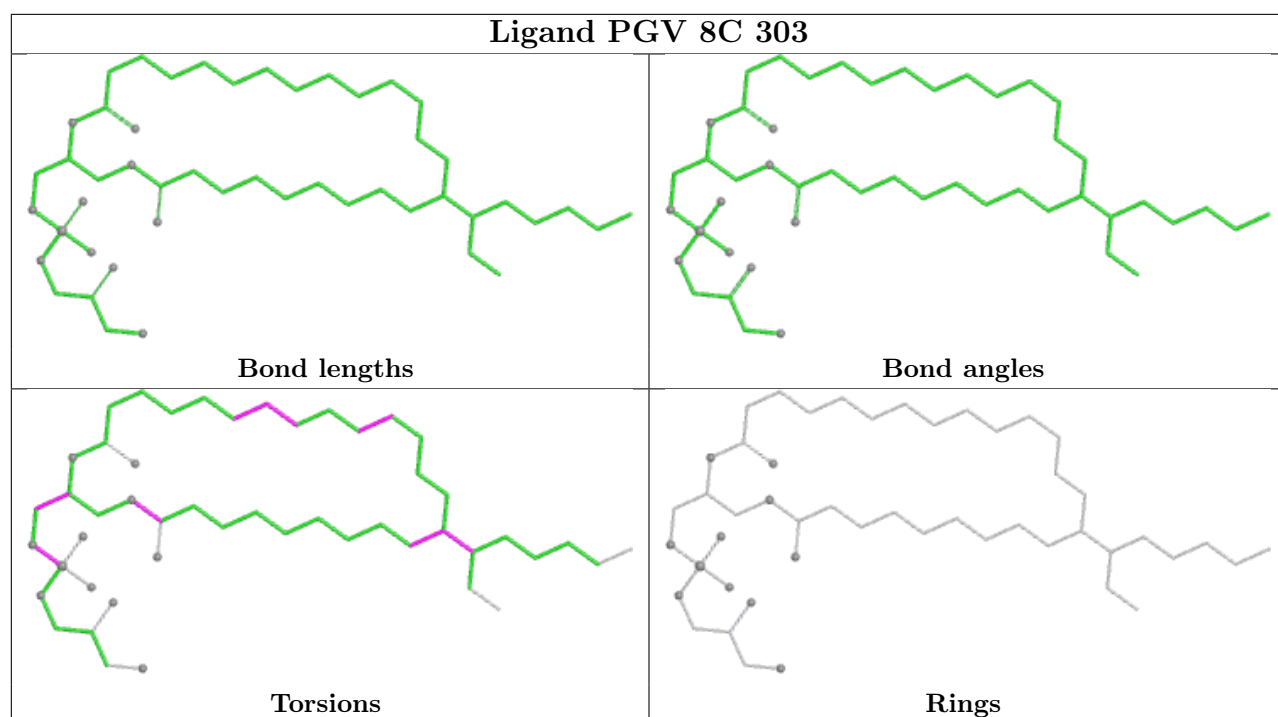




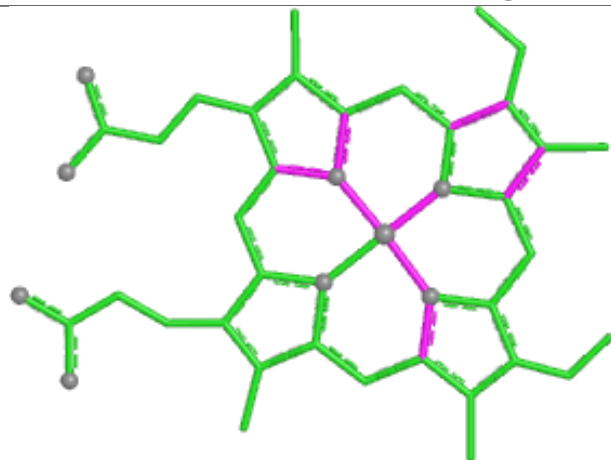




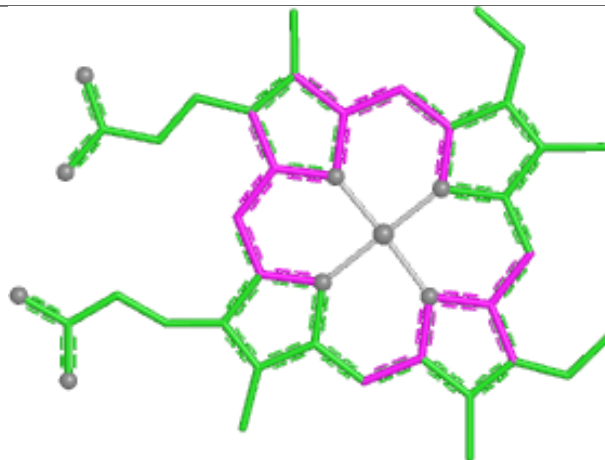




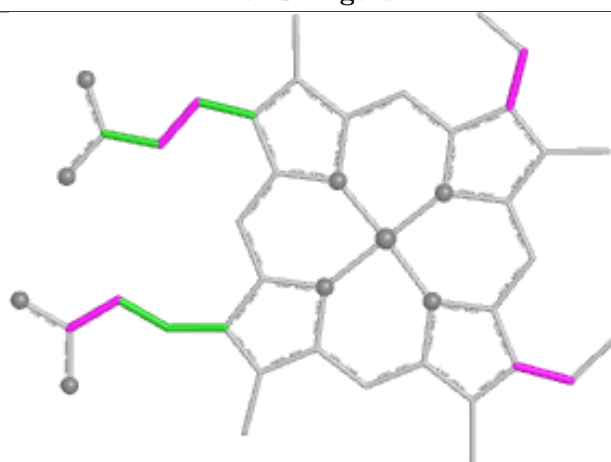
## Ligand HEM 3C 501



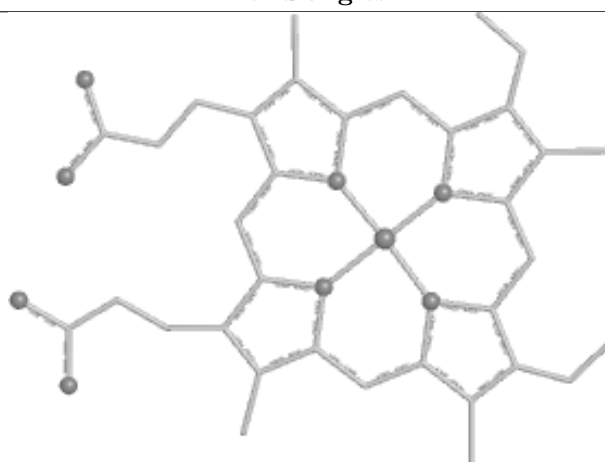
Bond lengths



Bond angles

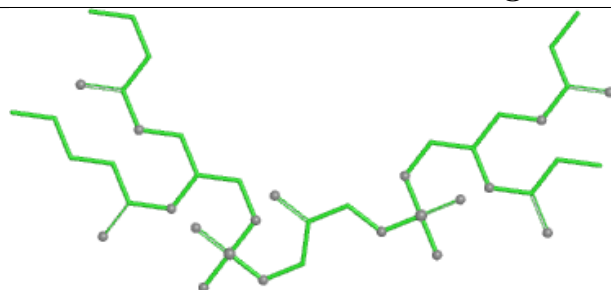


Torsions

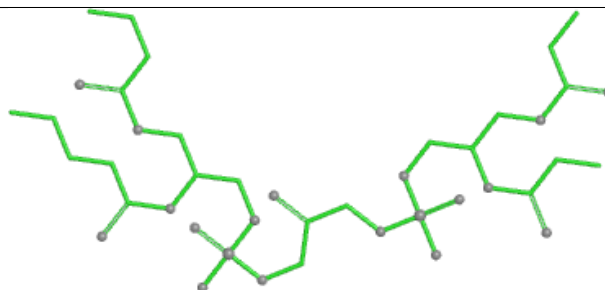


Rings

## Ligand CDL 3N 502



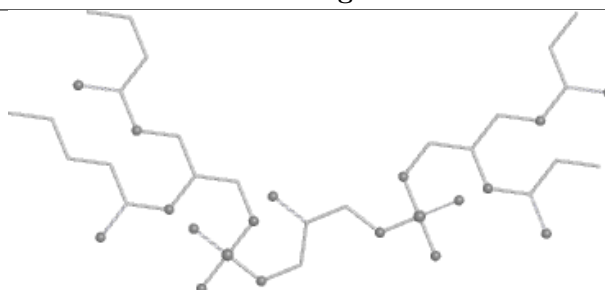
Bond lengths



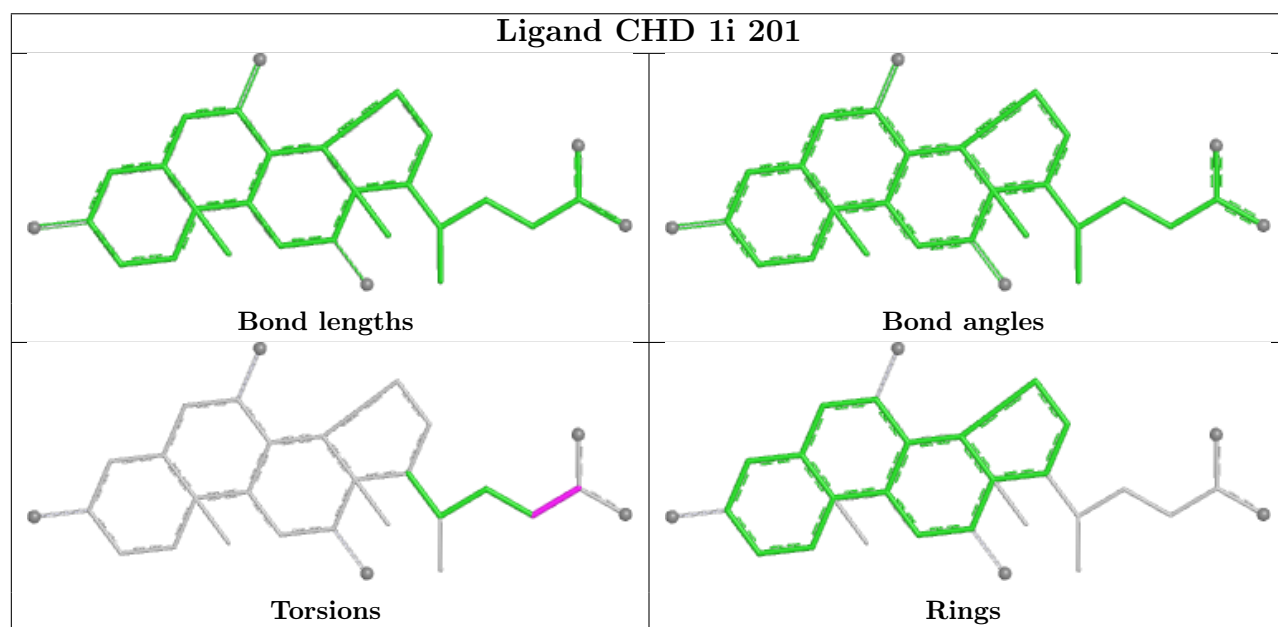
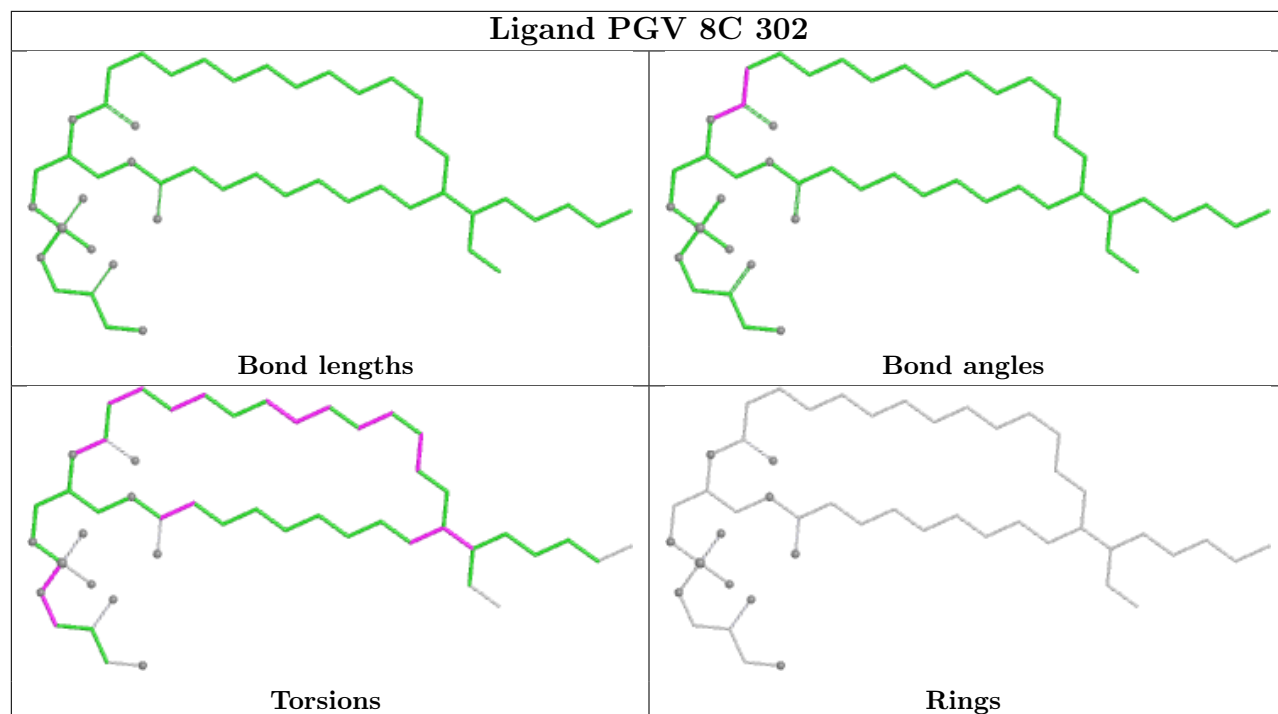
Bond angles

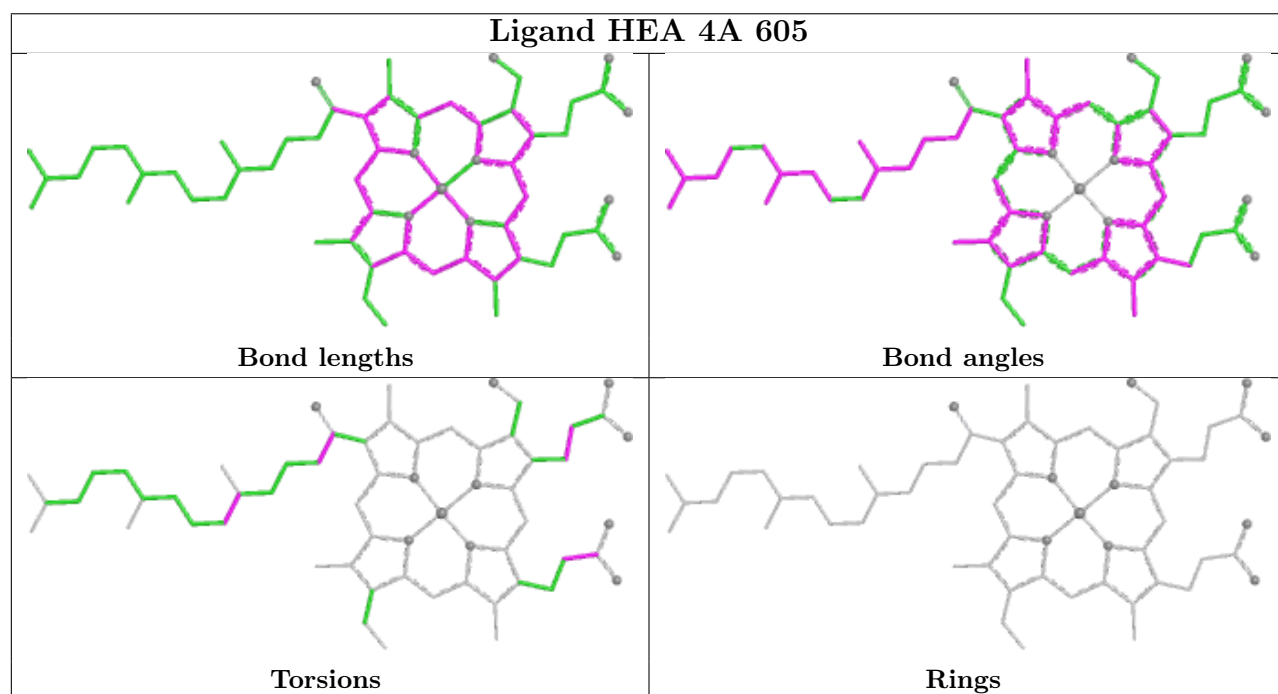
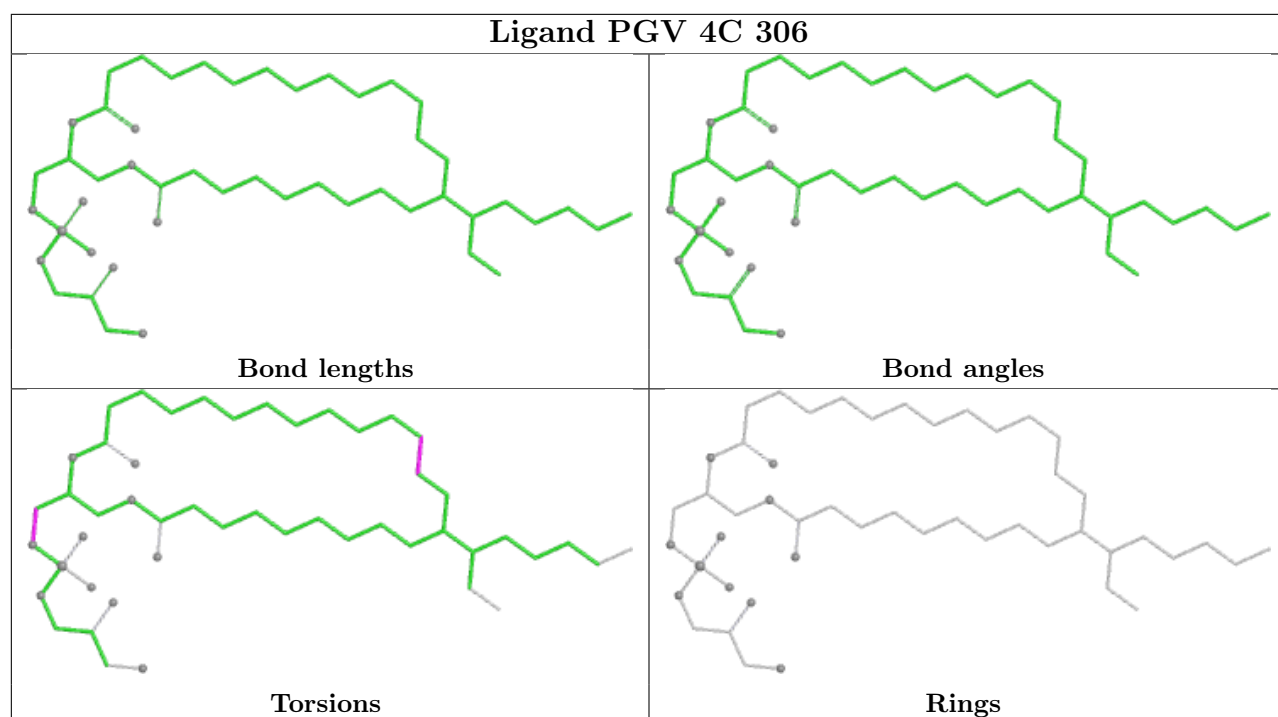


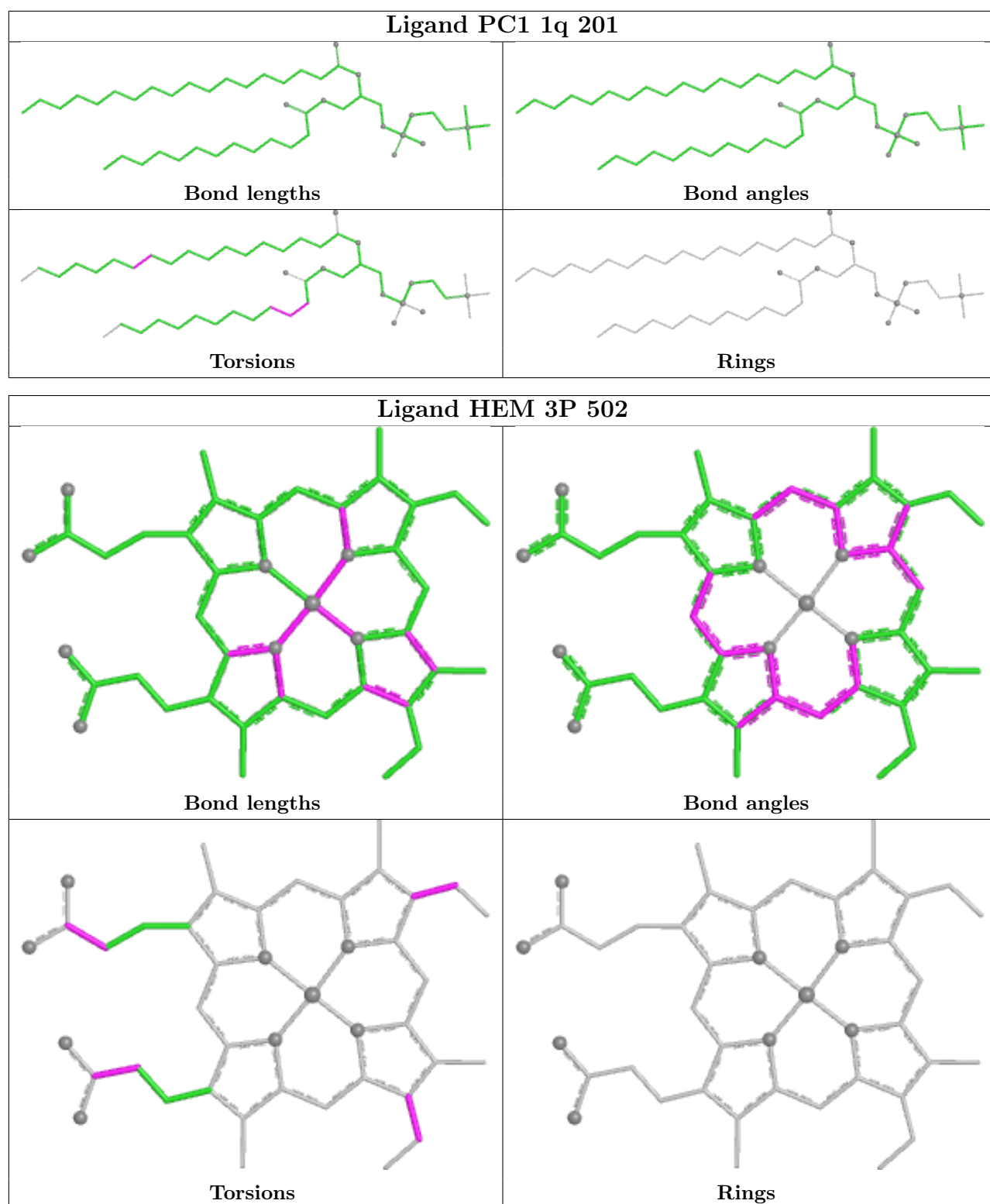
Torsions

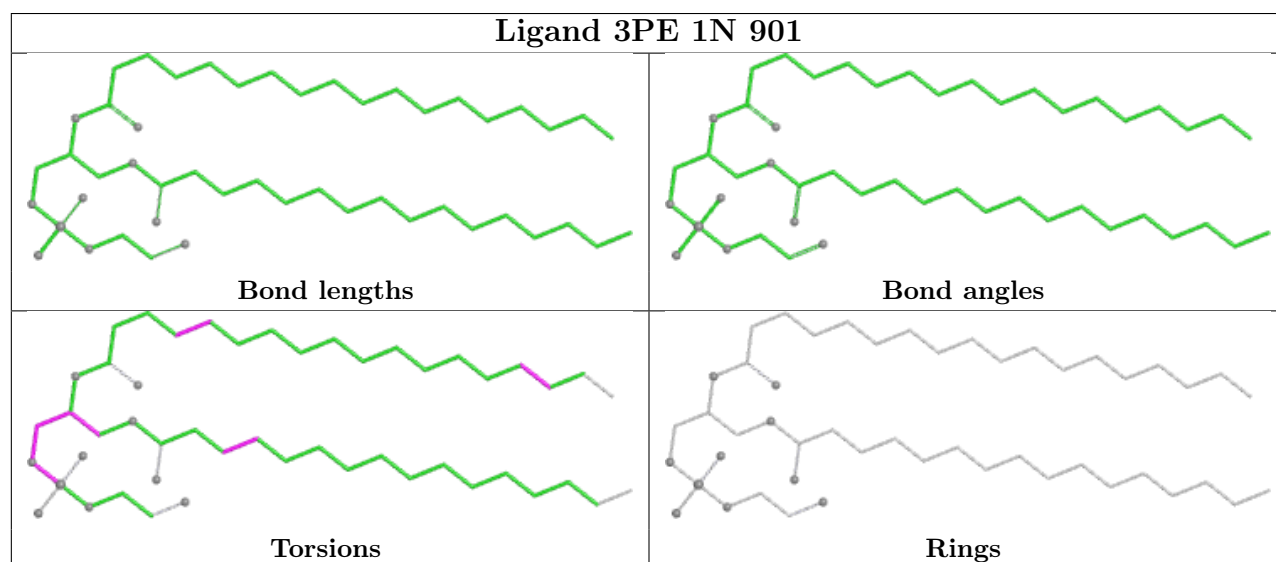
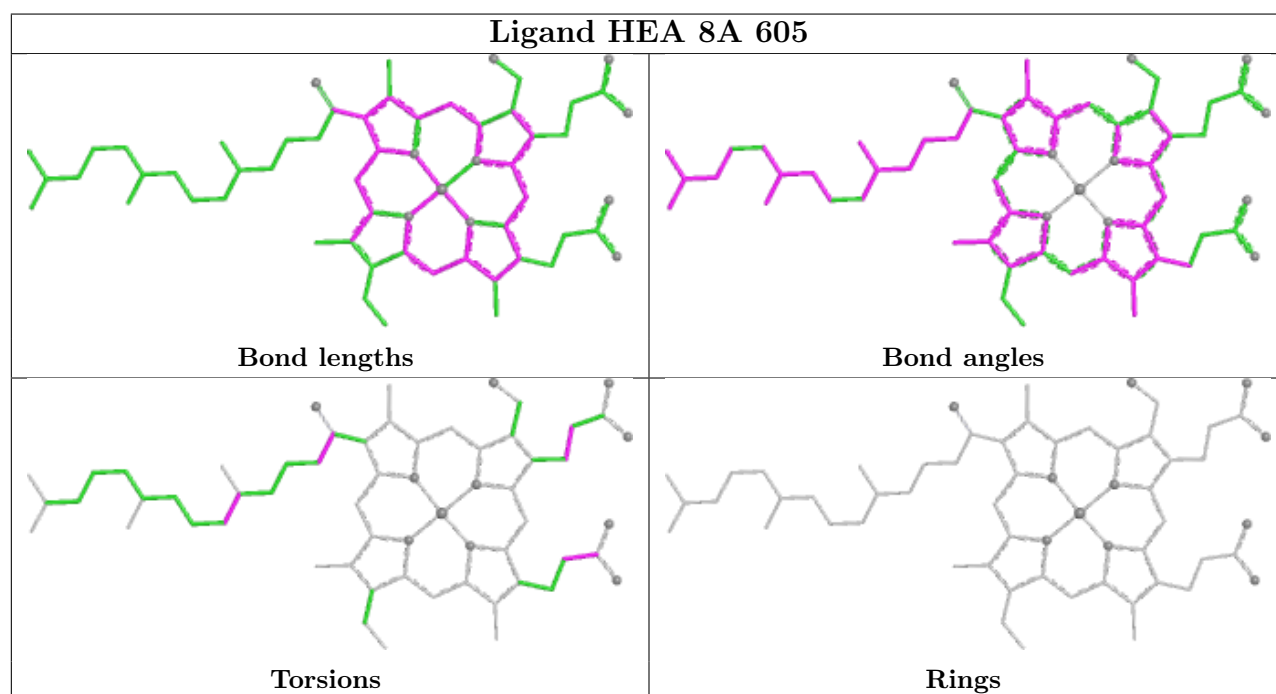
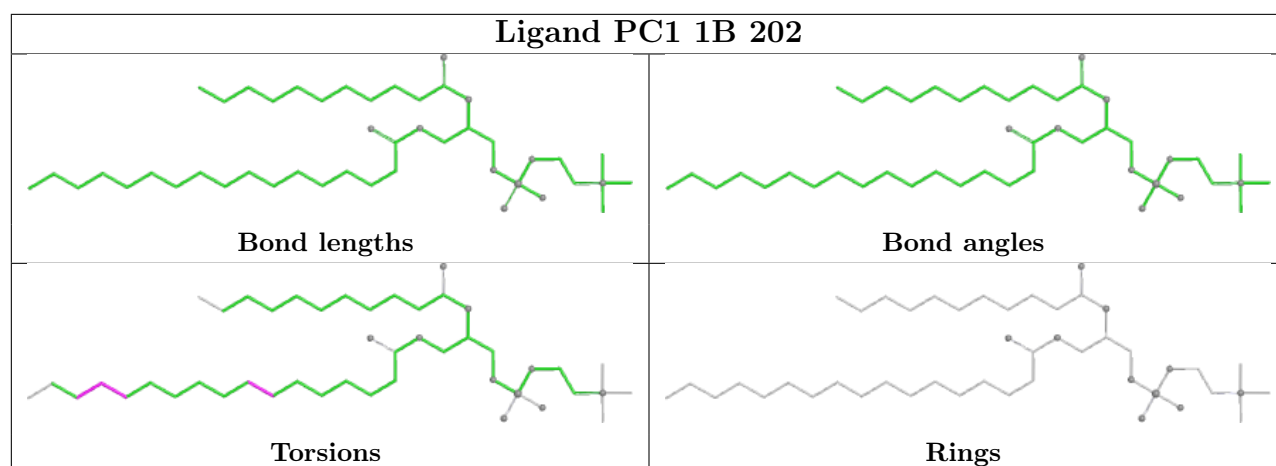


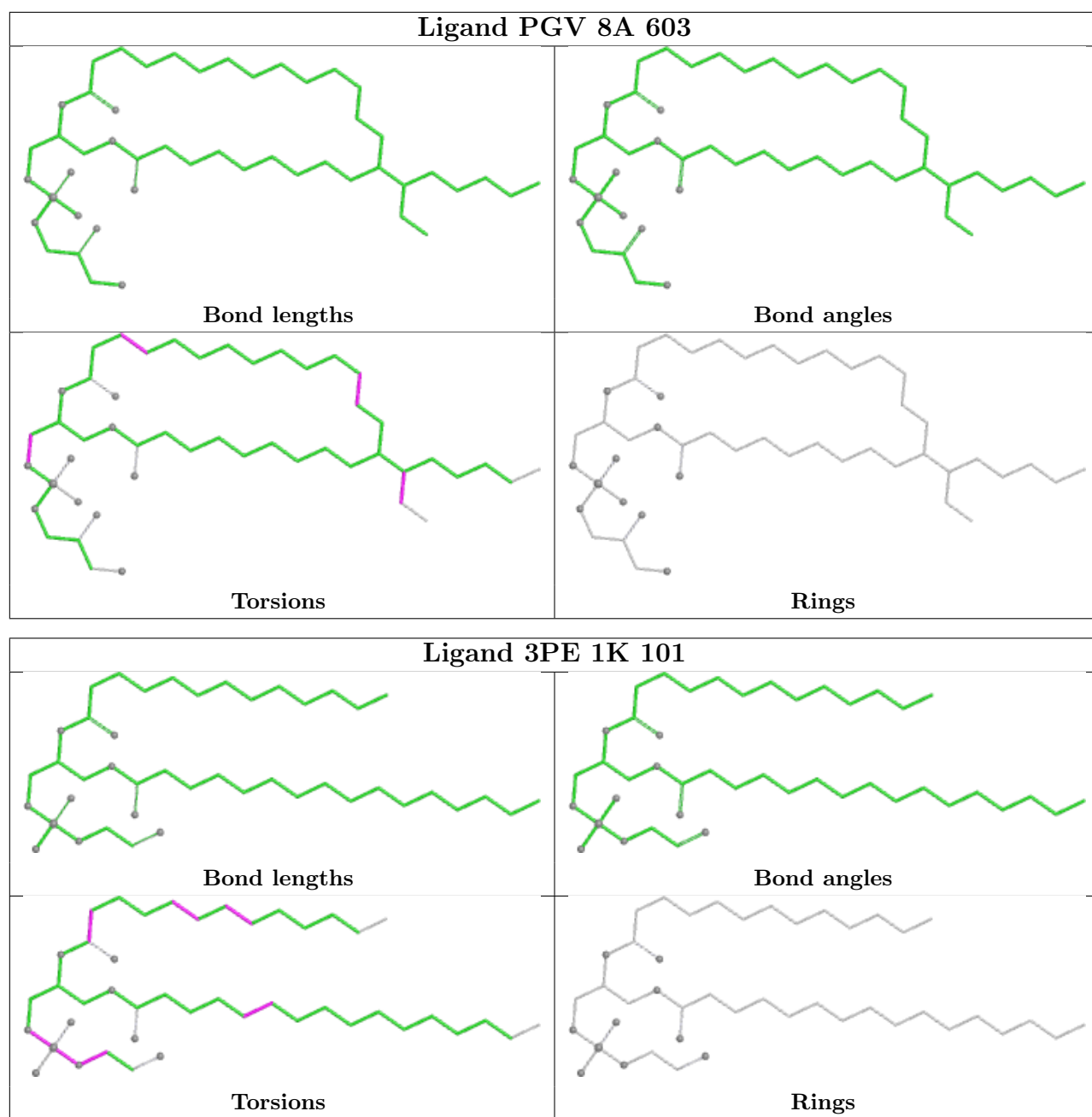
Rings

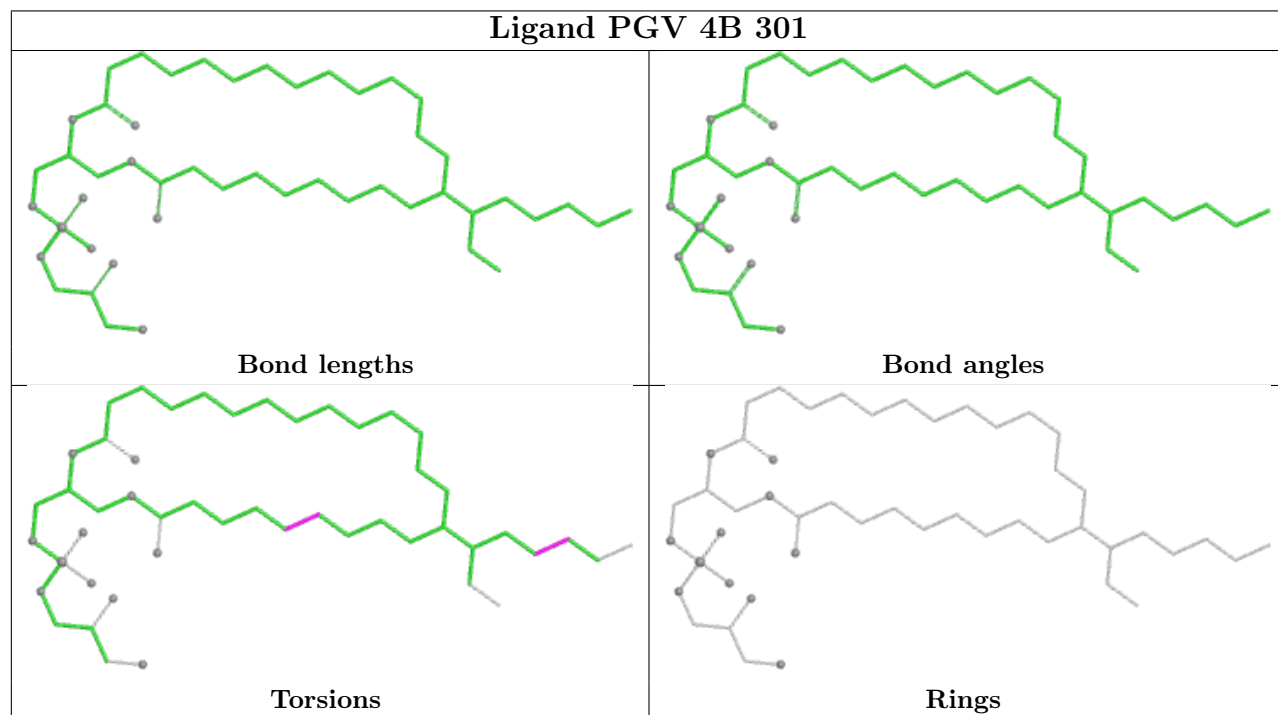
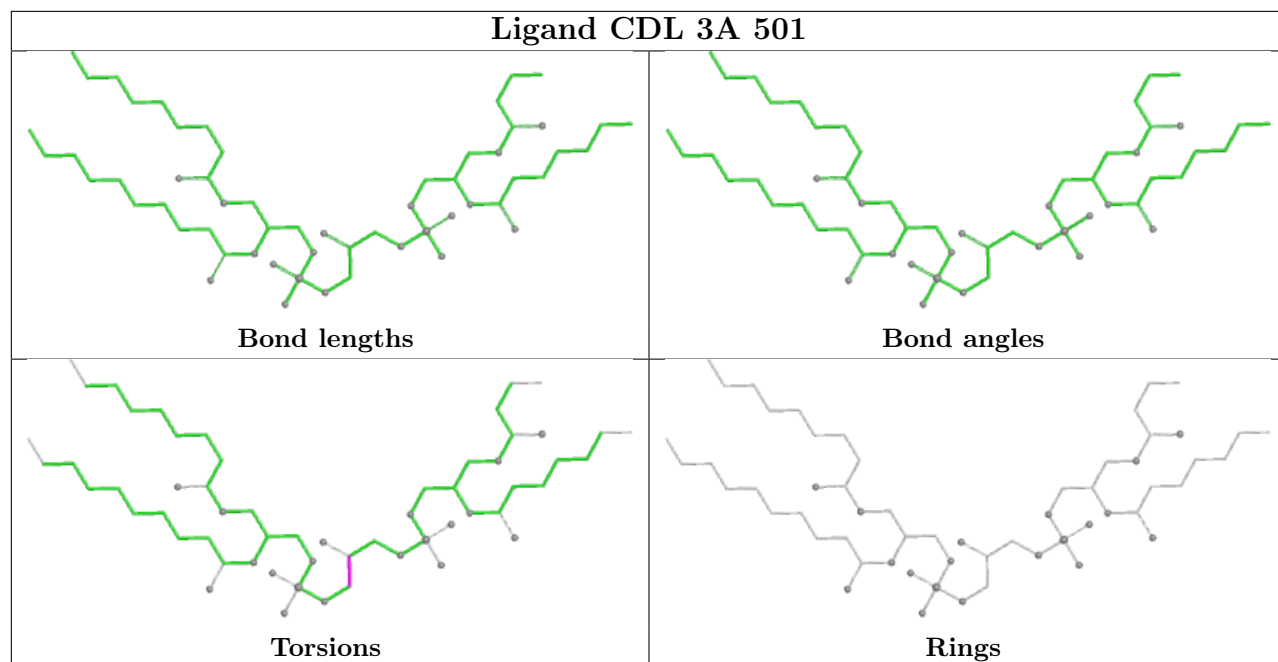


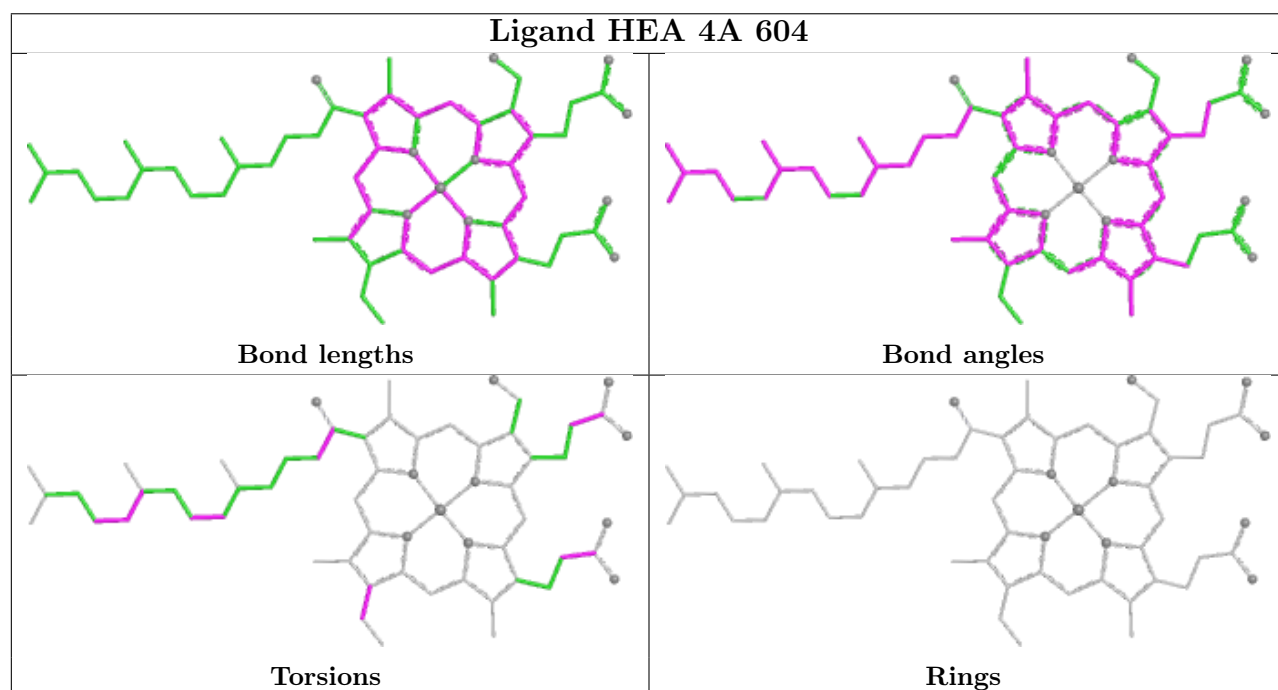
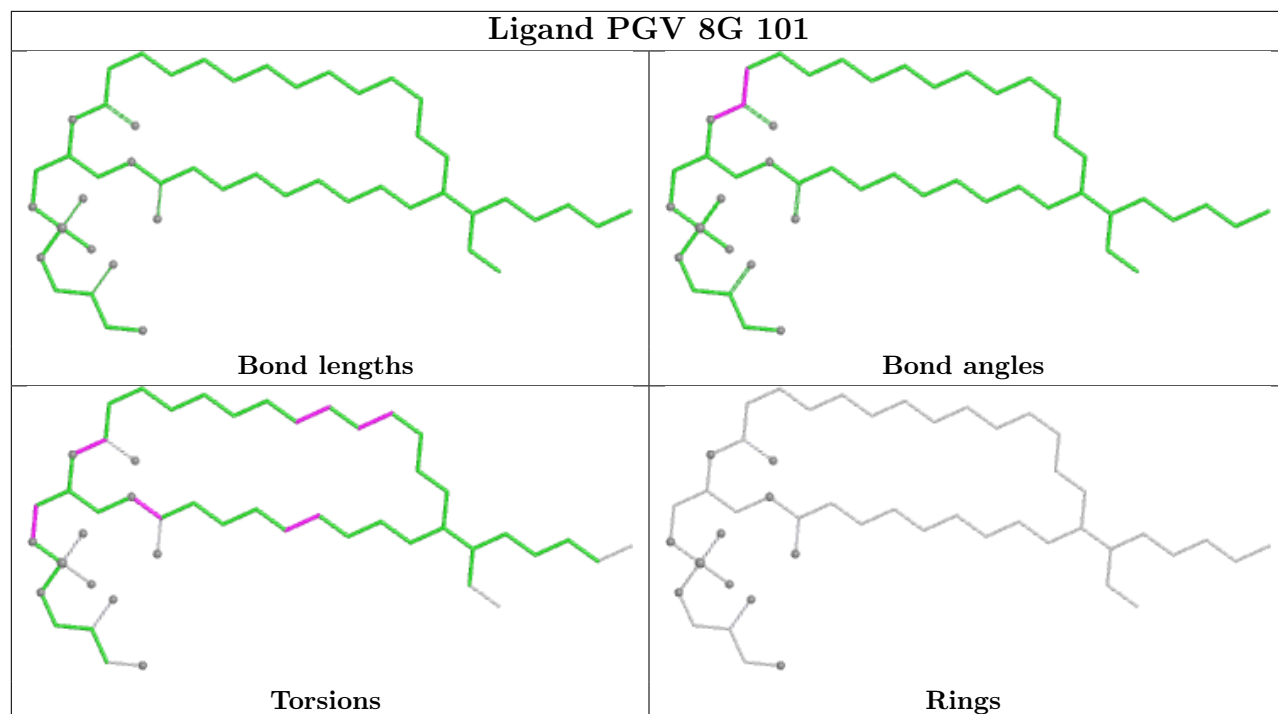


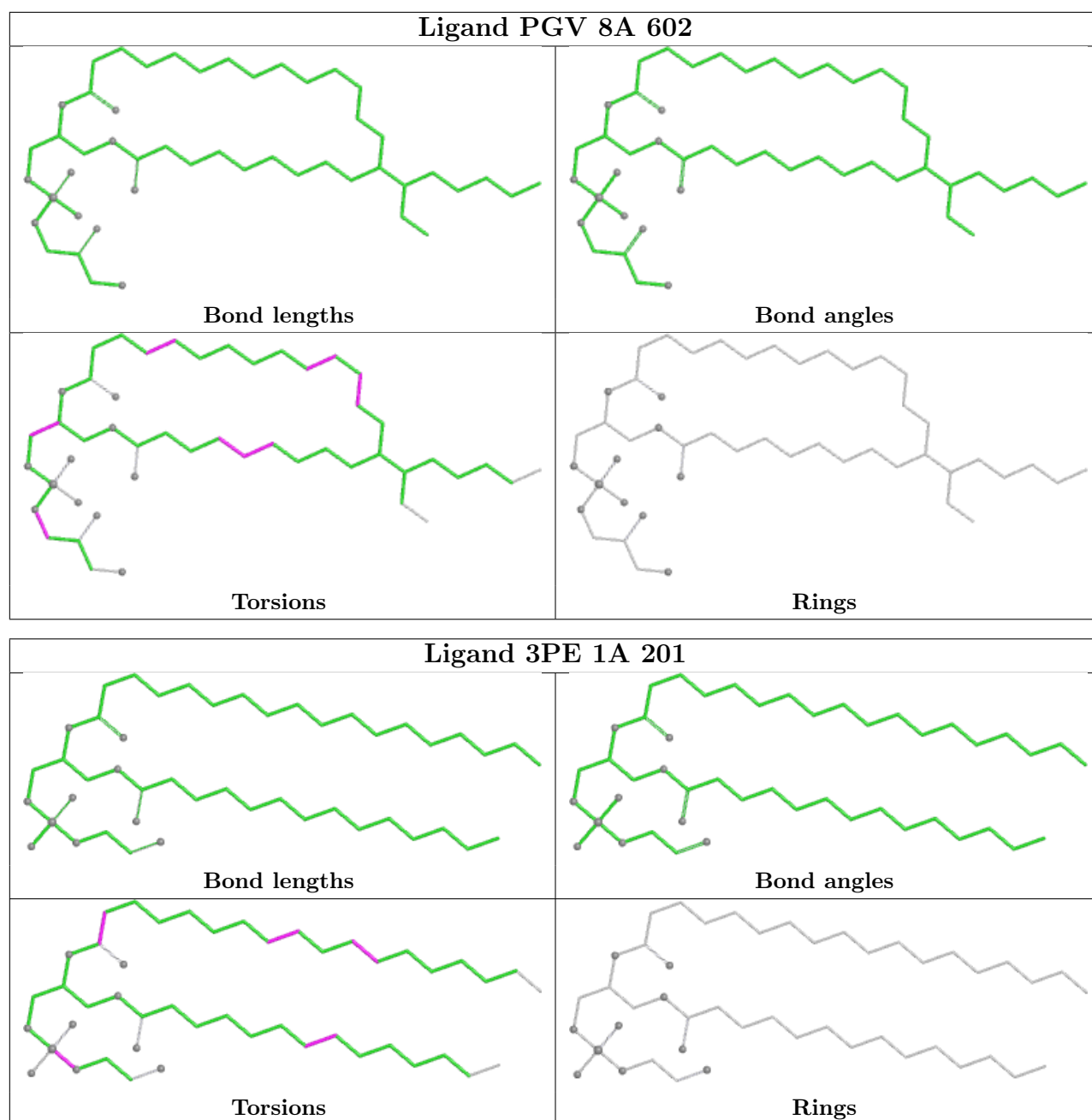


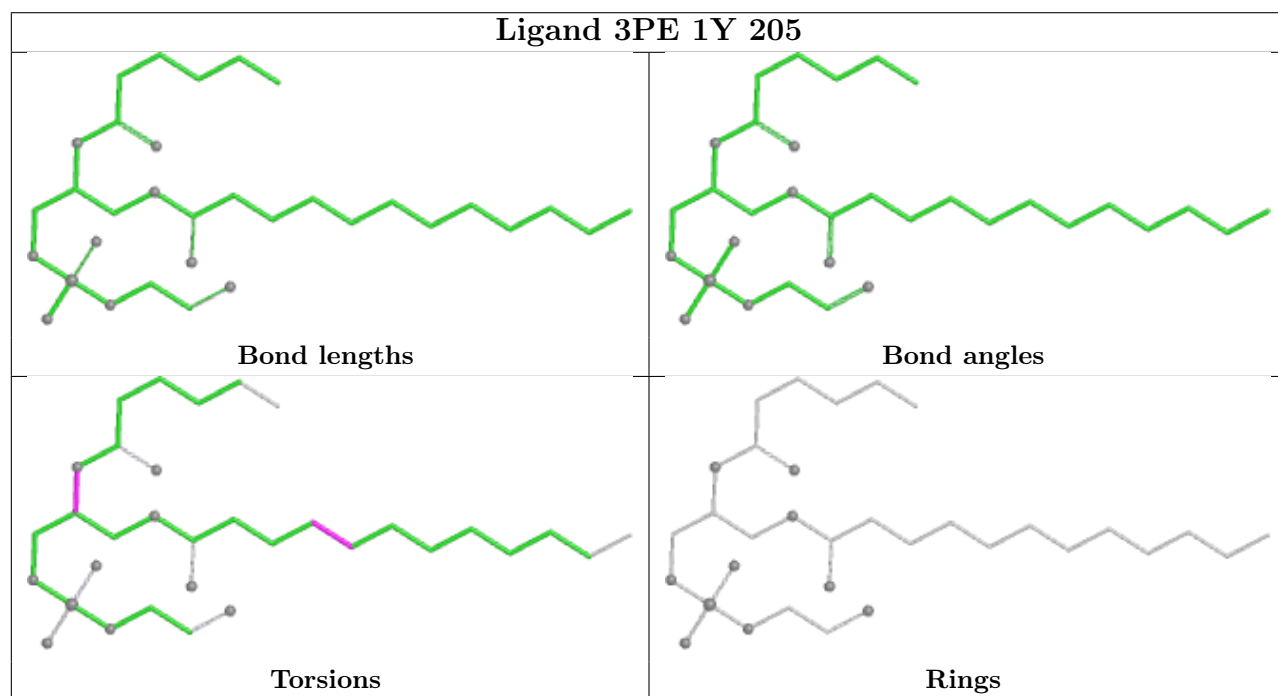
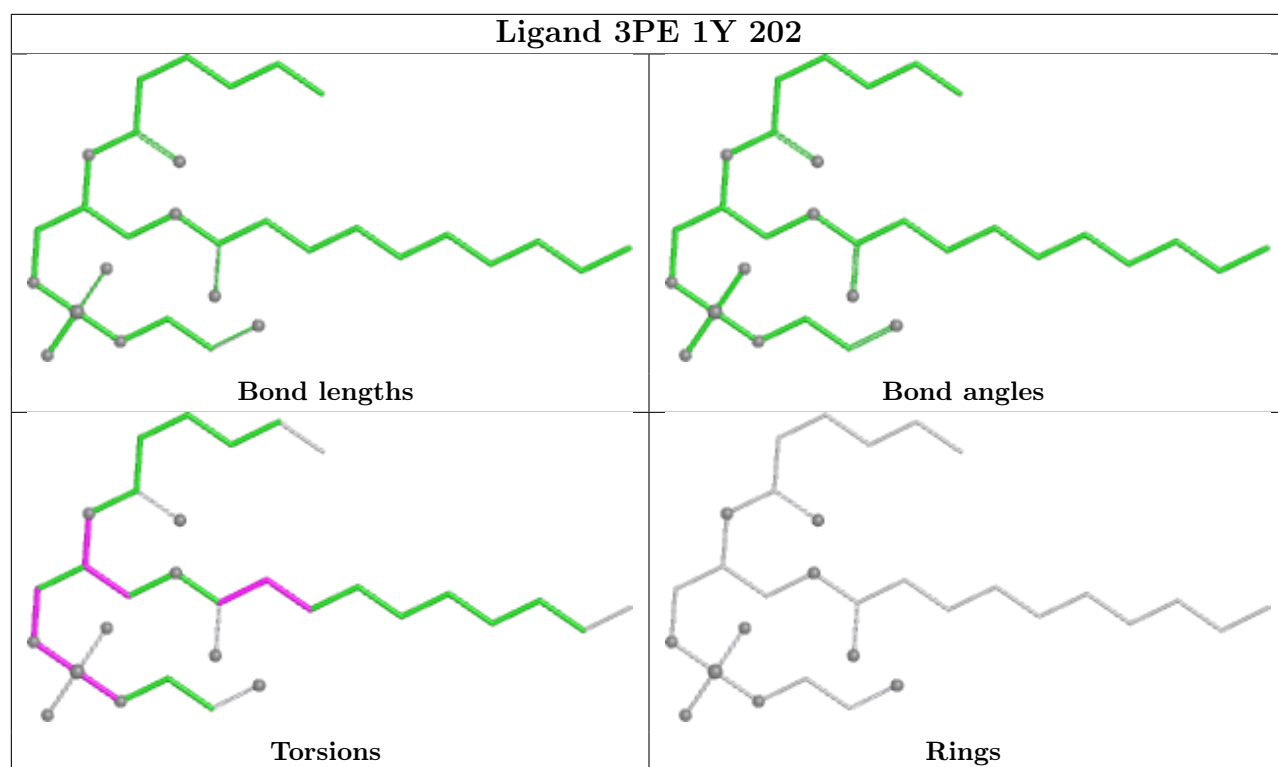




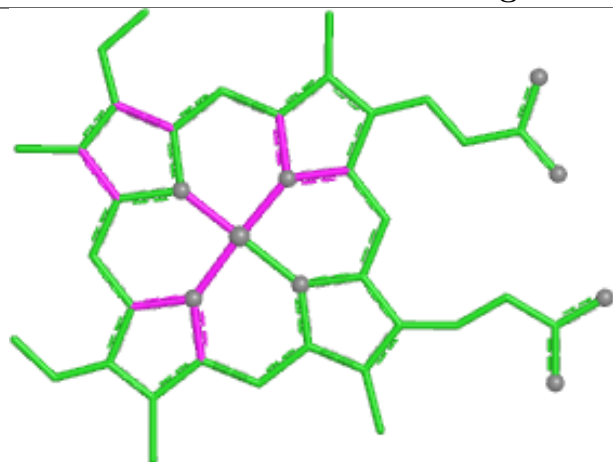




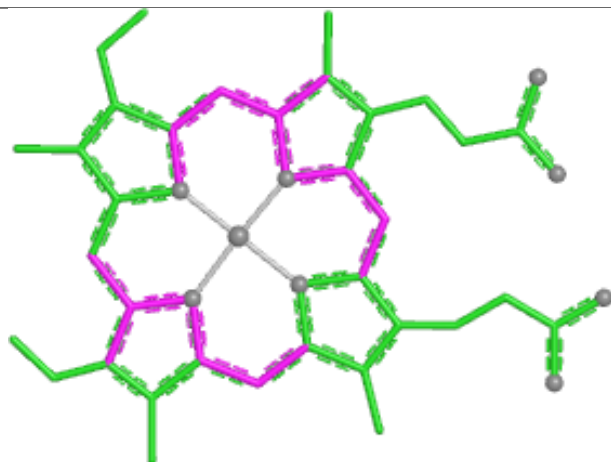




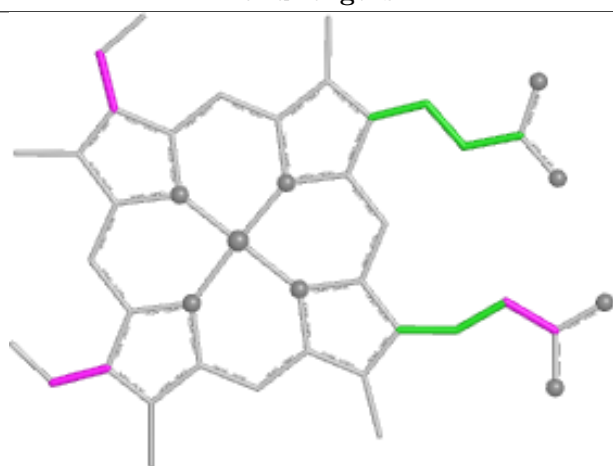
## Ligand HEM 3C 502



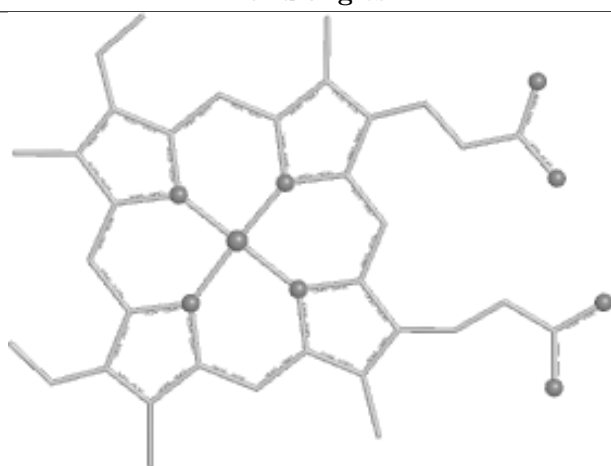
Bond lengths



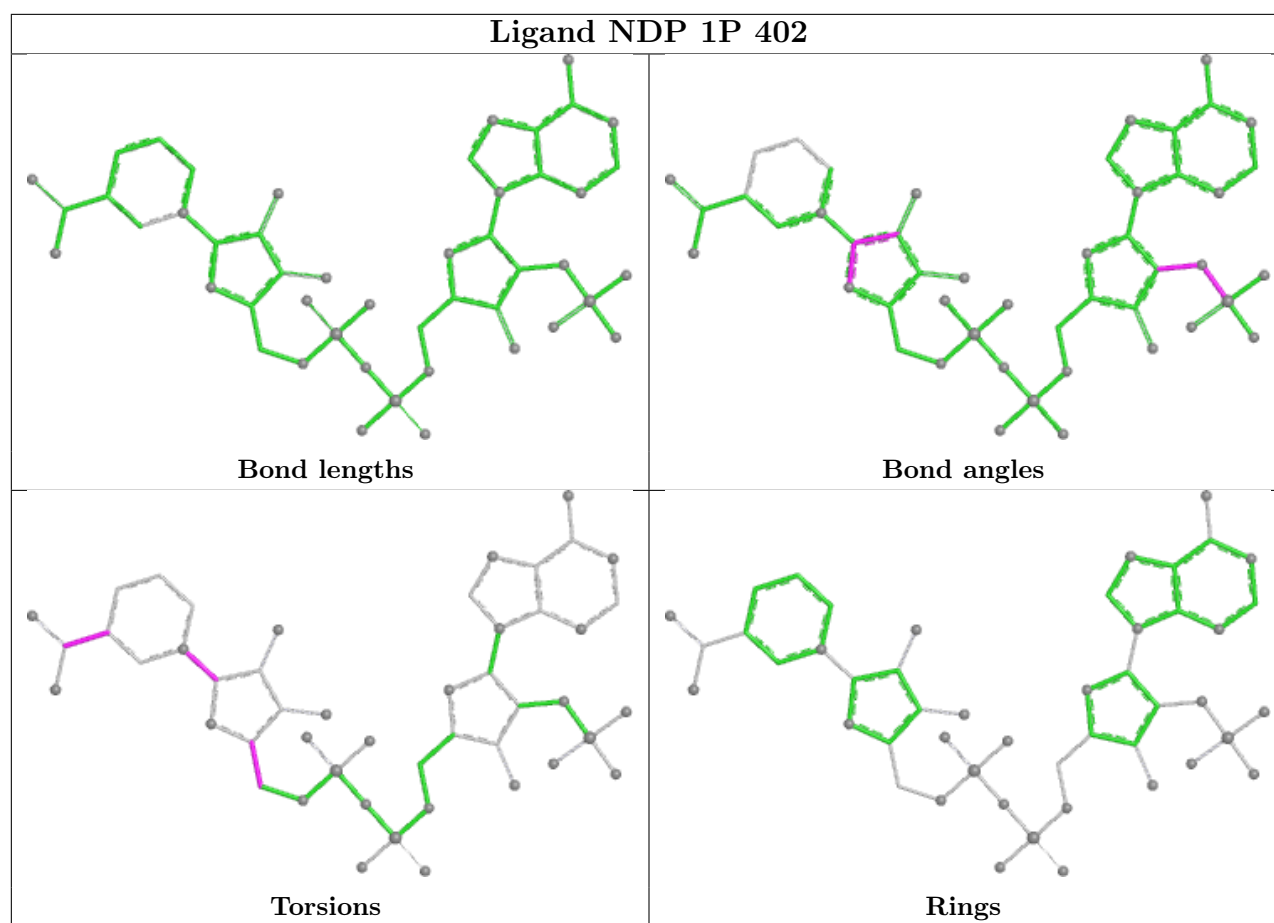
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 49  | 3V    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 3V    | 49:VAL    | C      | 50:LEU    | N      | 1.69         |
| 1     | 3V    | 48:SER    | C      | 49:VAL    | N      | 1.19         |

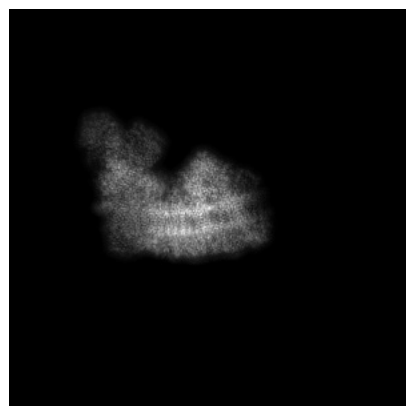
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42227. These allow visual inspection of the internal detail of the map and identification of artifacts.

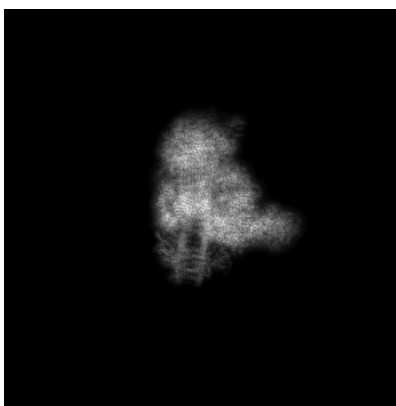
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

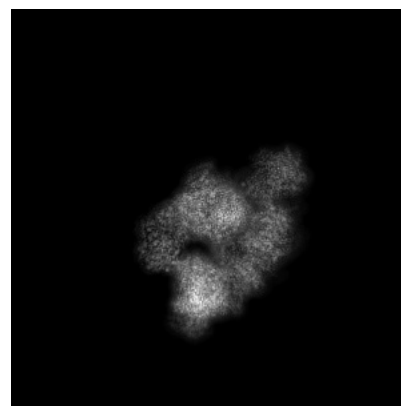
#### 6.1.1 Primary map



X

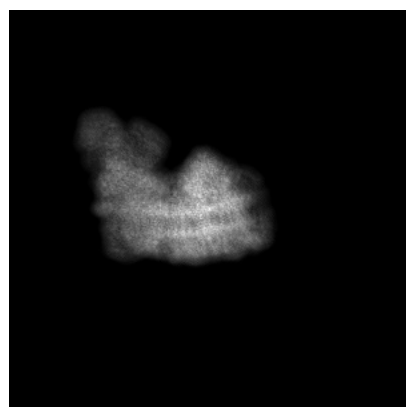


Y

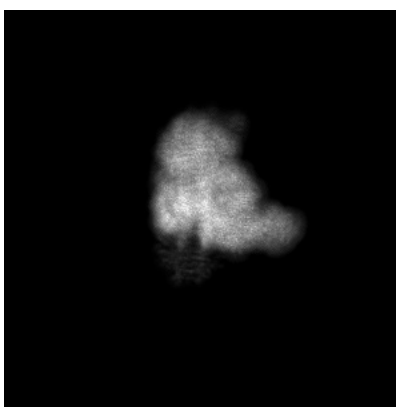


Z

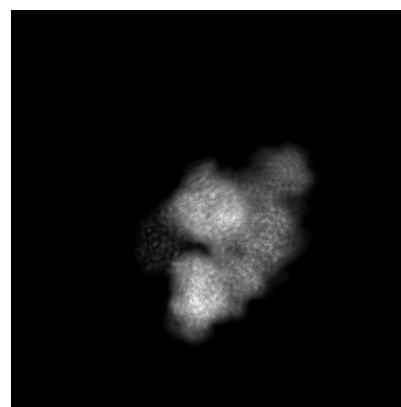
#### 6.1.2 Raw map



X



Y

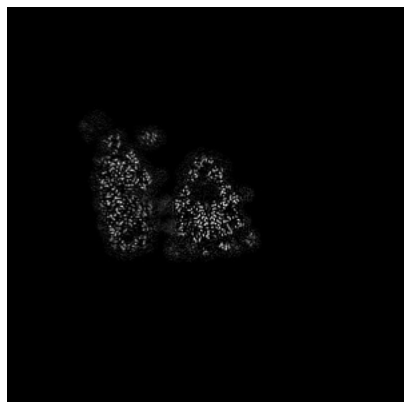


Z

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

## 6.2 Central slices [i](#)

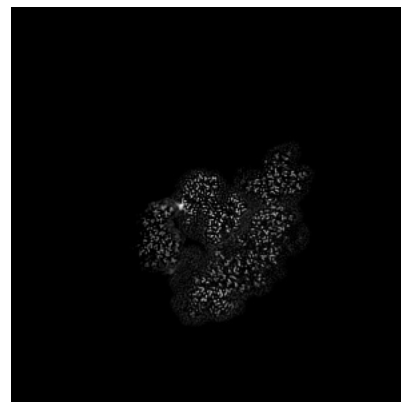
### 6.2.1 Primary map



X Index: 275

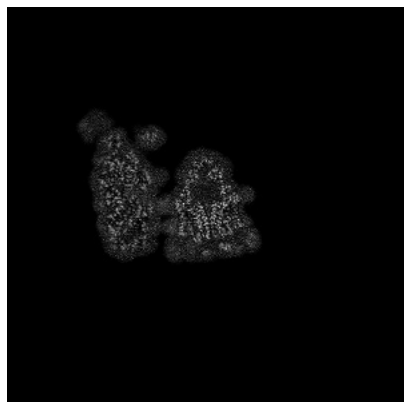


Y Index: 275

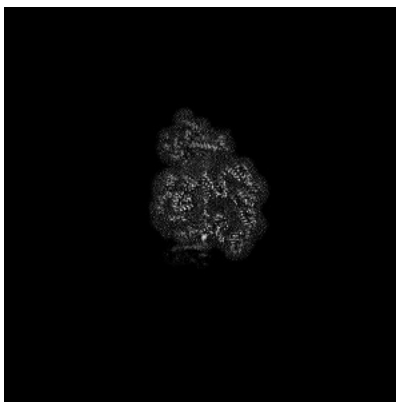


Z Index: 275

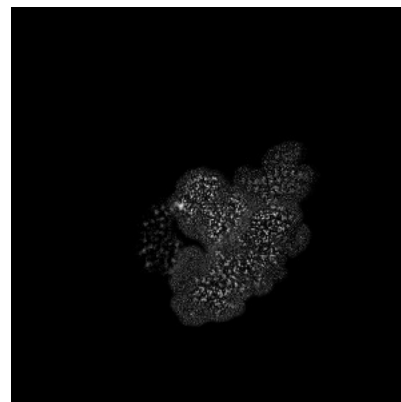
### 6.2.2 Raw map



X Index: 275



Y Index: 275

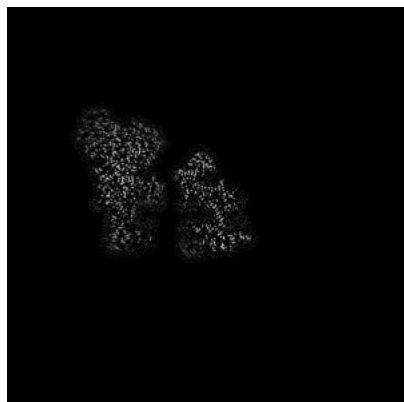


Z Index: 275

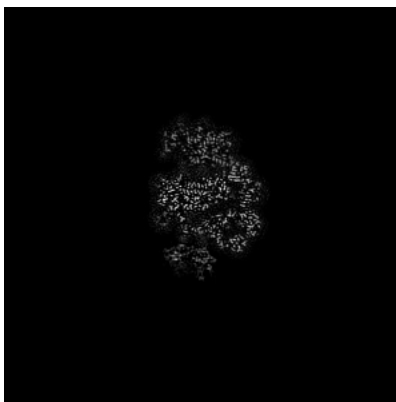
The images above show central slices of the map in three orthogonal directions.

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

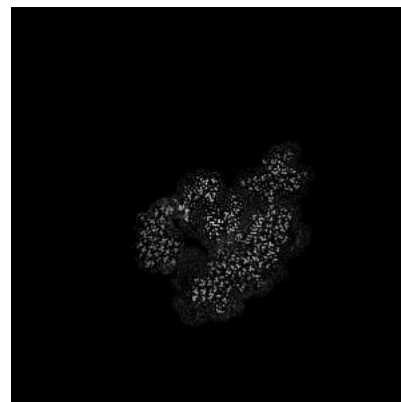
### 6.3.1 Primary map



X Index: 256

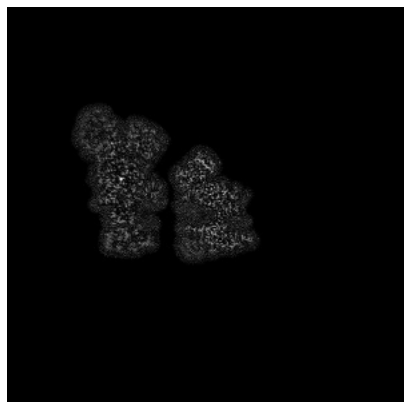


Y Index: 264

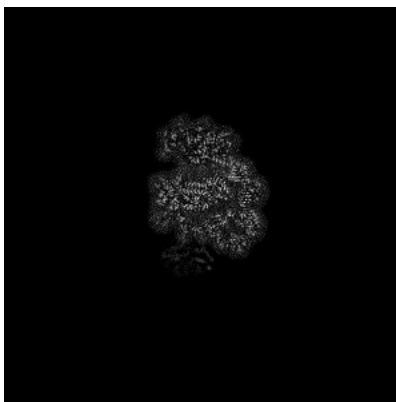


Z Index: 272

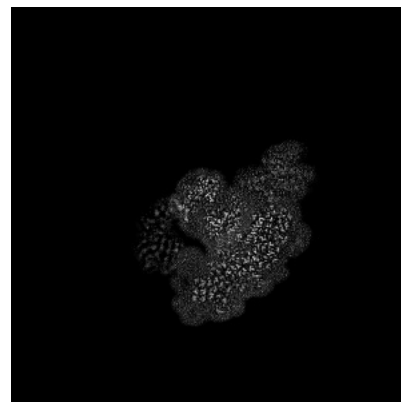
### 6.3.2 Raw map



X Index: 260



Y Index: 264

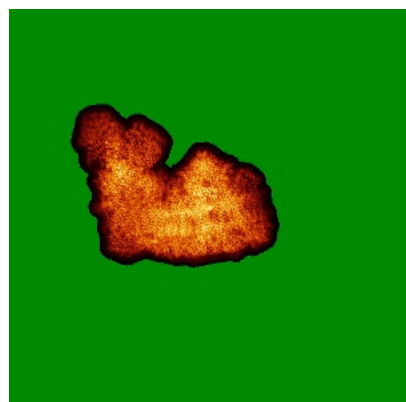


Z Index: 272

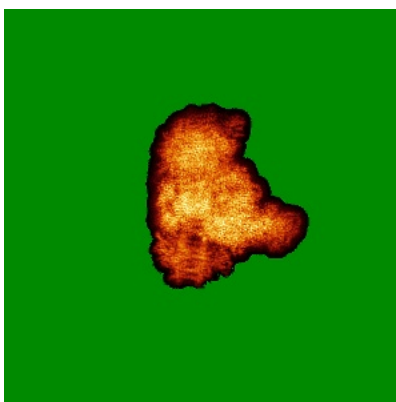
The images above show the largest variance slices of the map in three orthogonal directions.

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

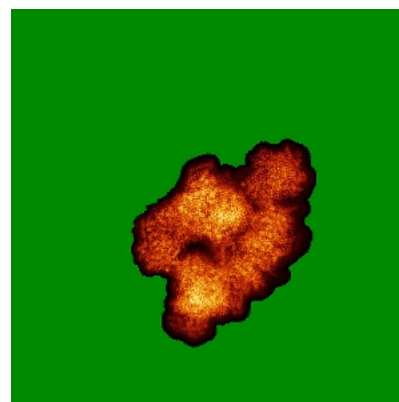
### 6.4.1 Primary map



X

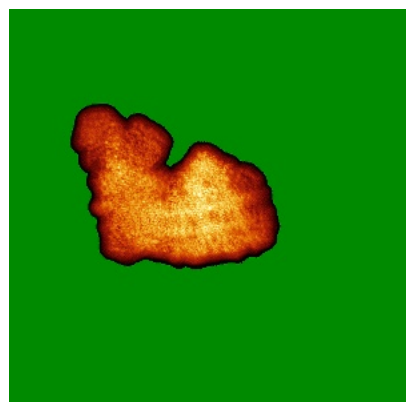


Y

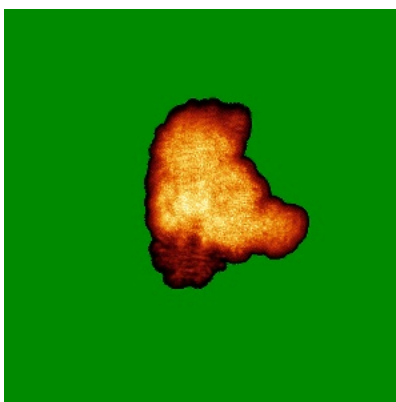


Z

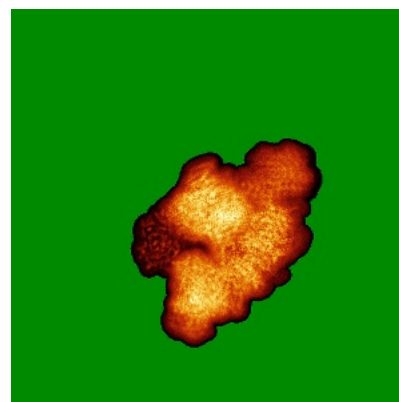
### 6.4.2 Raw map



X



Y

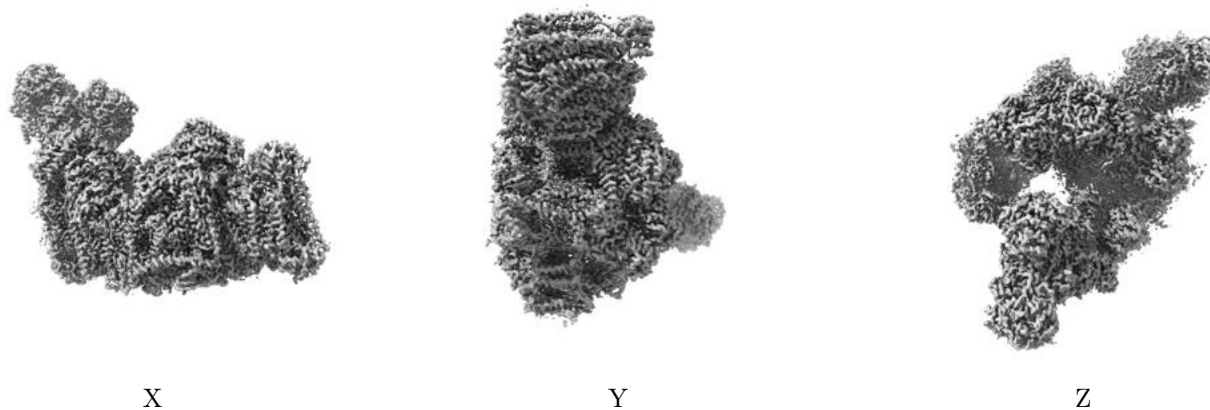


Z

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

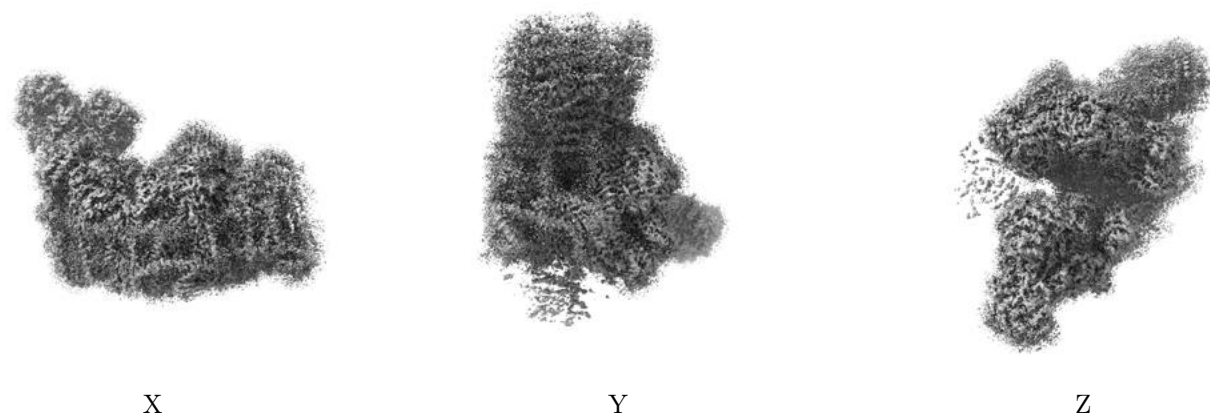
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

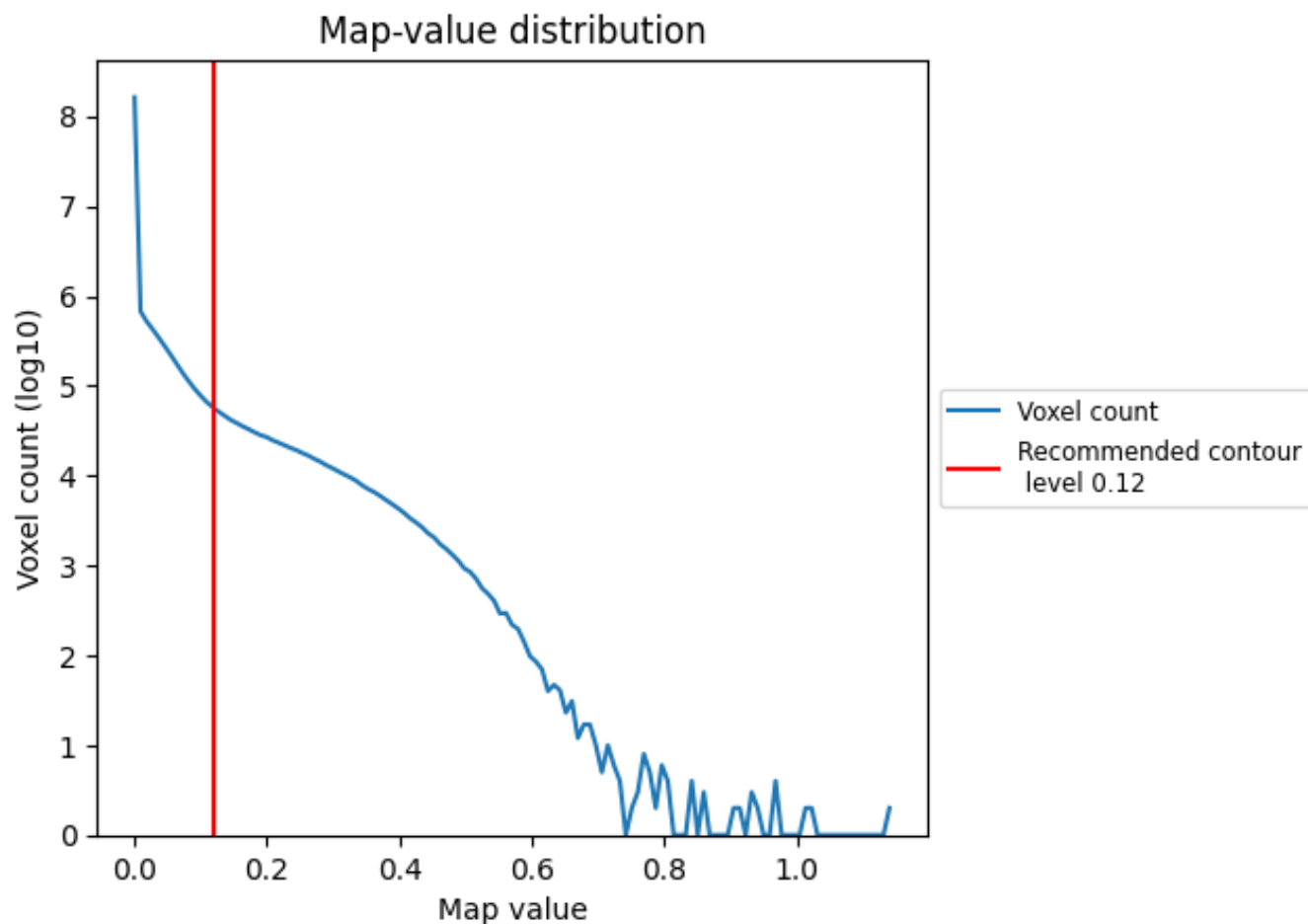
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

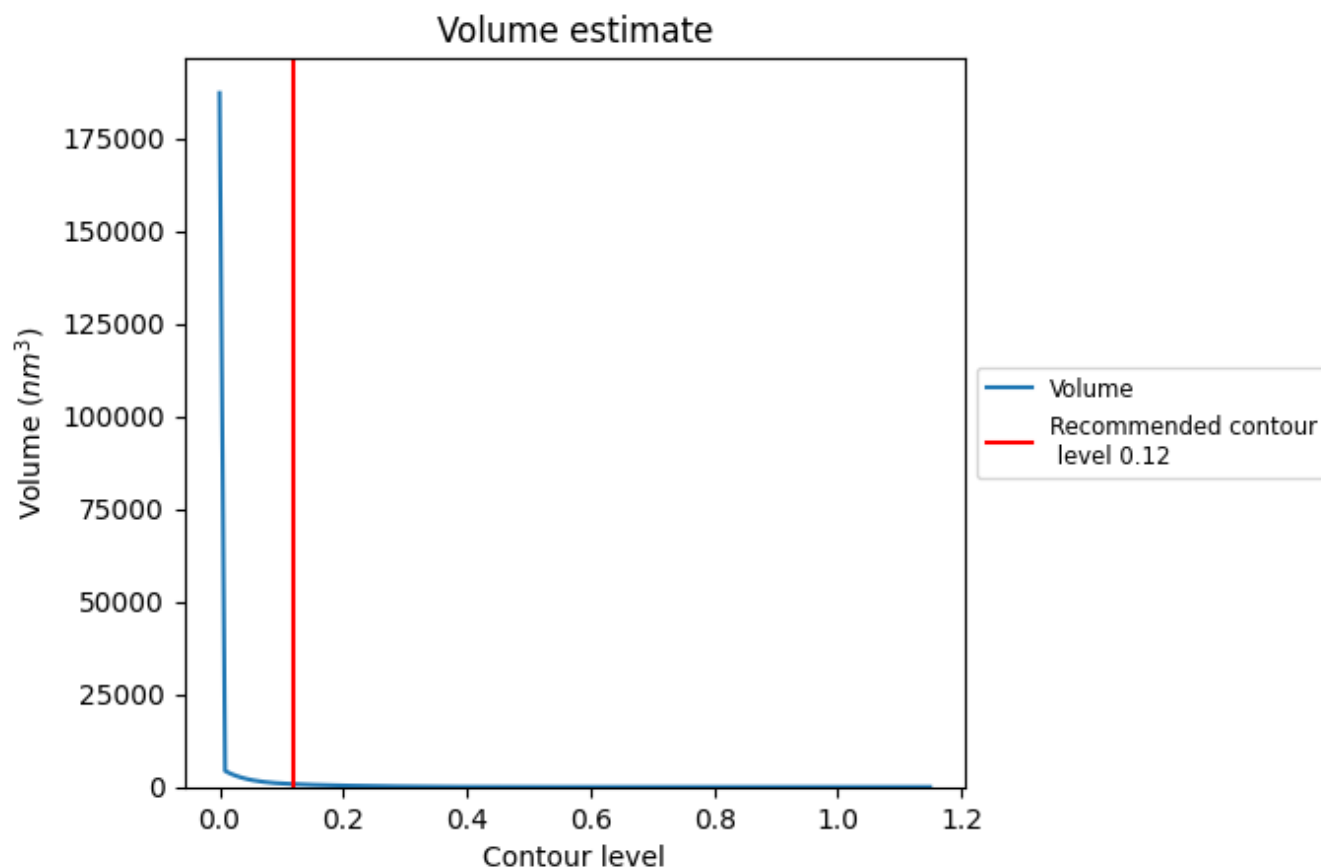
This section contains the results of statistical analysis of the map.

### 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.

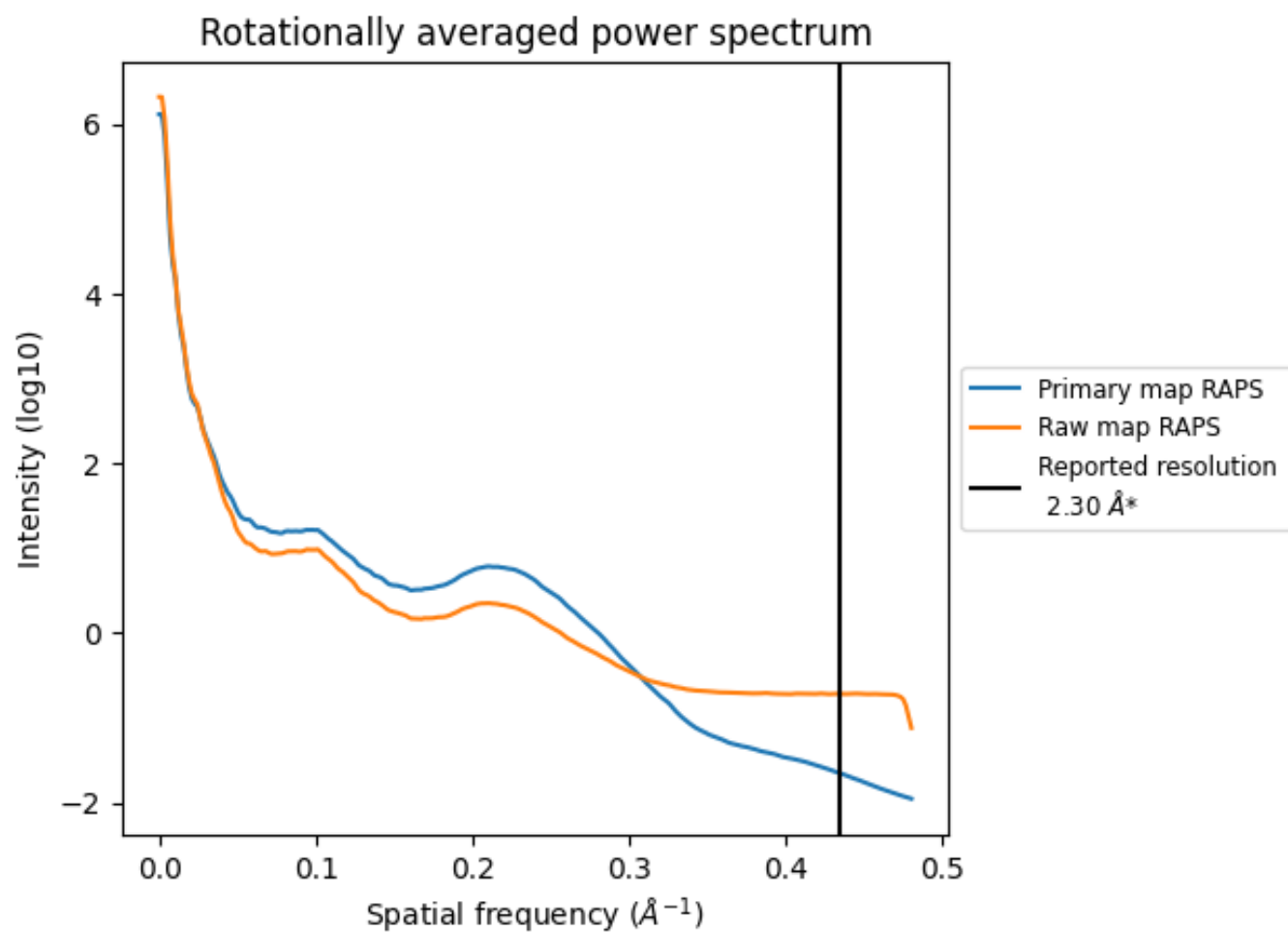
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 771  $\text{nm}^3$ ; this corresponds to an approximate mass of 696 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 ⓘ

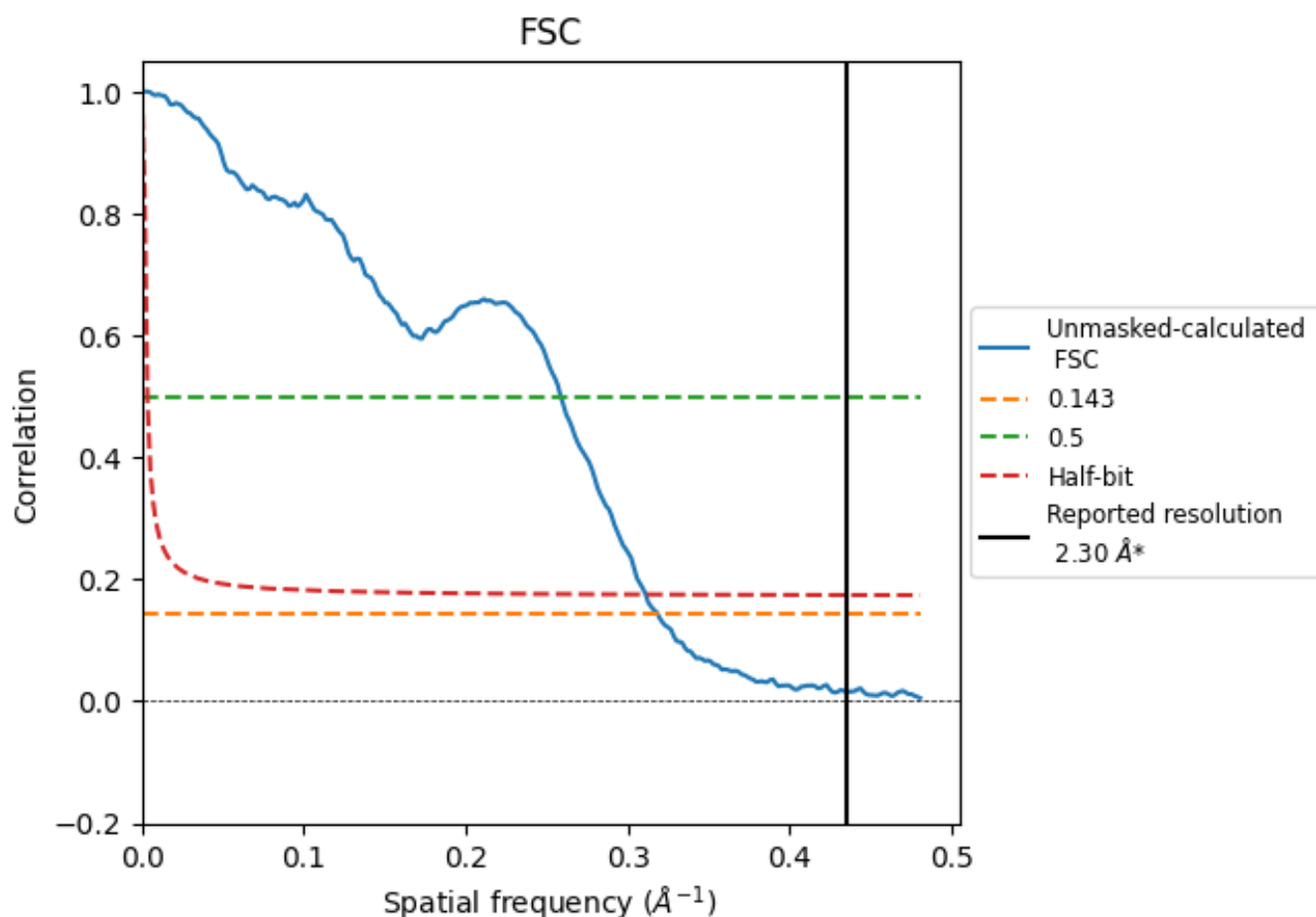


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.435 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

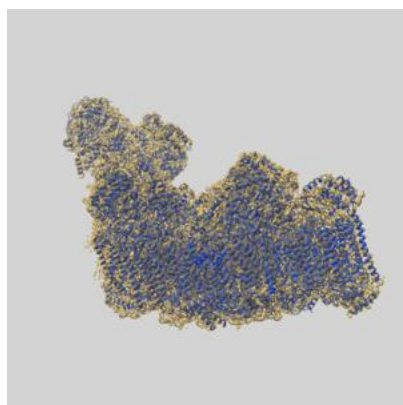
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.30                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.14                               | 3.86 | 3.21     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.14 differs from the reported value 2.3 by more than 10 %

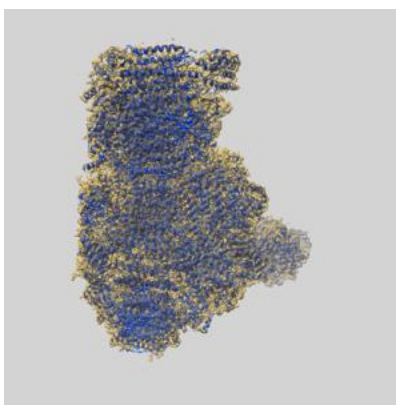
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42227 and PDB model 8UGJ. Per-residue inclusion information can be found in section 3 on page 38.

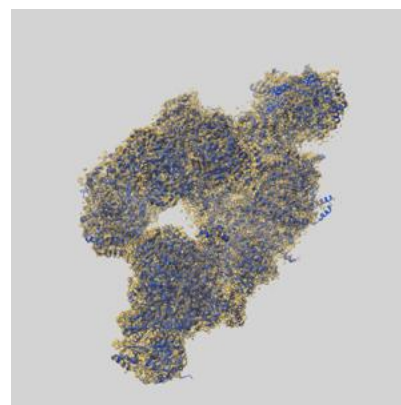
### 9.1 Map-model overlay [i](#)



X



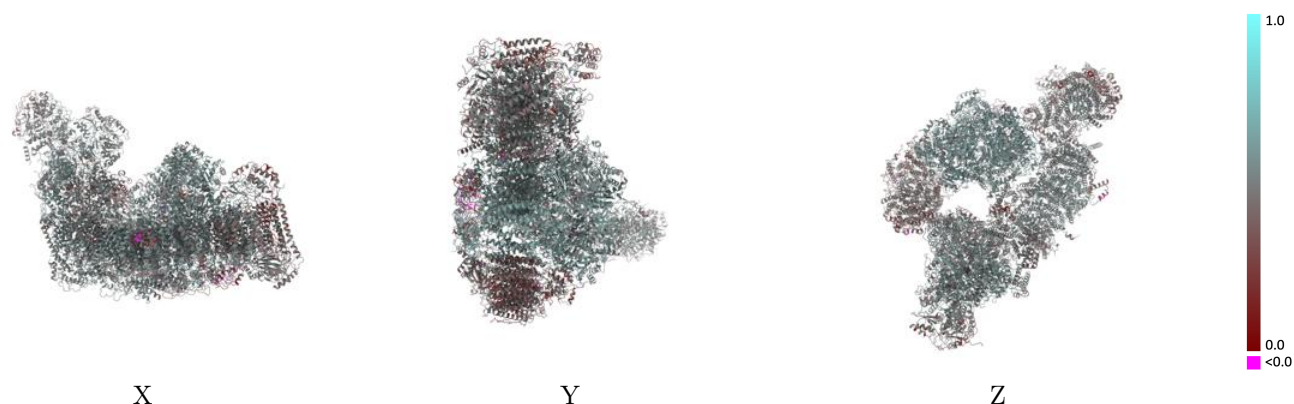
Y



Z

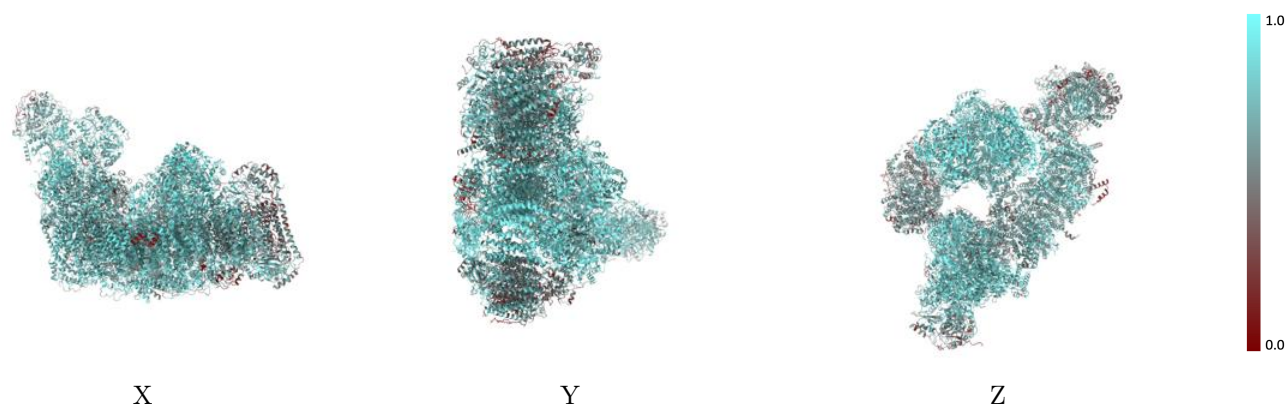
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



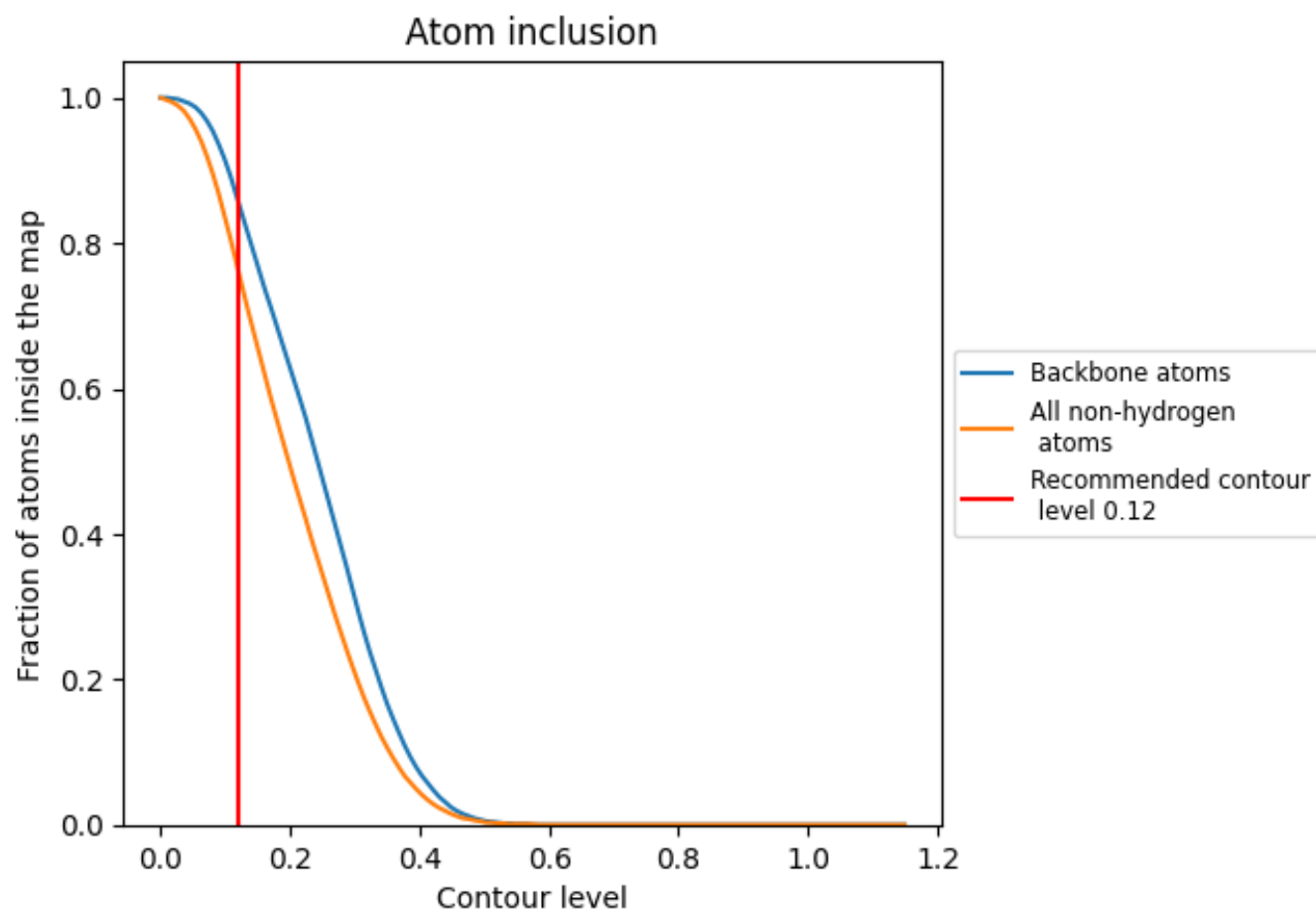
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (0.12) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7620   |  0.4950   |
| 1A    |  0.6590   |  0.4580   |
| 1B    |  0.8660   |  0.5350   |
| 1C    |  0.8720   |  0.5560   |
| 1D    |  0.8450   |  0.5410   |
| 1E    |  0.6430   |  0.4590   |
| 1F    |  0.6550   |  0.4660   |
| 1G    |  0.8050   |  0.5150   |
| 1H    |  0.8060   |  0.5140   |
| 1I    |  0.8950   |  0.5560   |
| 1J    |  0.6710   |  0.4620   |
| 1K    |  0.7730   |  0.5060   |
| 1L    |  0.8300   |  0.5200   |
| 1M    |  0.8490   |  0.5390   |
| 1N    |  0.8340  |  0.5390  |
| 1O    |  0.7540 |  0.4680 |
| 1P    |  0.7610 |  0.4890 |
| 1Q    |  0.7830 |  0.5130 |
| 1R    |  0.8030 |  0.5350 |
| 1S    |  0.7300 |  0.4740 |
| 1T    |  0.5330 |  0.3490 |
| 1U    |  0.7690 |  0.4940 |
| 1V    |  0.7410 |  0.4990 |
| 1W    |  0.8070 |  0.5110 |
| 1X    |  0.7450 |  0.5010 |
| 1Y    |  0.7760 |  0.4830 |
| 1Z    |  0.7800 |  0.5210 |
| 1a    |  0.8400 |  0.5270 |
| 1b    |  0.7490 |  0.4940 |
| 1c    |  0.7170 |  0.4900 |
| 1d    |  0.7770 |  0.5180 |
| 1e    |  0.7480 |  0.5190 |
| 1f    |  0.6950 |  0.4990 |
| 1g    |  0.7700 |  0.5060 |
| 1h    |  0.7590 |  0.5160 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 1i    |  0.5600   |  0.4240   |
| 1j    |  0.6760   |  0.4540   |
| 1k    |  0.6750   |  0.4500   |
| 1l    |  0.8060   |  0.5080   |
| 1m    |  0.8060   |  0.5160   |
| 1n    |  0.8200   |  0.5110   |
| 1o    |  0.7010   |  0.4450   |
| 1p    |  0.7580   |  0.5020   |
| 1q    |  0.7880   |  0.5240   |
| 1r    |  0.8190   |  0.5450   |
| 1s    |  0.6280   |  0.4670   |
| 3A    |  0.8560   |  0.5540   |
| 3B    |  0.8650   |  0.5550   |
| 3C    |  0.9140   |  0.5770   |
| 3D    |  0.9080   |  0.5710   |
| 3E    |  0.5160   |  0.3660   |
| 3F    |  0.8710   |  0.5680   |
| 3G    |  0.8490  |  0.5510  |
| 3H    |  0.7930 |  0.5240 |
| 3I    |  0.4830 |  0.4250 |
| 3J    |  0.8800 |  0.5130 |
| 3N    |  0.9010 |  0.5680 |
| 3O    |  0.8710 |  0.5560 |
| 3P    |  0.9170 |  0.5790 |
| 3Q    |  0.9170 |  0.5760 |
| 3R    |  0.5040 |  0.3410 |
| 3S    |  0.8830 |  0.5740 |
| 3T    |  0.9110 |  0.5600 |
| 3U    |  0.8120 |  0.5130 |
| 3V    |  0.7290 |  0.5270 |
| 3W    |  0.9180 |  0.5770 |
| 3X    |  0.8590 |  0.5500 |
| 3Y    |  0.8180 |  0.5350 |
| 4A    |  0.7670 |  0.4960 |
| 4B    |  0.6290 |  0.4440 |
| 4C    |  0.6810 |  0.4580 |
| 4D    |  0.5470 |  0.4050 |
| 4E    |  0.5240 |  0.3980 |
| 4F    |  0.6500 |  0.4690 |
| 4G    |  0.5720 |  0.4200 |
| 4H    |  0.7020 |  0.4510 |
| 4I    |  0.5490 |  0.4430 |

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| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| 4J    |  0.6570  |  0.4500  |
| 4K    |  0.4960  |  0.4260  |
| 4L    |  0.6710  |  0.4540  |
| 4M    |  0.5840  |  0.4440  |
| 4N    |  0.4840  |  0.4220  |
| 8A    |  0.7010  |  0.4270  |
| 8B    |  0.6480  |  0.3960  |
| 8C    |  0.6210  |  0.3890  |
| 8D    |  0.5890  |  0.3680  |
| 8E    |  0.5910  |  0.3680  |
| 8F    |  0.4800  |  0.3690  |
| 8G    |  0.5780  |  0.3700  |
| 8H    |  0.7180  |  0.4000  |
| 8I    |  0.7430  |  0.4120  |
| 8J    |  0.5710  |  0.3790  |
| 8K    |  0.6140  |  0.3890  |
| 8L    |  0.5740  |  0.3870  |
| 8M    |  0.6250  |  0.3910  |
| 8N    |  0.6560 |  0.3990 |