



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:56 PM UTC

PDB ID : 8UET / pdb\_00008uet  
EMDB ID : EMD-42170  
Title : In-situ complex I, Deactive class02  
Authors : Zheng, W.; Zhu, J.; Zhang, K.  
Deposited on : 2023-10-02  
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

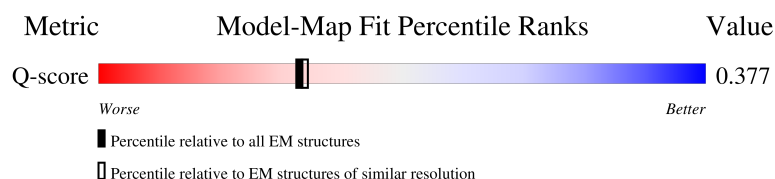
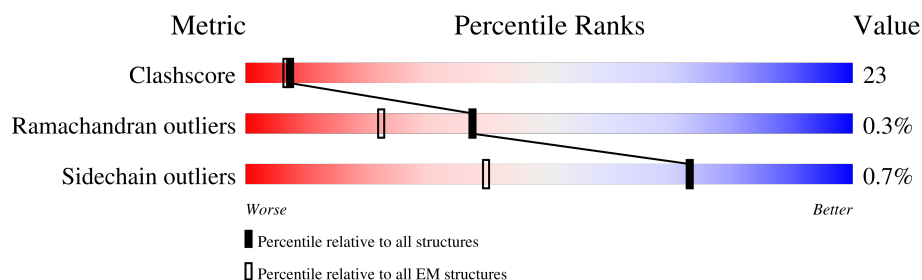
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

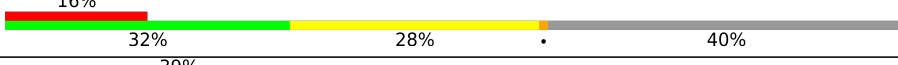
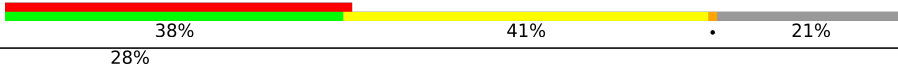
The reported resolution of this entry is 3.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | 1A    | 115    |  |
| 2   | 1B    | 258    |  |
| 3   | 1C    | 264    |  |
| 4   | 1D    | 476    |  |

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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    | 123    |                  |
| 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    | 114    |                  |
| 44  | 1s    | 471    |                  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 46  | SF4  | 1B    | 201 | -         | -        | X       | -                |
| 46  | SF4  | 1I    | 201 | -         | -        | X       | -                |

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67180 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    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 700   | 479 | 100 | 116 | 5 |         |       |

- 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    | 418      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3376  | 2159 | 577 | 616 | 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    | 175      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1339  | 898 | 190 | 238 | 13 |         |       |

- 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    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 648 | 172 | 170 | 6 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference      |
|-------|---------|----------|--------|-------------|----------------|
| 1d    | -2      | ACE      | -      | acetylation | UNP A0A480JRW3 |

- 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    | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 723 | 194 | 181 | 2 |         |       |

- 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 |         |       |

- 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    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 767   | 483 | 144 | 137 | 3 |         |       |

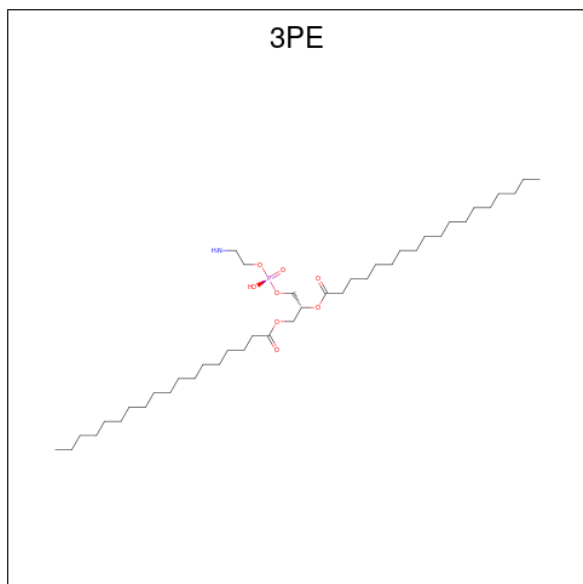
There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference      |
|-------|---------|----------|--------|-----------|----------------|
| 1r    | 0       | ACE      | -      | insertion | UNP A0A8W4F7N8 |

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

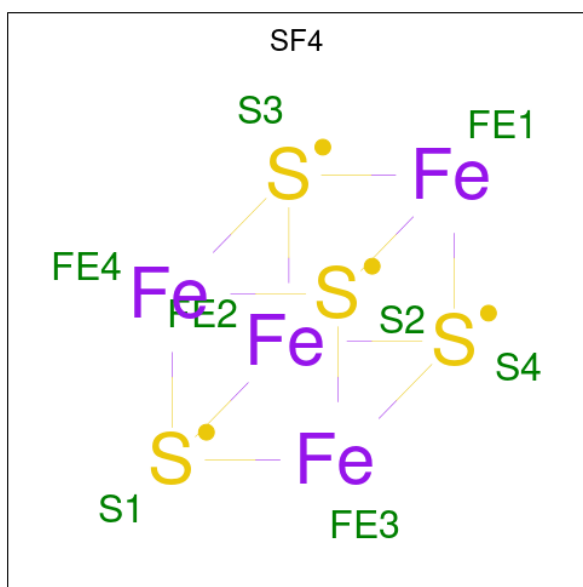
| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 44  | 1s    | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 382   | 238 | 70 | 73 | 1 |         |       |

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



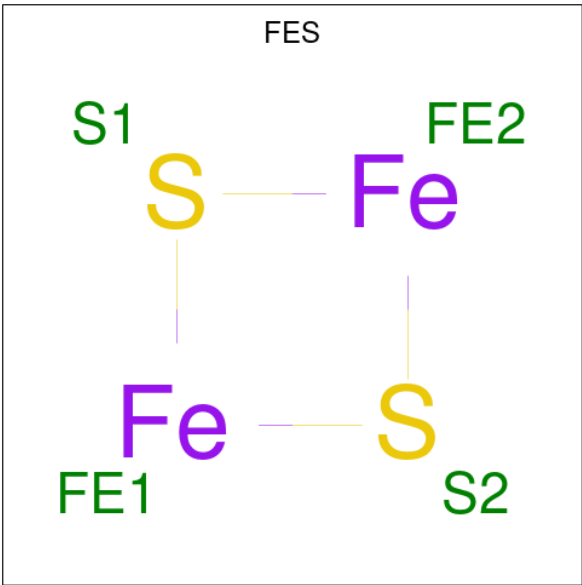
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 45  | 1A    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 47    | 37 | 1 | 8 | 1 |         |
| 45  | 1L    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |
| 45  | 1L    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 21 | 1 | 8 | 1 |         |
| 45  | 1L    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 42    | 32 | 1 | 8 | 1 |         |
| 45  | 1N    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |
| 45  | 1Y    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 51    | 41 | 1 | 8 | 1 |         |

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $Fe_4S_4$ ).



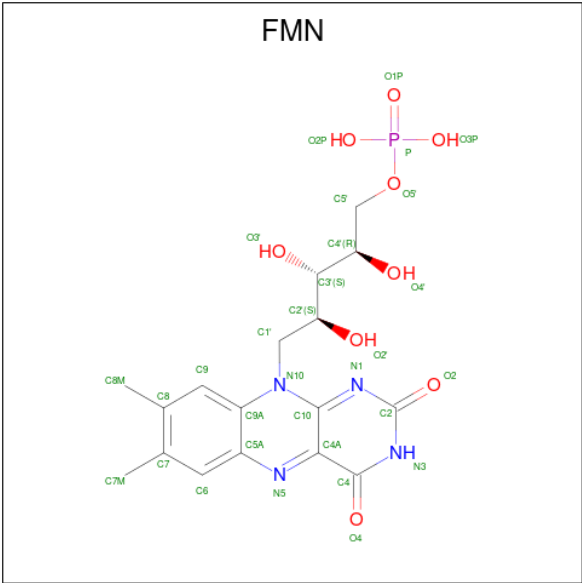
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 46  | 1B    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 46  | 1F    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 46  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 46  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 46  | 1I    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 46  | 1I    | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 47  | 1E    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |
| 47  | 1G    | 1        | Total | Fe | S | 0       |
|     |       |          | 4     | 2  | 2 |         |

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).

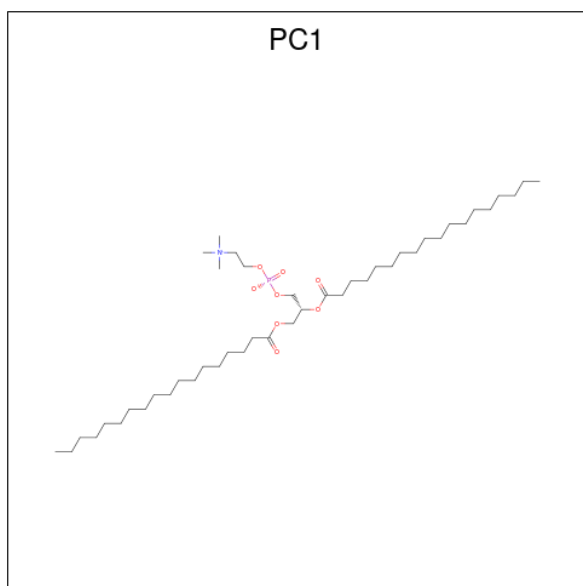


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 48  | 1F    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 31    | 17 | 4 | 9 | 1 |         |

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

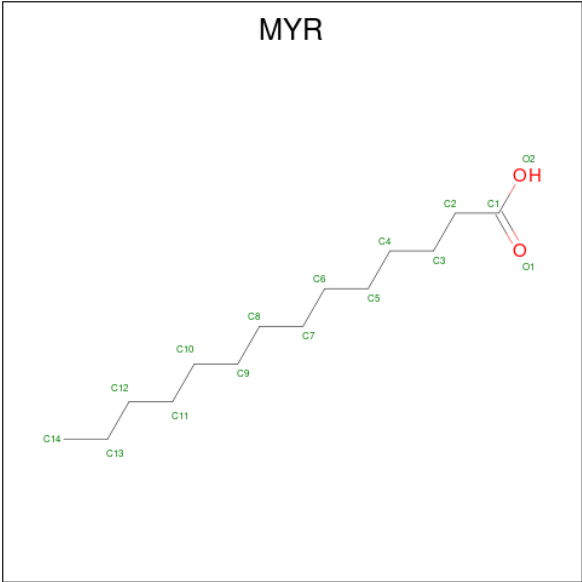
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 49  | 1G    | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



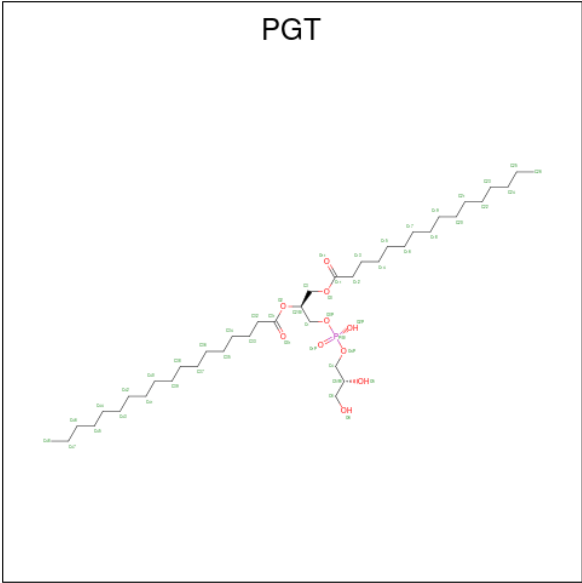
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 50  | 1H    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 54    | 44 | 1 | 8 | 1 |         |
| 50  | 1I    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 50  | 1J    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 35    | 25 | 1 | 8 | 1 |         |
| 50  | 1M    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 44    | 34 | 1 | 8 | 1 |         |
| 50  | 1f    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 46    | 36 | 1 | 8 | 1 |         |

- Molecule 51 is MYRISTIC ACID (CCD ID: MYR) (formula:  $C_{14}H_{28}O_2$ ).



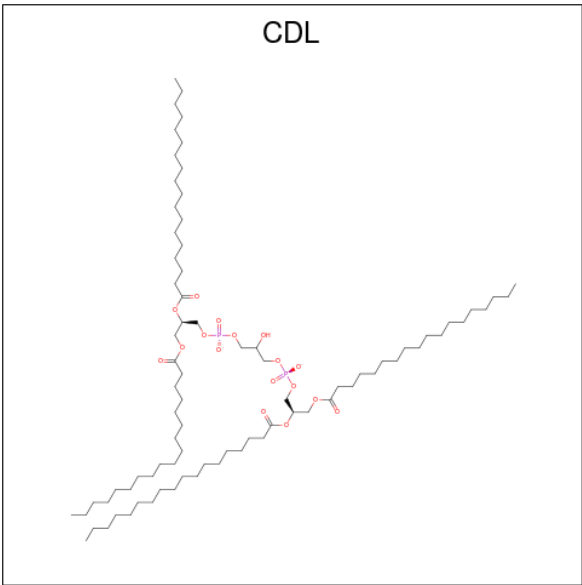
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 51  | 1L    | 1        | Total | C  | O | 0       |
|     |       |          | 15    | 14 | 1 |         |

- Molecule 52 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



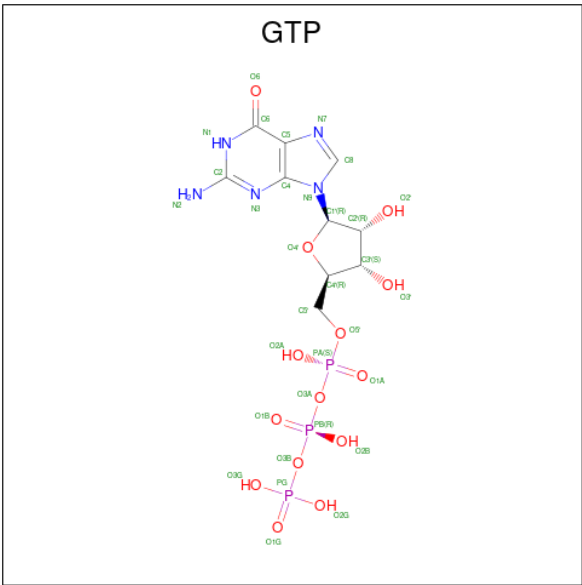
| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 52  | 1M    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 51    | 40 | 10 | 1 |         |

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 53  | 1N    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 77    | 58 | 17 | 2 |         |
| 53  | 1a    | 1        | Total | C  | O  | P | 0       |
|     |       |          | 61    | 42 | 17 | 2 |         |

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

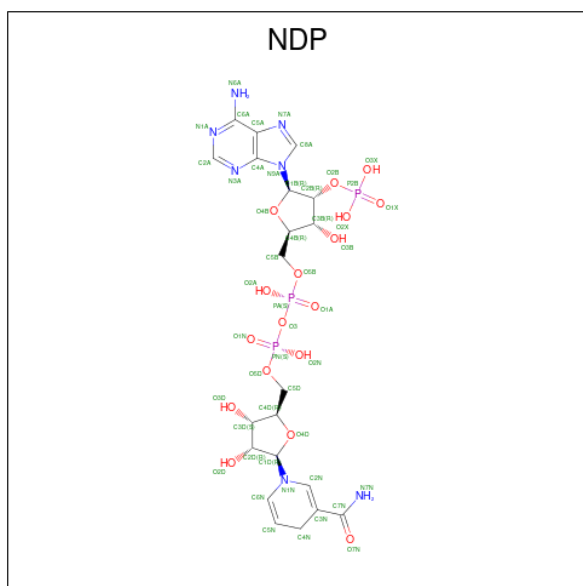


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 54  | 1O    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).

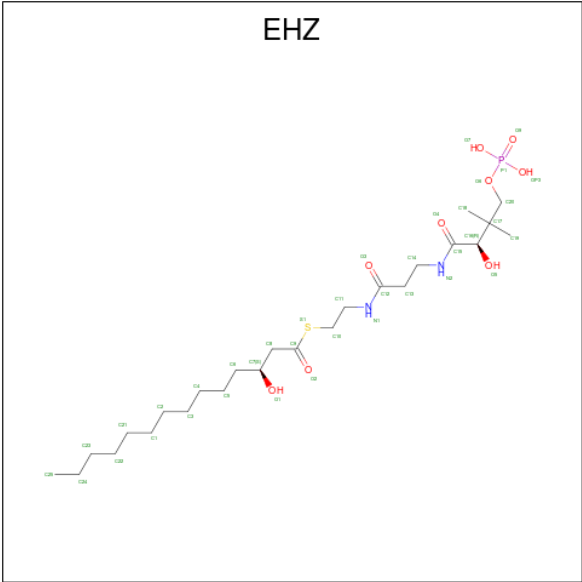


| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 56  | 1P    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 48    | 21 | 7 | 17 | 3 |         |

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

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

- Molecule 58 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:  $C_{25}H_{49}N_2O_9PS$ ).

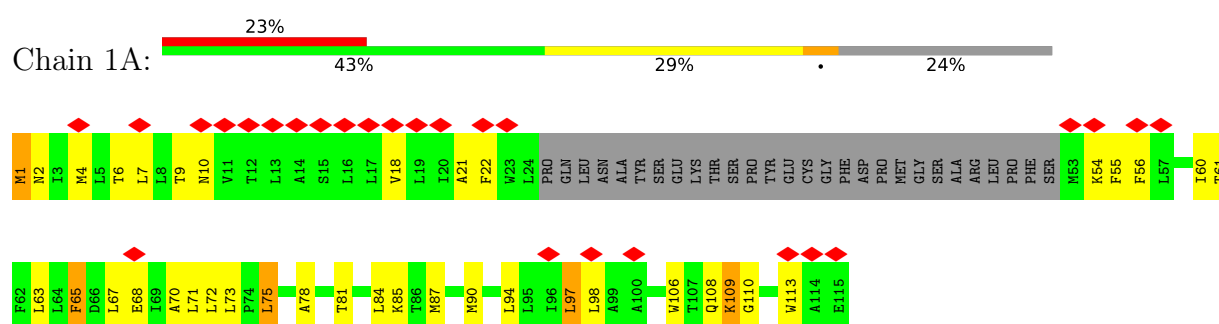


| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 58  | 1W    | 1        | Total | C  | N | O | P | S       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1       |
| 58  | 1n    | 1        | Total | C  | N | O | P | S       |
|     |       |          | 37    | 25 | 2 | 8 | 1 | 1       |

### 3 Residue-property plots

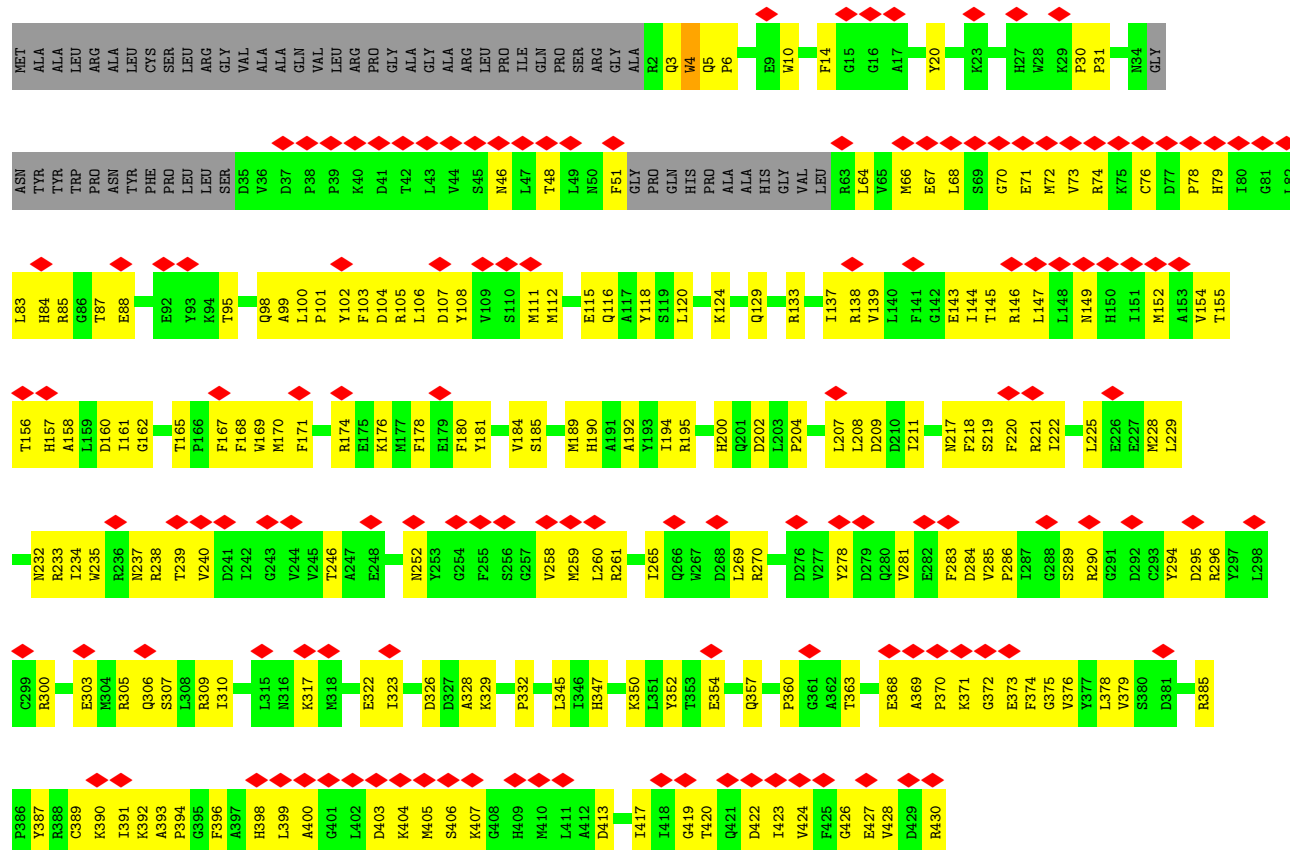
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

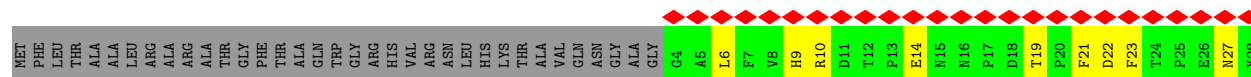
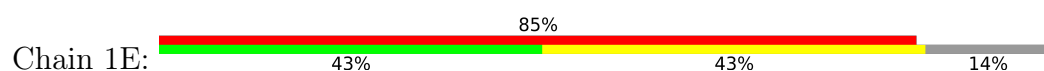




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

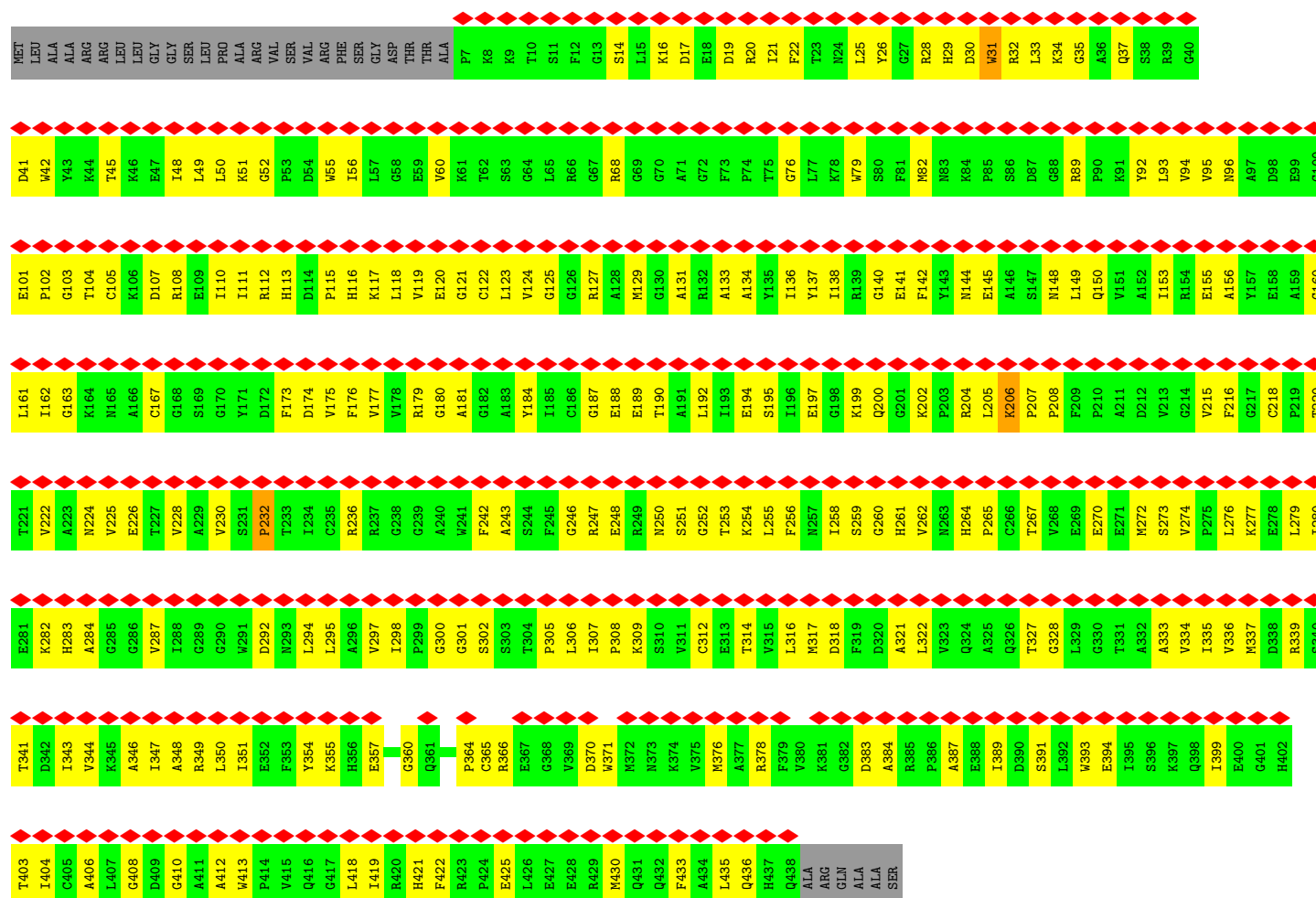
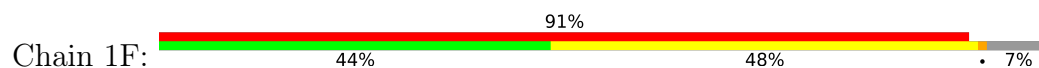


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





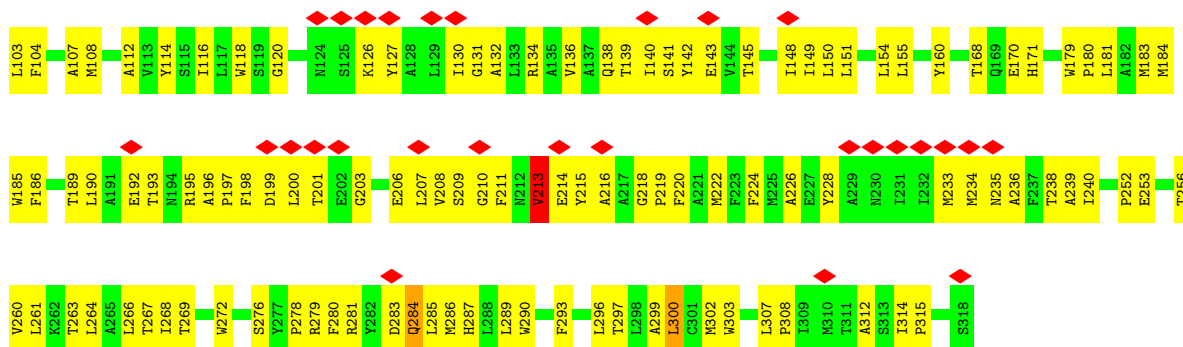
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



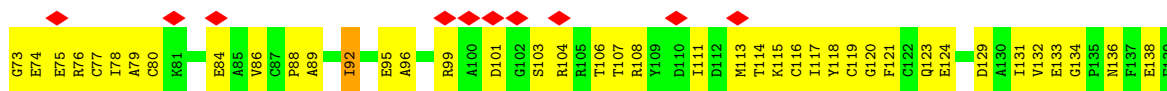
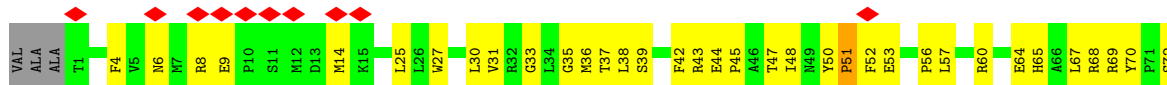
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial







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

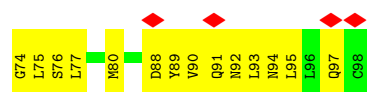


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

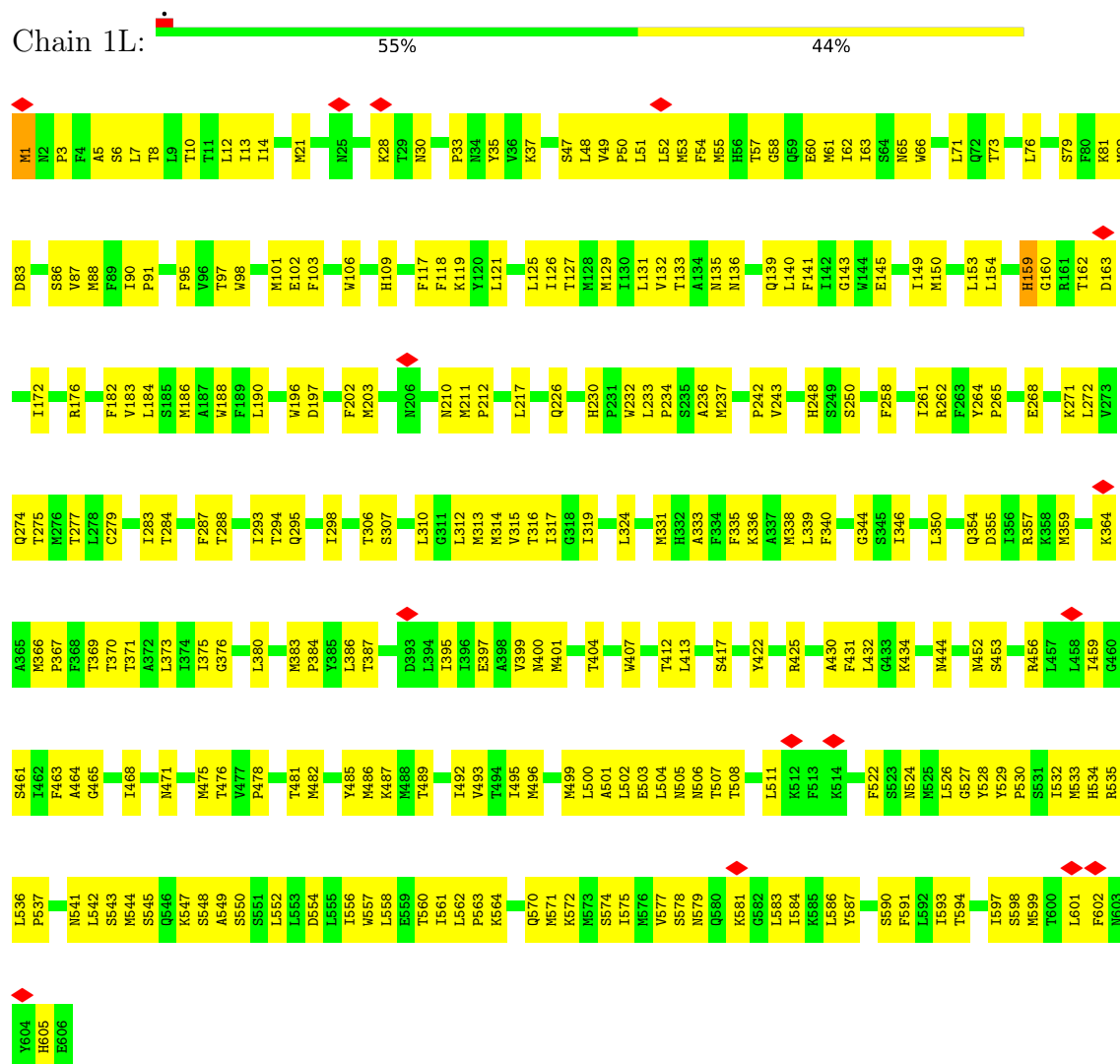


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

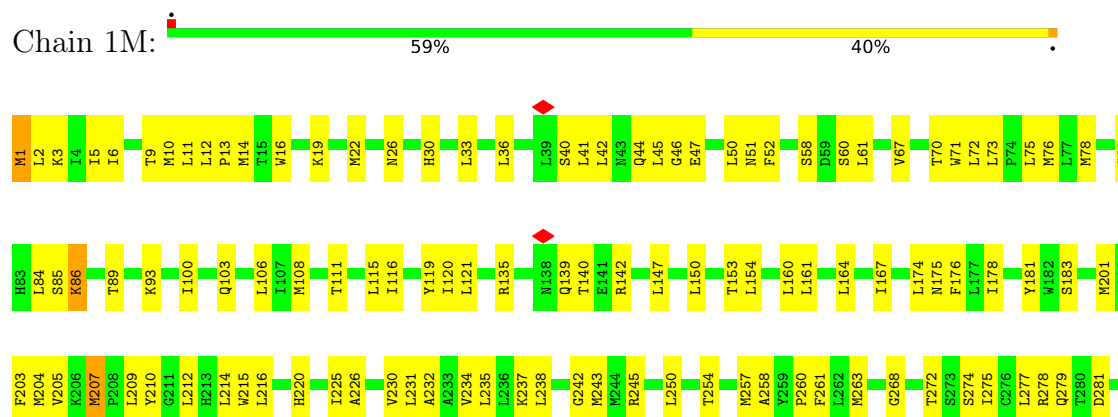




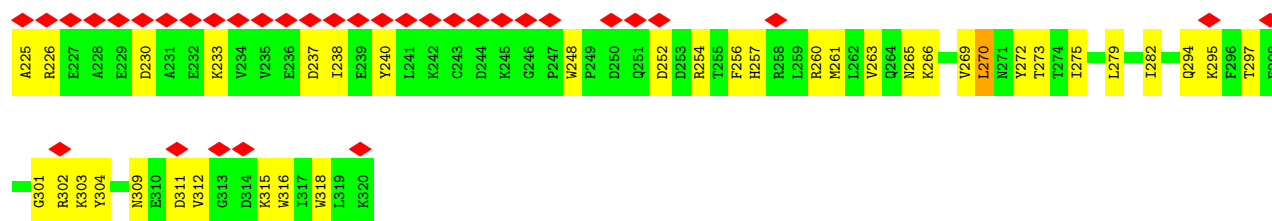
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



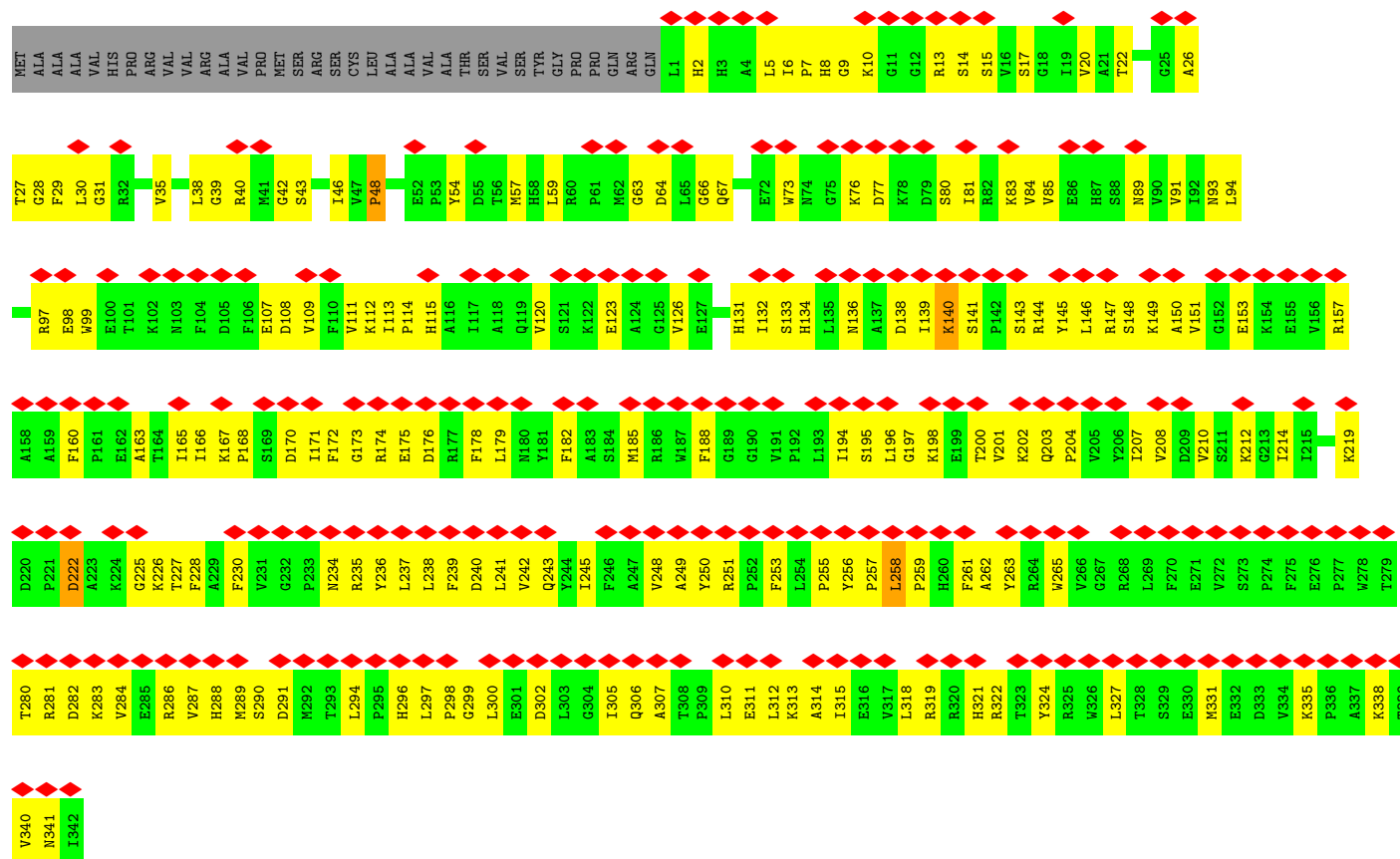
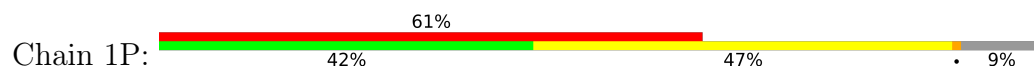
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



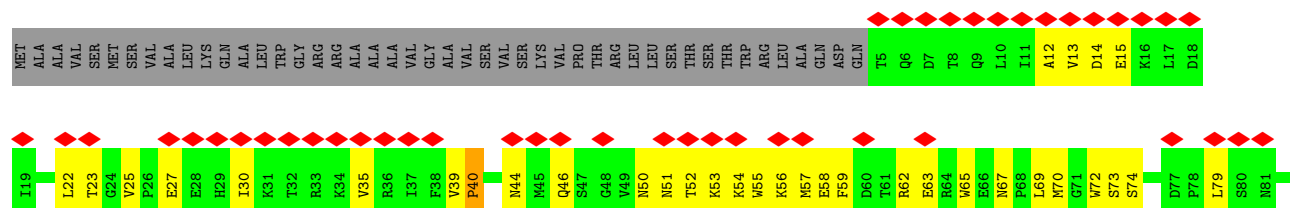
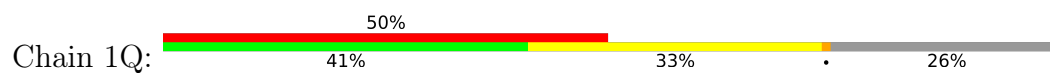


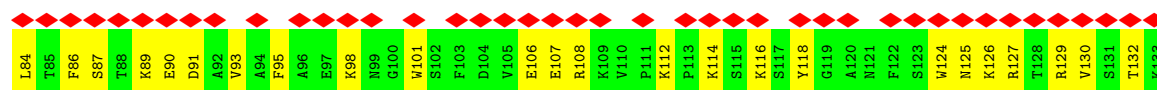


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



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

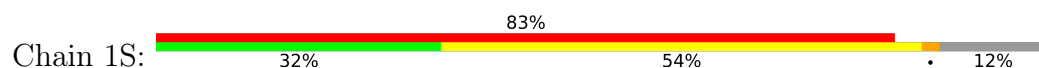




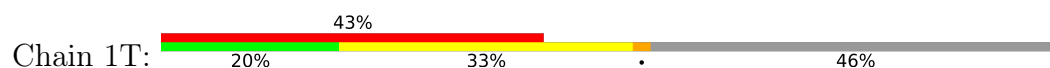
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



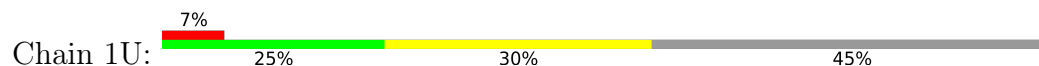
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

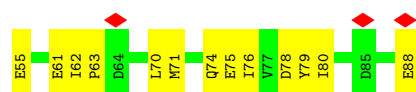


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

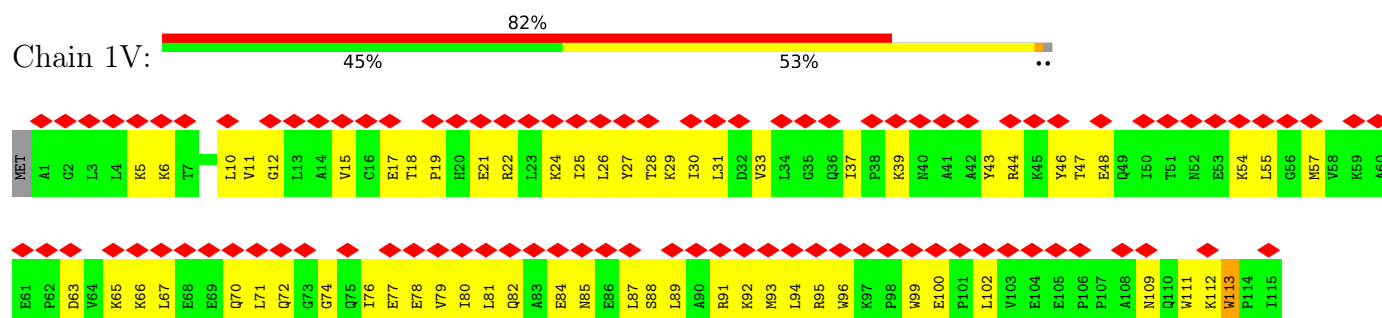


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

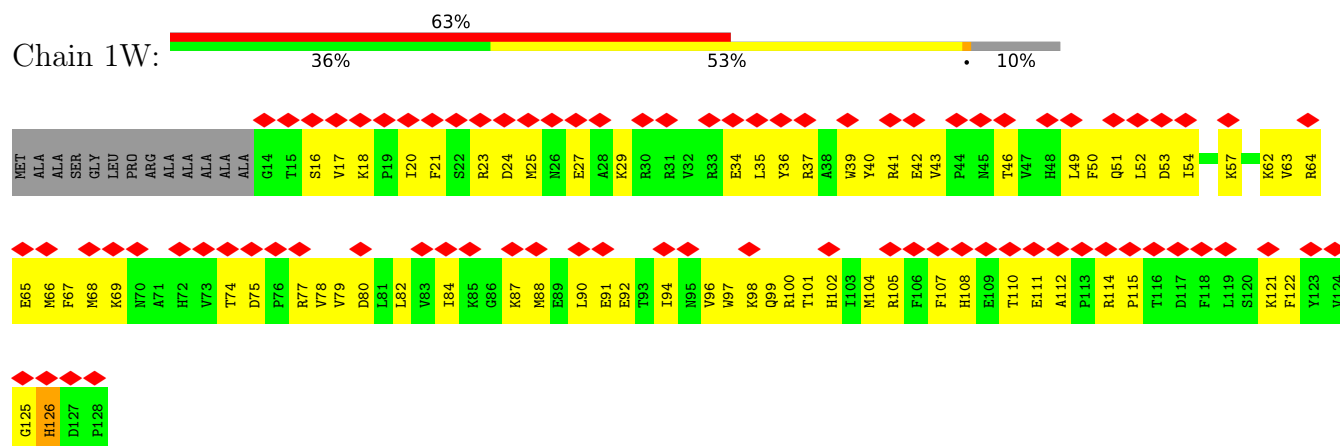




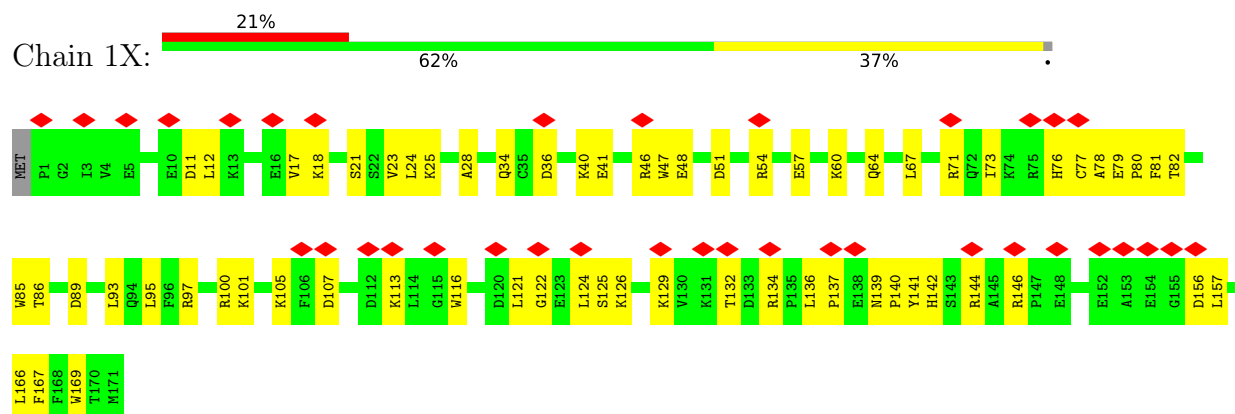
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



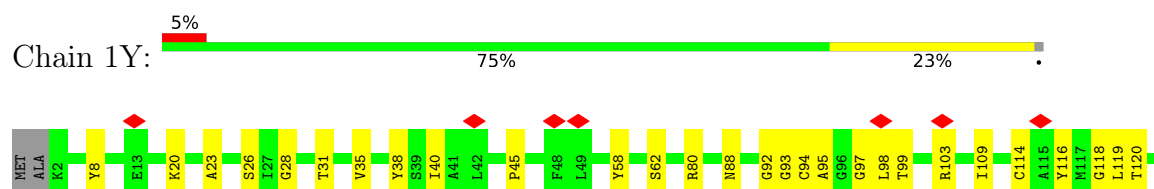
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

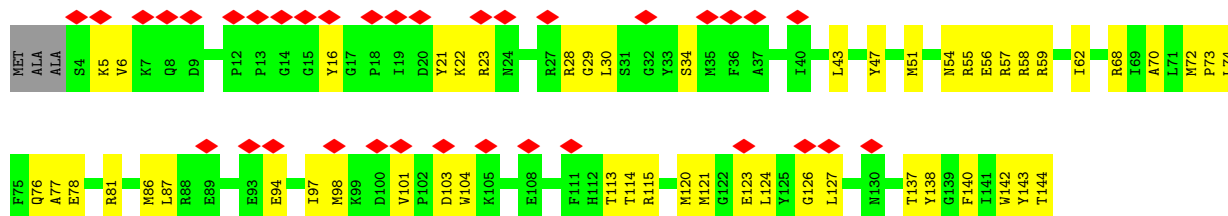


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





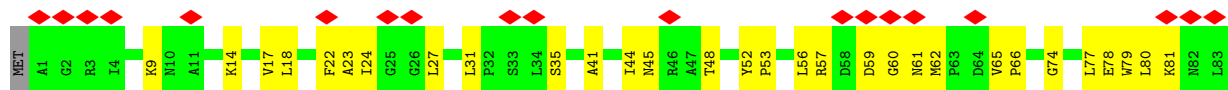
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



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



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

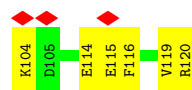


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

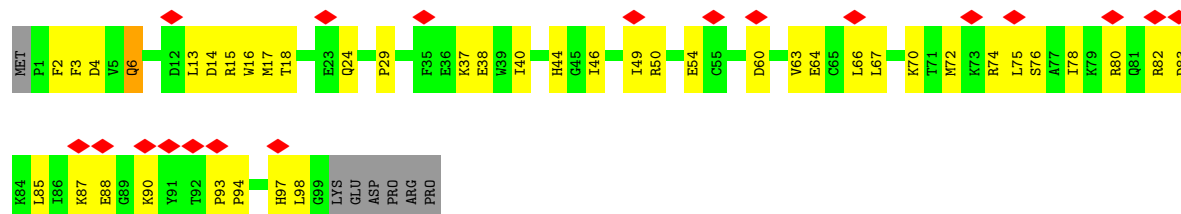


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

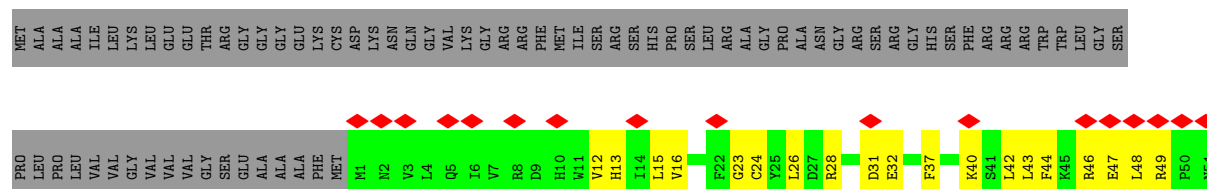




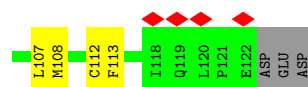
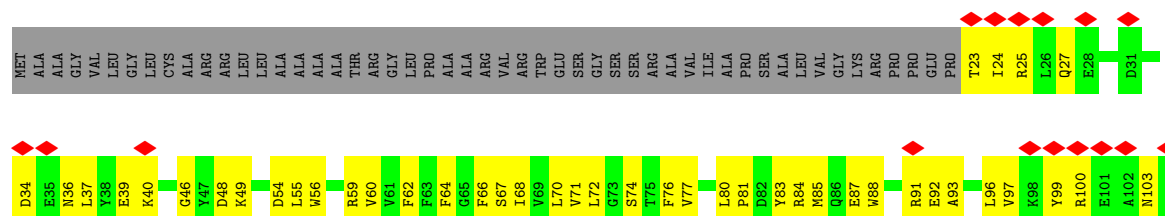
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

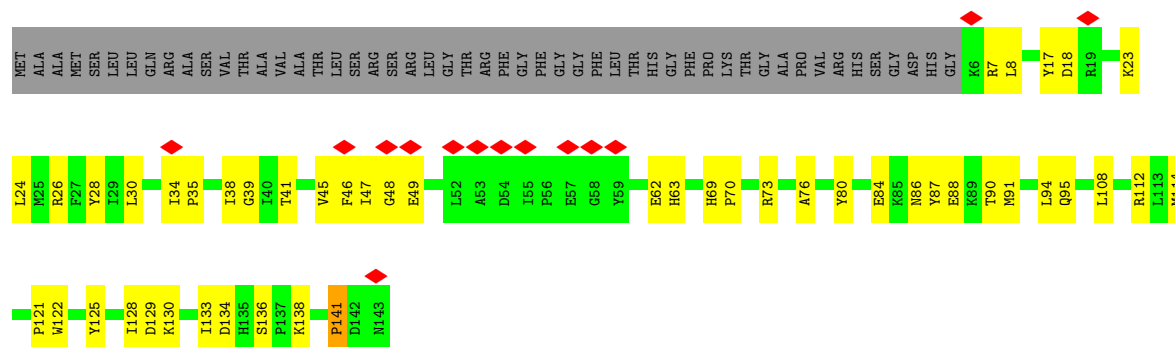


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

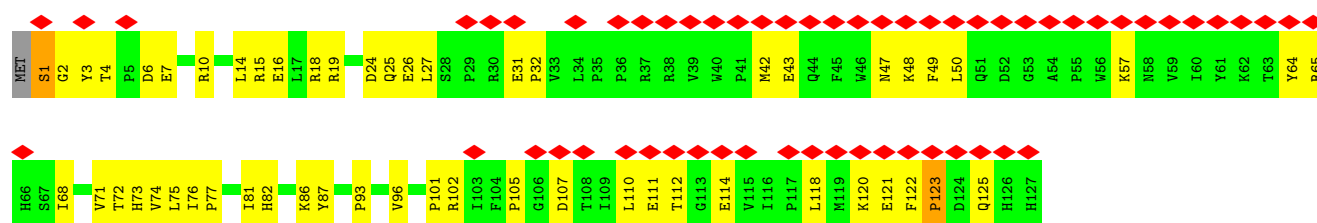


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

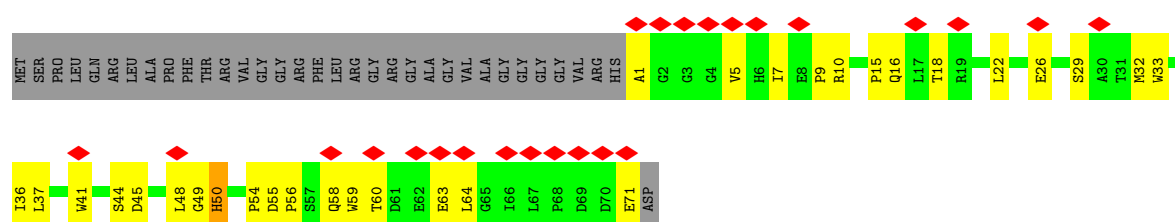




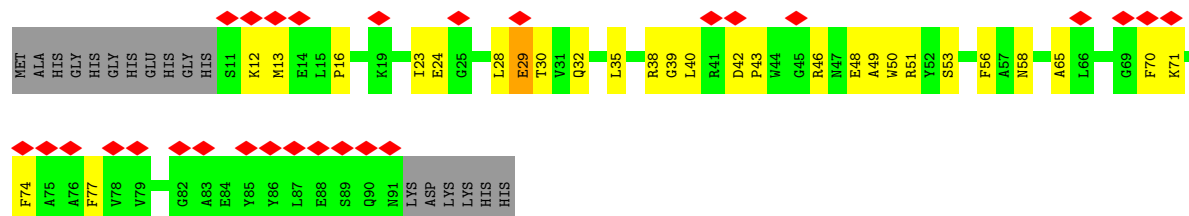
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

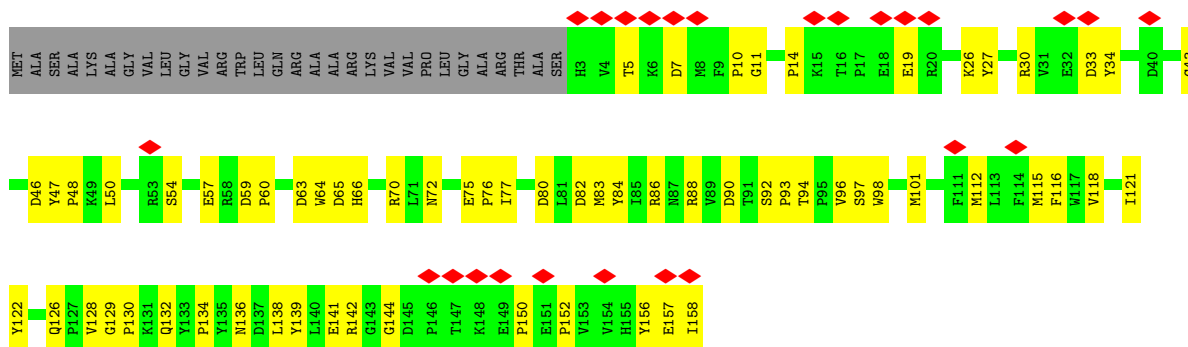


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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





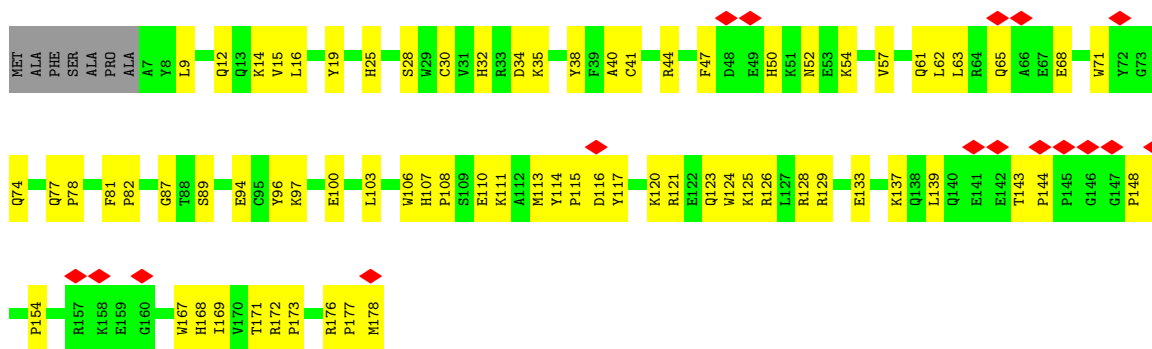
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 6% 62% 37%



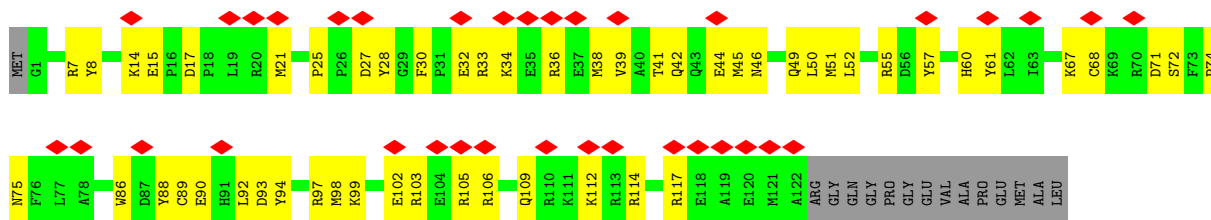
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 9% 55% 41%

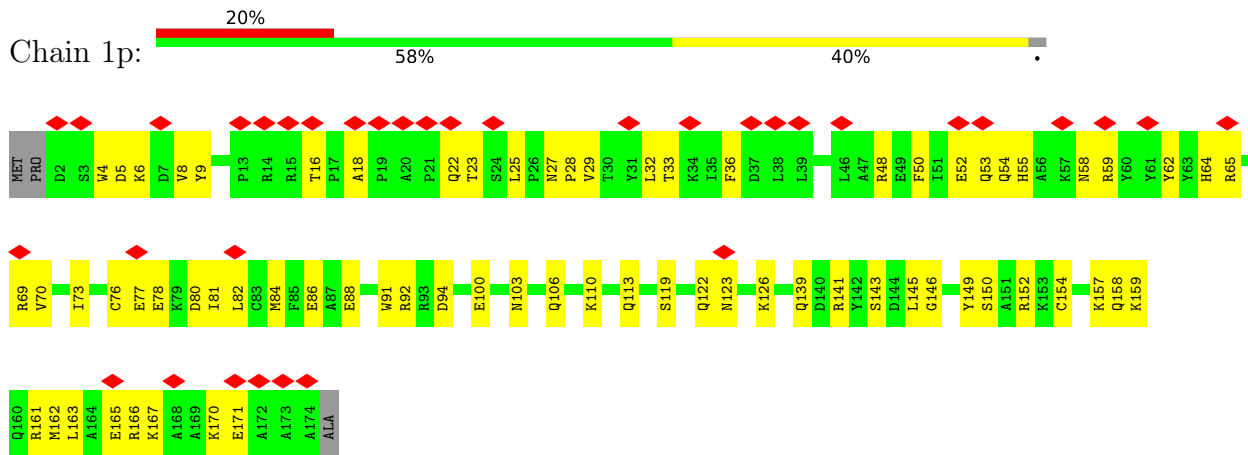


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

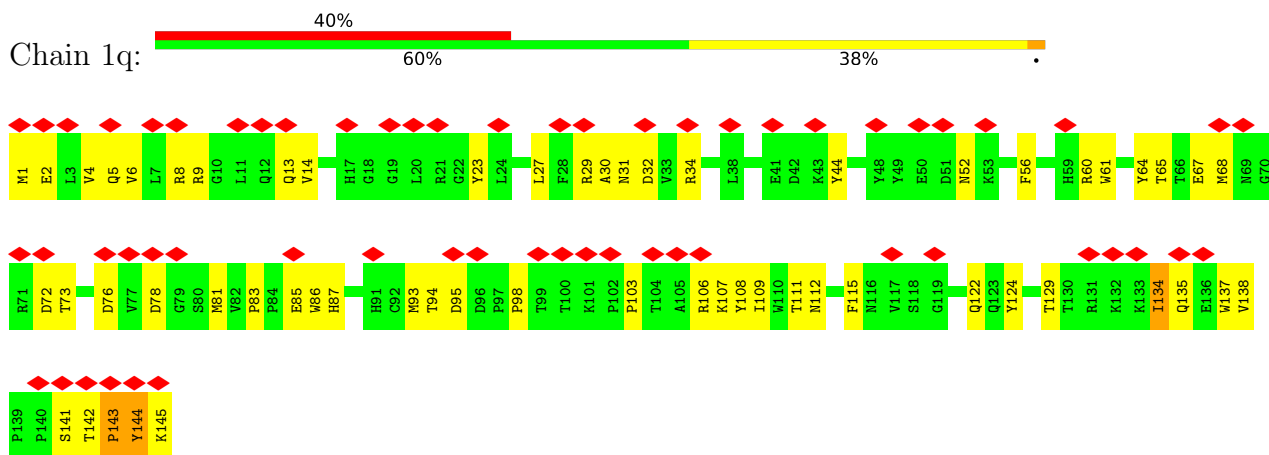
Chain 1o: 26% 50% 39% 11%



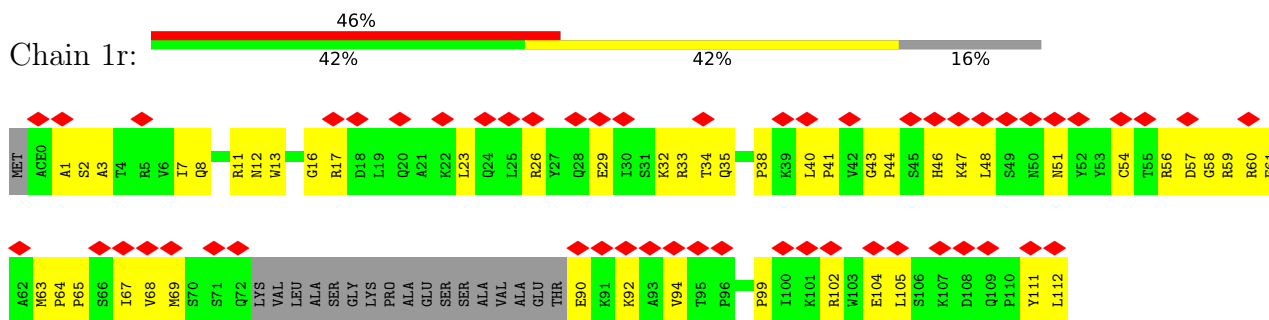
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



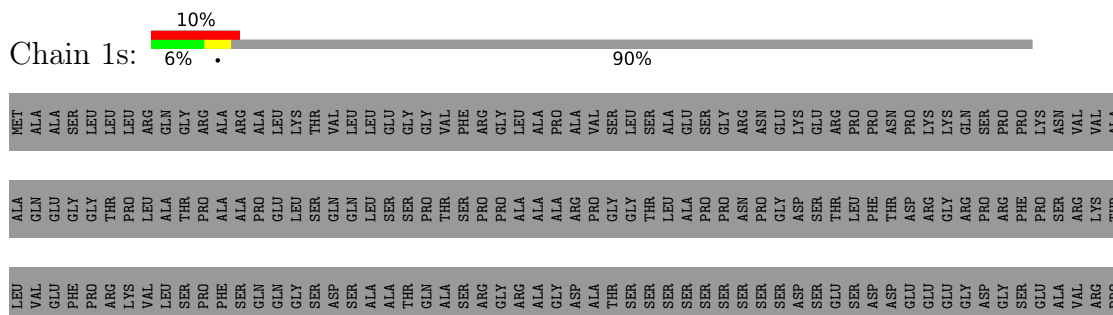
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



[illegible]

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 45000                                   | 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                    | 0.935                                   | Depositor |
| Minimum map value                    | -0.432                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.026                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size (Å)                         | 425.6, 425.6, 425.6                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.33, 1.33, 1.33                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, 3PE, PC1, K, ZN, NDP, FMN, GTP, MYR, PGT, FES, SAC, EH2, ACE, CDL, FME

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    | 0.17         | 0/705         | 0.42        | 0/963         |
| 2   | 1B    | 0.20         | 0/1273        | 0.43        | 0/1722        |
| 3   | 1C    | 0.17         | 0/1791        | 0.40        | 0/2439        |
| 4   | 1D    | 0.18         | 0/3464        | 0.39        | 0/4692        |
| 5   | 1E    | 0.15         | 0/1698        | 0.38        | 0/2311        |
| 6   | 1F    | 0.15         | 0/3401        | 0.40        | 1/4595 (0.0%) |
| 7   | 1G    | 0.20         | 1/5451 (0.0%) | 0.49        | 5/7387 (0.1%) |
| 8   | 1H    | 0.19         | 0/2566        | 0.42        | 0/3509        |
| 9   | 1I    | 0.31         | 1/1443 (0.1%) | 0.62        | 4/1952 (0.2%) |
| 10  | 1J    | 0.17         | 0/1364        | 0.43        | 0/1850        |
| 11  | 1K    | 0.18         | 0/751         | 0.46        | 0/1018        |
| 12  | 1L    | 0.17         | 0/4939        | 0.38        | 0/6718        |
| 13  | 1M    | 0.18         | 0/3713        | 0.35        | 0/5063        |
| 14  | 1N    | 0.19         | 0/2765        | 0.41        | 0/3758        |
| 15  | 1O    | 0.15         | 0/2650        | 0.38        | 1/3588 (0.0%) |
| 16  | 1P    | 0.17         | 0/2828        | 0.42        | 1/3834 (0.0%) |
| 17  | 1Q    | 0.20         | 0/1070        | 0.50        | 1/1446 (0.1%) |
| 18  | 1R    | 0.15         | 0/755         | 0.40        | 0/1018        |
| 19  | 1S    | 0.20         | 0/711         | 0.60        | 1/956 (0.1%)  |
| 20  | 1T    | 0.25         | 0/701         | 0.67        | 2/946 (0.2%)  |
| 20  | 1U    | 0.14         | 0/706         | 0.42        | 0/954         |
| 21  | 1V    | 0.18         | 0/946         | 0.49        | 0/1281        |
| 22  | 1W    | 0.19         | 0/995         | 0.50        | 0/1340        |
| 23  | 1X    | 0.13         | 0/1436        | 0.32        | 0/1938        |
| 24  | 1Y    | 0.15         | 0/1037        | 0.32        | 0/1404        |
| 25  | 1Z    | 0.17         | 0/1199        | 0.38        | 0/1617        |
| 26  | 1a    | 0.18         | 0/577         | 0.39        | 0/777         |
| 27  | 1b    | 0.15         | 0/664         | 0.40        | 0/912         |
| 28  | 1c    | 0.18         | 0/430         | 0.45        | 1/581 (0.2%)  |
| 29  | 1d    | 0.15         | 0/1024        | 0.33        | 0/1383        |
| 30  | 1e    | 0.15         | 0/836         | 0.34        | 0/1118        |
| 31  | 1f    | 0.13         | 0/499         | 0.42        | 0/673         |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 32  | 1g    | 0.16         | 0/858          | 0.42        | 0/1165          |
| 33  | 1h    | 0.25         | 0/1184         | 0.52        | 2/1603 (0.1%)   |
| 34  | 1i    | 0.17         | 0/1131         | 0.45        | 1/1541 (0.1%)   |
| 35  | 1j    | 0.14         | 0/627          | 0.45        | 2/858 (0.2%)    |
| 36  | 1k    | 0.15         | 0/668          | 0.36        | 0/903           |
| 37  | 1l    | 0.14         | 0/1365         | 0.38        | 0/1867          |
| 38  | 1m    | 0.14         | 0/1092         | 0.35        | 0/1481          |
| 39  | 1n    | 0.13         | 0/1549         | 0.30        | 0/2098          |
| 40  | 1o    | 0.15         | 0/1069         | 0.36        | 0/1430          |
| 41  | 1p    | 0.14         | 0/1481         | 0.30        | 0/1997          |
| 42  | 1q    | 0.23         | 0/1253         | 0.54        | 2/1704 (0.1%)   |
| 43  | 1r    | 0.17         | 0/782          | 0.50        | 0/1057          |
| 44  | 1s    | 0.15         | 0/394          | 0.35        | 0/533           |
| All | All   | 0.18         | 2/67841 (0.0%) | 0.42        | 24/91980 (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                   |
| 7   | 1G    | 0                   | 2                   |
| 13  | 1M    | 0                   | 1                   |
| 21  | 1V    | 0                   | 1                   |
| All | All   | 0                   | 5                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | 1I    | 51  | PRO  | CG-CD | -6.39 | 1.34        | 1.51     |
| 7   | 1G    | 389 | PRO  | CG-CD | -5.13 | 1.33        | 1.50     |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 9   | 1I    | 51  | PRO  | N-CD-CG  | -12.35 | 88.98       | 103.80   |
| 33  | 1h    | 141 | PRO  | CA-N-CD  | -11.05 | 96.53       | 112.00   |
| 9   | 1I    | 51  | PRO  | CA-N-CD  | -10.46 | 96.86       | 111.50   |
| 20  | 1T    | 27  | PRO  | CA-N-CD  | -9.81  | 98.26       | 112.00   |
| 7   | 1G    | 389 | PRO  | CA-N-CD  | -8.75  | 99.75       | 112.00   |
| 9   | 1I    | 51  | PRO  | CA-CB-CG | -8.37  | 88.11       | 104.00   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 15  | 1O    | 175 | PRO  | CA-N-CD  | -7.94 | 100.89      | 112.00   |
| 7   | 1G    | 389 | PRO  | N-CD-CG  | -6.87 | 92.89       | 103.20   |
| 33  | 1h    | 141 | PRO  | N-CD-CG  | -6.85 | 92.93       | 103.20   |
| 19  | 1S    | 25  | ARG  | CA-CB-CG | 6.50  | 127.11      | 114.10   |
| 6   | 1F    | 232 | PRO  | CA-N-CD  | -6.45 | 102.97      | 112.00   |
| 7   | 1G    | 289 | GLY  | N-CA-C   | 6.33  | 128.19      | 113.18   |
| 35  | 1j    | 54  | PRO  | CA-C-N   | 5.96  | 128.95      | 120.49   |
| 35  | 1j    | 54  | PRO  | C-N-CA   | 5.96  | 128.95      | 120.49   |
| 16  | 1P    | 48  | PRO  | CA-N-CD  | -5.95 | 103.68      | 112.00   |
| 42  | 1q    | 143 | PRO  | CA-N-CD  | -5.71 | 104.01      | 112.00   |
| 7   | 1G    | 287 | GLU  | N-CA-C   | 5.67  | 122.87      | 110.80   |
| 20  | 1T    | 27  | PRO  | N-CD-CG  | -5.62 | 94.76       | 103.20   |
| 7   | 1G    | 338 | VAL  | N-CA-C   | -5.56 | 106.40      | 112.80   |
| 28  | 1c    | 7   | PRO  | CA-N-CD  | -5.56 | 104.22      | 112.00   |
| 9   | 1I    | 51  | PRO  | CB-CG-CD | -5.35 | 93.10       | 105.40   |
| 34  | 1i    | 123 | PRO  | CA-N-CD  | -5.25 | 104.65      | 112.00   |
| 42  | 1q    | 144 | TYR  | N-CA-C   | 5.24  | 117.04      | 110.91   |
| 17  | 1Q    | 40  | PRO  | CA-N-CD  | -5.23 | 104.68      | 112.00   |

There are no chirality outliers.

All (5) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 6   | 1F    | 206 | LYS  | Peptide |
| 7   | 1G    | 284 | ILE  | Peptide |
| 7   | 1G    | 286 | ASN  | Peptide |
| 13  | 1M    | 207 | MET  | Peptide |
| 21  | 1V    | 113 | TRP  | 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    | 700   | 0        | 749      | 47      | 0            |
| 2   | 1B    | 1242  | 0        | 1249     | 84      | 0            |
| 3   | 1C    | 1740  | 0        | 1691     | 125     | 0            |
| 4   | 1D    | 3376  | 0        | 3316     | 203     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | 1E    | 1658  | 0        | 1662     | 105     | 0            |
| 6   | 1F    | 3325  | 0        | 3288     | 200     | 0            |
| 7   | 1G    | 5362  | 0        | 5387     | 366     | 0            |
| 8   | 1H    | 2504  | 0        | 2602     | 152     | 0            |
| 9   | 1I    | 1412  | 0        | 1365     | 116     | 0            |
| 10  | 1J    | 1339  | 0        | 1337     | 72      | 0            |
| 11  | 1K    | 750   | 0        | 794      | 55      | 0            |
| 12  | 1L    | 4818  | 0        | 4956     | 229     | 0            |
| 13  | 1M    | 3632  | 0        | 3836     | 175     | 0            |
| 14  | 1N    | 2712  | 0        | 2872     | 151     | 0            |
| 15  | 1O    | 2590  | 0        | 2556     | 106     | 0            |
| 16  | 1P    | 2751  | 0        | 2776     | 174     | 0            |
| 17  | 1Q    | 1047  | 0        | 1042     | 67      | 0            |
| 18  | 1R    | 741   | 0        | 704      | 34      | 0            |
| 19  | 1S    | 700   | 0        | 719      | 56      | 0            |
| 20  | 1T    | 689   | 0        | 687      | 61      | 0            |
| 20  | 1U    | 694   | 0        | 691      | 46      | 0            |
| 21  | 1V    | 927   | 0        | 972      | 73      | 0            |
| 22  | 1W    | 971   | 0        | 975      | 77      | 0            |
| 23  | 1X    | 1398  | 0        | 1378     | 53      | 0            |
| 24  | 1Y    | 1016  | 0        | 1020     | 24      | 0            |
| 25  | 1Z    | 1168  | 0        | 1161     | 56      | 0            |
| 26  | 1a    | 562   | 0        | 557      | 29      | 0            |
| 27  | 1b    | 643   | 0        | 645      | 32      | 0            |
| 28  | 1c    | 417   | 0        | 425      | 9       | 0            |
| 29  | 1d    | 996   | 0        | 990      | 31      | 0            |
| 30  | 1e    | 816   | 0        | 823      | 40      | 0            |
| 31  | 1f    | 487   | 0        | 497      | 22      | 0            |
| 32  | 1g    | 835   | 0        | 795      | 48      | 0            |
| 33  | 1h    | 1151  | 0        | 1164     | 55      | 0            |
| 34  | 1i    | 1100  | 0        | 1106     | 60      | 0            |
| 35  | 1j    | 601   | 0        | 546      | 29      | 0            |
| 36  | 1k    | 649   | 0        | 626      | 21      | 0            |
| 37  | 1l    | 1310  | 0        | 1204     | 76      | 0            |
| 38  | 1m    | 1062  | 0        | 1075     | 48      | 0            |
| 39  | 1n    | 1495  | 0        | 1434     | 64      | 0            |
| 40  | 1o    | 1045  | 0        | 1018     | 70      | 0            |
| 41  | 1p    | 1449  | 0        | 1416     | 69      | 0            |
| 42  | 1q    | 1212  | 0        | 1174     | 69      | 0            |
| 43  | 1r    | 767   | 0        | 789      | 63      | 0            |
| 44  | 1s    | 382   | 0        | 351      | 17      | 0            |
| 45  | 1A    | 47    | 0        | 71       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 45  | 1L    | 119   | 0        | 163      | 18      | 0            |
| 45  | 1N    | 51    | 0        | 82       | 6       | 0            |
| 45  | 1Y    | 51    | 0        | 82       | 1       | 0            |
| 46  | 1B    | 8     | 0        | 0        | 2       | 0            |
| 46  | 1F    | 8     | 0        | 0        | 1       | 0            |
| 46  | 1G    | 16    | 0        | 0        | 1       | 0            |
| 46  | 1I    | 16    | 0        | 0        | 2       | 0            |
| 47  | 1E    | 4     | 0        | 0        | 0       | 0            |
| 47  | 1G    | 4     | 0        | 0        | 0       | 0            |
| 48  | 1F    | 31    | 0        | 19       | 4       | 0            |
| 49  | 1G    | 1     | 0        | 0        | 1       | 0            |
| 50  | 1H    | 54    | 0        | 88       | 7       | 0            |
| 50  | 1I    | 44    | 0        | 60       | 2       | 0            |
| 50  | 1J    | 35    | 0        | 44       | 2       | 0            |
| 50  | 1M    | 44    | 0        | 62       | 2       | 0            |
| 50  | 1f    | 46    | 0        | 69       | 6       | 0            |
| 51  | 1L    | 15    | 0        | 27       | 2       | 0            |
| 52  | 1M    | 51    | 0        | 78       | 8       | 0            |
| 53  | 1N    | 77    | 0        | 98       | 2       | 0            |
| 53  | 1a    | 61    | 0        | 66       | 4       | 0            |
| 54  | 1O    | 32    | 0        | 12       | 3       | 0            |
| 55  | 1O    | 1     | 0        | 0        | 0       | 0            |
| 56  | 1P    | 48    | 0        | 26       | 5       | 0            |
| 57  | 1R    | 1     | 0        | 0        | 0       | 0            |
| 58  | 1W    | 37    | 0        | 0        | 0       | 0            |
| 58  | 1n    | 37    | 0        | 0        | 0       | 0            |
| All | All   | 67180 | 0        | 67467    | 3144    | 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 23.

All (3144) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:1G:290:LEU:N    | 42:1q:142:THR:O   | 2.01                     | 0.93              |
| 34:1i:76:ILE:HD12 | 34:1i:77:PRO:HD3  | 1.50                     | 0.91              |
| 2:1B:125:TYR:HE1  | 9:1L:88:PRO:HB2   | 1.36                     | 0.91              |
| 7:1G:288:LYS:H    | 42:1q:143:PRO:HD2 | 1.36                     | 0.90              |
| 37:1l:134:PRO:HB3 | 40:1o:38:MET:HE2  | 1.55                     | 0.89              |
| 7:1G:290:LEU:HD23 | 42:1q:141:SER:HA  | 1.55                     | 0.89              |
| 5:1E:151:ALA:HB3  | 5:1E:163:ASP:HA   | 1.54                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:1i:1:SAC:HG     | 34:1i:2:GLY:N      | 1.71                     | 0.88              |
| 2:1B:166:LYS:HE3   | 9:1I:142:GLU:HG2   | 1.55                     | 0.87              |
| 7:1G:25:THR:HA     | 7:1G:72:PRO:HA     | 1.56                     | 0.87              |
| 40:1o:14:LYS:HD2   | 40:1o:109:GLN:HG3  | 1.57                     | 0.86              |
| 7:1G:289:GLY:N     | 42:1q:143:PRO:O    | 2.08                     | 0.85              |
| 9:1I:70:TYR:HE2    | 18:1R:87:CYS:HA    | 1.41                     | 0.85              |
| 16:1P:40:ARG:HH21  | 22:1W:110:THR:HG23 | 1.42                     | 0.84              |
| 7:1G:640:ASN:OD1   | 7:1G:641:TYR:N     | 2.09                     | 0.84              |
| 2:1B:79:SER:HB3    | 8:1H:209:SER:HB2   | 1.60                     | 0.84              |
| 7:1G:290:LEU:H     | 42:1q:143:PRO:HA   | 1.43                     | 0.84              |
| 14:1N:25:HIS:NE2   | 30:1e:17:MET:SD    | 2.51                     | 0.83              |
| 11:1K:95:LEU:HB3   | 14:1N:54:GLU:HG3   | 1.60                     | 0.83              |
| 15:1O:237:ASP:HA   | 15:1O:240:TYR:HB2  | 1.60                     | 0.82              |
| 4:1D:138:ARG:HG3   | 4:1D:194:ILE:HD12  | 1.60                     | 0.82              |
| 21:1V:74:GLY:HA2   | 43:1r:102:ARG:HH12 | 1.42                     | 0.82              |
| 7:1G:389:PRO:HD2   | 7:1G:390:LEU:H     | 1.43                     | 0.81              |
| 7:1G:289:GLY:H     | 42:1q:143:PRO:C    | 1.90                     | 0.79              |
| 14:1N:230:LEU:HD11 | 14:1N:244:MET:HE1  | 1.61                     | 0.79              |
| 17:1Q:127:ARG:HG2  | 44:1s:70:ARG:HH12  | 1.47                     | 0.79              |
| 39:1n:62:LEU:HA    | 39:1n:65:GLN:HE22  | 1.47                     | 0.79              |
| 14:1N:322:GLN:O    | 29:1d:49:ARG:NH2   | 2.15                     | 0.79              |
| 8:1H:102:VAL:HG21  | 8:1H:154:LEU:HD21  | 1.64                     | 0.79              |
| 6:1F:95:VAL:HB     | 6:1F:136:ILE:HG22  | 1.65                     | 0.78              |
| 6:1F:399:ILE:HD11  | 6:1F:412:ALA:HB2   | 1.65                     | 0.78              |
| 7:1G:190:MET:HE2   | 7:1G:190:MET:HA    | 1.65                     | 0.78              |
| 12:1L:190:LEU:HD23 | 13:1M:383:THR:HG21 | 1.64                     | 0.78              |
| 7:1G:286:ASN:O     | 42:1q:144:TYR:HB2  | 1.82                     | 0.78              |
| 18:1R:84:CYS:HB3   | 18:1R:87:CYS:SG    | 2.23                     | 0.78              |
| 7:1G:670:ASP:O     | 7:1G:672:TYR:N     | 2.16                     | 0.78              |
| 16:1P:200:THR:HB   | 16:1P:238:LEU:HB2  | 1.65                     | 0.77              |
| 6:1F:79:TRP:HA     | 6:1F:82:MET:HE3    | 1.67                     | 0.77              |
| 16:1P:245:ILE:HG13 | 16:1P:318:LEU:HD11 | 1.65                     | 0.77              |
| 5:1E:100:ILE:HB    | 5:1E:139:LEU:HA    | 1.64                     | 0.77              |
| 6:1F:21:ILE:HG21   | 6:1F:230:VAL:HG12  | 1.67                     | 0.77              |
| 6:1F:120:GLU:HB2   | 6:1F:232:PRO:HG3   | 1.65                     | 0.77              |
| 16:1P:262:ALA:HA   | 16:1P:265:TRP:HD1  | 1.50                     | 0.77              |
| 6:1F:142:PHE:HB3   | 6:1F:145:GLU:HB2   | 1.66                     | 0.77              |
| 7:1G:325:ALA:HA    | 7:1G:328:LEU:HD12  | 1.66                     | 0.77              |
| 7:1G:537:LEU:HD22  | 7:1G:538:PRO:HD2   | 1.67                     | 0.77              |
| 2:1B:34:ASP:OD1    | 2:1B:38:ASN:ND2    | 2.17                     | 0.76              |
| 45:1L:702:3PE:H242 | 37:1l:88:ARG:HD3   | 1.67                     | 0.76              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:1R:81:THR:OG1   | 18:1R:91:PHE:O     | 2.03                     | 0.76              |
| 6:1F:355:LYS:HD2   | 6:1F:370:ASP:HA    | 1.67                     | 0.76              |
| 23:1X:18:LYS:HA    | 26:1a:54:ILE:HD11  | 1.66                     | 0.76              |
| 6:1F:190:THR:HB    | 6:1F:204:ARG:HB2   | 1.67                     | 0.76              |
| 40:1o:109:GLN:OE1  | 40:1o:109:GLN:N    | 2.19                     | 0.76              |
| 12:1L:508:THR:O    | 39:1n:35:LYS:NZ    | 2.18                     | 0.76              |
| 5:1E:30:ARG:HG2    | 44:1s:52:LEU:HB3   | 1.68                     | 0.76              |
| 14:1N:316:GLN:HB3  | 15:1O:63:THR:HG21  | 1.68                     | 0.76              |
| 2:1B:66:ARG:HH22   | 43:1r:26:ARG:HH22  | 1.32                     | 0.75              |
| 7:1G:288:LYS:HG3   | 42:1q:142:THR:HB   | 1.68                     | 0.75              |
| 15:1O:200:GLN:O    | 15:1O:204:ASN:ND2  | 2.19                     | 0.75              |
| 14:1N:128:LEU:HD11 | 14:1N:213:LEU:HD13 | 1.68                     | 0.75              |
| 4:1D:158:ALA:HB2   | 4:1D:229:LEU:HD11  | 1.67                     | 0.75              |
| 19:1S:62:PRO:HG2   | 19:1S:79:ASN:HA    | 1.66                     | 0.75              |
| 6:1F:96:ASN:ND2    | 6:1F:187:GLY:O     | 2.20                     | 0.75              |
| 12:1L:597:ILE:HD12 | 12:1L:601:LEU:HB3  | 1.67                     | 0.75              |
| 6:1F:387:ALA:HB1   | 43:1r:48:LEU:HD21  | 1.67                     | 0.75              |
| 21:1V:66:LYS:O     | 21:1V:70:GLN:NE2   | 2.20                     | 0.75              |
| 30:1e:40:ILE:HD11  | 33:1h:128:ILE:HB   | 1.67                     | 0.75              |
| 19:1S:14:GLY:HA2   | 19:1S:97:LYS:HB2   | 1.68                     | 0.74              |
| 38:1m:44:ARG:HH12  | 38:1m:48:LEU:HG    | 1.52                     | 0.74              |
| 4:1D:161:ILE:HG23  | 8:1H:278:PRO:HB3   | 1.69                     | 0.74              |
| 7:1G:652:VAL:HG22  | 7:1G:653:ASN:H     | 1.53                     | 0.74              |
| 5:1E:39:PRO:HA     | 44:1s:65:GLN:HB3   | 1.70                     | 0.74              |
| 16:1P:138:ASP:HB2  | 16:1P:141:SER:HB3  | 1.68                     | 0.74              |
| 4:1D:107:ASP:HB3   | 4:1D:427:GLU:HB2   | 1.69                     | 0.74              |
| 7:1G:228:ILE:HG13  | 7:1G:581:GLN:HB3   | 1.68                     | 0.74              |
| 4:1D:66:MET:HE3    | 4:1D:76:CYS:HB3    | 1.70                     | 0.74              |
| 2:1B:113:VAL:HG13  | 2:1B:142:VAL:HA    | 1.69                     | 0.73              |
| 4:1D:413:ASP:OD1   | 8:1H:281:ARG:NH1   | 2.21                     | 0.73              |
| 6:1F:384:ALA:HB3   | 6:1F:430:MET:HE2   | 1.70                     | 0.73              |
| 3:1C:50:ILE:HD11   | 3:1C:107:VAL:HG12  | 1.70                     | 0.73              |
| 16:1P:160:PHE:HB3  | 16:1P:163:ALA:HB2  | 1.70                     | 0.73              |
| 38:1m:116:GLN:NE2  | 38:1m:117:GLU:OE2  | 2.20                     | 0.73              |
| 26:1a:23:THR:O     | 26:1a:27:HIS:ND1   | 2.21                     | 0.73              |
| 3:1C:30:ALA:HA     | 3:1C:37:VAL:HG21   | 1.70                     | 0.73              |
| 6:1F:347:ILE:HA    | 6:1F:350:LEU:HB2   | 1.71                     | 0.73              |
| 12:1L:556:ILE:HD11 | 38:1m:75:ILE:HG12  | 1.70                     | 0.73              |
| 13:1M:135:ARG:NH1  | 14:1N:304:MET:SD   | 2.61                     | 0.73              |
| 10:1J:18:VAL:HG11  | 10:1J:96:GLY:HA3   | 1.70                     | 0.73              |
| 10:1J:146:LEU:HA   | 11:1K:58:MET:HE1   | 1.69                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:1W:84:ILE:HA    | 22:1W:87:LYS:HB3   | 1.71                     | 0.73              |
| 5:1E:131:THR:HG21  | 5:1E:135:LYS:HD2   | 1.71                     | 0.72              |
| 6:1F:105:CYS:HB3   | 6:1F:108:ARG:HH21  | 1.54                     | 0.72              |
| 33:1h:62:GLU:OE1   | 33:1h:63:HIS:N     | 2.22                     | 0.72              |
| 6:1F:403:THR:HG21  | 6:1F:408:GLY:HA3   | 1.70                     | 0.72              |
| 12:1L:578:SER:HB2  | 14:1N:172:GLN:HE21 | 1.53                     | 0.72              |
| 56:1P:501:NDP:H8A  | 56:1P:501:NDP:H51A | 1.71                     | 0.72              |
| 32:1g:23:THR:O     | 32:1g:25:ARG:N     | 2.17                     | 0.72              |
| 20:1T:36:PHE:HA    | 20:1T:40:LEU:HB2   | 1.72                     | 0.72              |
| 37:1l:54:SER:HA    | 37:1l:84:TYR:HB3   | 1.70                     | 0.72              |
| 3:1C:48:LEU:HB3    | 3:1C:105:ILE:HG22  | 1.72                     | 0.72              |
| 15:1O:315:LYS:HD2  | 15:1O:316:TRP:H    | 1.54                     | 0.72              |
| 34:1i:105:PRO:O    | 40:1o:67:LYS:NZ    | 2.22                     | 0.72              |
| 10:1J:152:TRP:HE1  | 14:1N:19:LEU:HD21  | 1.55                     | 0.71              |
| 14:1N:26:TRP:HB3   | 14:1N:74:ILE:HD13  | 1.71                     | 0.71              |
| 17:1Q:22:LEU:HD23  | 22:1W:78:VAL:HG23  | 1.71                     | 0.71              |
| 16:1P:134:HIS:H    | 16:1P:149:LYS:HE3  | 1.54                     | 0.71              |
| 20:1T:54:MET:HE3   | 20:1T:76:ILE:HG21  | 1.70                     | 0.71              |
| 12:1L:106:TRP:O    | 12:1L:109:HIS:ND1  | 2.23                     | 0.71              |
| 13:1M:41:LEU:O     | 13:1M:44:GLN:NE2   | 2.23                     | 0.71              |
| 52:1M:501:PGT:H362 | 14:1N:280:THR:HG21 | 1.73                     | 0.71              |
| 15:1O:233:LYS:HD3  | 21:1V:91:ARG:NH2   | 2.06                     | 0.71              |
| 24:1Y:94:CYS:O     | 24:1Y:98:LEU:N     | 2.14                     | 0.71              |
| 27:1b:60:GLY:O     | 27:1b:61:ASN:ND2   | 2.23                     | 0.71              |
| 8:1H:215:TYR:HB3   | 8:1H:220:PHE:HB2   | 1.73                     | 0.71              |
| 12:1L:237:MET:HE3  | 12:1L:237:MET:HA   | 1.71                     | 0.71              |
| 12:1L:283:ILE:HD13 | 37:1l:112:MET:HG2  | 1.72                     | 0.71              |
| 16:1P:20:VAL:HB    | 16:1P:89:ASN:H     | 1.54                     | 0.71              |
| 38:1m:117:GLU:OE2  | 38:1m:117:GLU:N    | 2.18                     | 0.71              |
| 15:1O:15:THR:HA    | 15:1O:18:LEU:HD12  | 1.70                     | 0.71              |
| 21:1V:57:MET:HE2   | 21:1V:70:GLN:HB3   | 1.70                     | 0.71              |
| 14:1N:265:MET:HA   | 14:1N:265:MET:HE3  | 1.72                     | 0.71              |
| 15:1O:26:THR:HB    | 15:1O:169:VAL:HG12 | 1.73                     | 0.71              |
| 16:1P:300:LEU:HD22 | 16:1P:307:ALA:HB2  | 1.72                     | 0.71              |
| 6:1F:250:ASN:HD22  | 6:1F:318:ASP:HB2   | 1.56                     | 0.71              |
| 14:1N:211:MET:SD   | 14:1N:333:SER:OG   | 2.49                     | 0.71              |
| 7:1G:504:ASP:OD1   | 19:1S:55:ARG:NH1   | 2.24                     | 0.70              |
| 10:1J:171:ILE:HD11 | 11:1K:76:SER:HB2   | 1.73                     | 0.70              |
| 21:1V:82:GLN:N     | 21:1V:82:GLN:OE1   | 2.24                     | 0.70              |
| 37:1l:156:TYR:HB3  | 40:1o:33:ARG:HG2   | 1.71                     | 0.70              |
| 42:1q:73:THR:HG21  | 42:1q:81:MET:HE1   | 1.73                     | 0.70              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:314:MET:HA   | 12:1L:317:ILE:HG22 | 1.74                     | 0.70              |
| 15:1O:18:LEU:HD11  | 15:1O:256:PHE:HE2  | 1.57                     | 0.70              |
| 32:1g:62:PHE:O     | 33:1h:28:TYR:OH    | 2.07                     | 0.70              |
| 20:1T:83:LYS:HZ2   | 20:1T:84:LYS:HB3   | 1.56                     | 0.70              |
| 2:1B:52:LEU:HD21   | 2:1B:96:MET:HG2    | 1.73                     | 0.70              |
| 37:1l:136:ASN:HB3  | 37:1l:152:PRO:HA   | 1.73                     | 0.70              |
| 14:1N:18:MET:HA    | 14:1N:18:MET:HE2   | 1.74                     | 0.70              |
| 20:1U:70:LEU:HD12  | 20:1U:76:ILE:HD12  | 1.74                     | 0.70              |
| 7:1G:107:ILE:HA    | 9:1I:104:ARG:HH21  | 1.55                     | 0.70              |
| 12:1L:545:SER:HG   | 13:1M:274:SER:HG   | 1.39                     | 0.70              |
| 7:1G:288:LYS:N     | 42:1q:143:PRO:O    | 2.25                     | 0.69              |
| 20:1U:6:LEU:HD13   | 20:1U:11:ILE:HD11  | 1.74                     | 0.69              |
| 5:1E:10:ARG:HH12   | 18:1R:77:LYS:HG2   | 1.56                     | 0.69              |
| 21:1V:30:ILE:HG22  | 21:1V:87:LEU:HB2   | 1.72                     | 0.69              |
| 3:1C:40:VAL:HG12   | 3:1C:50:ILE:HG22   | 1.75                     | 0.69              |
| 9:1I:9:GLU:OE1     | 9:1I:9:GLU:N       | 2.23                     | 0.69              |
| 13:1M:164:LEU:HA   | 13:1M:167:ILE:HD12 | 1.75                     | 0.69              |
| 7:1G:43:HIS:HB3    | 7:1G:46:LEU:HB3    | 1.75                     | 0.69              |
| 22:1W:54:ILE:HG21  | 22:1W:107:PHE:HE1  | 1.57                     | 0.69              |
| 4:1D:238:ARG:HG2   | 8:1H:284:GLN:HE22  | 1.57                     | 0.69              |
| 7:1G:257:ASP:HB3   | 7:1G:369:ALA:HB2   | 1.74                     | 0.69              |
| 12:1L:533:MET:HA   | 12:1L:533:MET:HE3  | 1.75                     | 0.69              |
| 13:1M:150:LEU:HD13 | 14:1N:294:MET:HE1  | 1.73                     | 0.69              |
| 13:1M:307:TRP:NE1  | 38:1m:127:SER:OG   | 2.25                     | 0.69              |
| 14:1N:85:THR:HG22  | 14:1N:87:THR:HG23  | 1.74                     | 0.69              |
| 5:1E:165:THR:HG23  | 5:1E:167:LYS:H     | 1.58                     | 0.69              |
| 8:1H:140:ILE:HG21  | 10:1J:66:VAL:HG11  | 1.74                     | 0.69              |
| 22:1W:62:LYS:HA    | 22:1W:65:GLU:HG3   | 1.75                     | 0.69              |
| 22:1W:62:LYS:NZ    | 22:1W:65:GLU:OE2   | 2.25                     | 0.69              |
| 8:1H:276:SER:HB2   | 9:1I:37:THR:HG21   | 1.75                     | 0.69              |
| 3:1C:86:ARG:HH22   | 21:1V:113:TRP:HB2  | 1.56                     | 0.68              |
| 7:1G:378:LEU:HD21  | 7:1G:439:PHE:HZ    | 1.57                     | 0.68              |
| 21:1V:78:GLU:OE2   | 21:1V:78:GLU:N     | 2.25                     | 0.68              |
| 40:1o:52:LEU:HD13  | 40:1o:55:ARG:HD2   | 1.75                     | 0.68              |
| 7:1G:289:GLY:HA2   | 42:1q:145:LYS:C    | 2.18                     | 0.68              |
| 14:1N:237:MET:HB2  | 14:1N:240:ILE:HG12 | 1.75                     | 0.68              |
| 20:1T:47:GLN:HA    | 20:1T:50:ILE:HG12  | 1.75                     | 0.68              |
| 53:1a:101:CDL:HB22 | 43:1r:3:ALA:HA     | 1.75                     | 0.68              |
| 9:1I:150:ASN:ND2   | 42:1q:124:TYR:OH   | 2.26                     | 0.68              |
| 12:1L:10:THR:O     | 12:1L:13:ILE:N     | 2.26                     | 0.68              |
| 12:1L:593:ILE:O    | 12:1L:597:ILE:HG22 | 1.92                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:1Z:73:PRO:HD3   | 27:1b:52:TYR:HE2   | 1.59                     | 0.68              |
| 5:1E:145:LEU:HD22  | 5:1E:155:GLN:HB2   | 1.75                     | 0.68              |
| 7:1G:106:PRO:HB3   | 9:1I:80:CYS:HB2    | 1.76                     | 0.68              |
| 20:1T:11:ILE:HD11  | 20:1T:84:LYS:HE3   | 1.76                     | 0.68              |
| 7:1G:307:LEU:HD11  | 7:1G:338:VAL:HG21  | 1.76                     | 0.68              |
| 7:1G:327:ALA:HB2   | 7:1G:596:ASP:HB3   | 1.76                     | 0.68              |
| 8:1H:183:MET:HB3   | 50:1H:401:PC1:H2F2 | 1.76                     | 0.68              |
| 4:1D:390:LYS:NZ    | 4:1D:391:ILE:O     | 2.26                     | 0.68              |
| 4:1D:394:PRO:O     | 4:1D:398:HIS:ND1   | 2.25                     | 0.68              |
| 32:1g:100:ARG:HG2  | 32:1g:107:LEU:HA   | 1.76                     | 0.68              |
| 38:1m:21:GLU:OE1   | 38:1m:21:GLU:N     | 2.26                     | 0.68              |
| 4:1D:307:SER:HA    | 4:1D:310:ILE:HD12  | 1.77                     | 0.67              |
| 24:1Y:93:GLY:HA3   | 24:1Y:118:GLY:HA2  | 1.74                     | 0.67              |
| 9:1I:64:GLU:OE2    | 9:1I:149:TYR:OH    | 2.12                     | 0.67              |
| 15:1O:148:CYS:HA   | 15:1O:279:LEU:HD21 | 1.75                     | 0.67              |
| 6:1F:224:ASN:ND2   | 48:1F:501:FMN:O2   | 2.27                     | 0.67              |
| 16:1P:29:PHE:CE1   | 16:1P:176:ASP:HA   | 2.29                     | 0.67              |
| 3:1C:190:LEU:O     | 17:1Q:74:SER:OG    | 2.11                     | 0.67              |
| 30:1e:94:PRO:HD2   | 30:1e:97:HIS:CD2   | 2.29                     | 0.67              |
| 35:1j:59:TRP:O     | 40:1o:106:ARG:NH2  | 2.27                     | 0.67              |
| 40:1o:102:GLU:O    | 40:1o:106:ARG:N    | 2.27                     | 0.67              |
| 2:1B:63:ALA:HA     | 2:1B:69:MET:HB2    | 1.76                     | 0.67              |
| 4:1D:306:GLN:OE1   | 4:1D:309:ARG:NH2   | 2.26                     | 0.67              |
| 1:1A:68:GLU:OE1    | 1:1A:68:GLU:N      | 2.19                     | 0.67              |
| 7:1G:198:ASN:ND2   | 7:1G:263:ILE:O     | 2.24                     | 0.67              |
| 12:1L:532:ILE:HD11 | 37:1l:101:MET:HB3  | 1.75                     | 0.66              |
| 24:1Y:109:ILE:HD12 | 24:1Y:109:ILE:H    | 1.60                     | 0.66              |
| 35:1j:45:ASP:HB2   | 35:1j:50:HIS:HB2   | 1.77                     | 0.66              |
| 14:1N:9:LEU:HD22   | 14:1N:42:PRO:HG3   | 1.77                     | 0.66              |
| 6:1F:137:TYR:HD2   | 6:1F:192:LEU:HG    | 1.60                     | 0.66              |
| 7:1G:358:LEU:HD23  | 7:1G:645:ALA:HB2   | 1.77                     | 0.66              |
| 17:1Q:15:GLU:HG3   | 22:1W:75:ASP:HB2   | 1.75                     | 0.66              |
| 29:1d:34:MET:HG3   | 29:1d:72:GLY:HA3   | 1.77                     | 0.66              |
| 3:1C:111:THR:HG21  | 3:1C:117:ILE:HD11  | 1.75                     | 0.66              |
| 8:1H:222:MET:SD    | 8:1H:222:MET:N     | 2.68                     | 0.66              |
| 14:1N:22:ILE:O     | 30:1e:6:GLN:NE2    | 2.29                     | 0.66              |
| 15:1O:233:LYS:HD3  | 21:1V:91:ARG:HH21  | 1.59                     | 0.66              |
| 37:1l:7:ASP:O      | 37:1l:26:LYS:NZ    | 2.27                     | 0.66              |
| 37:1l:141:GLU:HA   | 41:1p:122:GLN:HB3  | 1.77                     | 0.66              |
| 6:1F:68:ARG:NH2    | 6:1F:253:THR:O     | 2.29                     | 0.66              |
| 12:1L:83:ASP:OD2   | 12:1L:262:ARG:NH1  | 2.28                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:134:GLN:O    | 14:1N:135:LYS:HD3  | 1.95                     | 0.66              |
| 30:1e:16:TRP:CD1   | 30:1e:16:TRP:H     | 2.14                     | 0.66              |
| 34:1i:110:LEU:HB3  | 41:1p:18:ALA:HB2   | 1.78                     | 0.66              |
| 22:1W:18:LYS:O     | 22:1W:77:ARG:NH1   | 2.24                     | 0.66              |
| 2:1B:55:CYS:HB3    | 2:1B:89:ALA:HB1    | 1.76                     | 0.66              |
| 15:1O:168:VAL:HG11 | 15:1O:238:ILE:HD12 | 1.78                     | 0.66              |
| 1:1A:73:LEU:O      | 8:1H:160:TYR:OH    | 2.14                     | 0.65              |
| 5:1E:6:LEU:O       | 5:1E:92:ARG:NH1    | 2.29                     | 0.65              |
| 17:1Q:58:GLU:OE1   | 17:1Q:58:GLU:N     | 2.28                     | 0.65              |
| 43:1r:32:LYS:O     | 43:1r:35:GLN:NE2   | 2.26                     | 0.65              |
| 7:1G:366:THR:OG1   | 7:1G:491:ASN:ND2   | 2.28                     | 0.65              |
| 14:1N:147:GLN:HB2  | 33:1h:125:TYR:CZ   | 2.31                     | 0.65              |
| 43:1r:63:MET:SD    | 43:1r:64:PRO:HD2   | 2.37                     | 0.65              |
| 8:1H:26:LYS:HG2    | 26:1a:5:ILE:HG12   | 1.77                     | 0.65              |
| 9:1I:45:PRO:HB2    | 9:1I:47:THR:HG23   | 1.77                     | 0.65              |
| 9:1I:57:LEU:O      | 43:1r:33:ARG:NH2   | 2.29                     | 0.65              |
| 19:1S:30:GLN:OE1   | 19:1S:33:ARG:NH1   | 2.29                     | 0.65              |
| 4:1D:165:THR:HA    | 8:1H:32:GLN:HB3    | 1.79                     | 0.65              |
| 6:1F:184:TYR:HB3   | 6:1F:357:GLU:HG2   | 1.77                     | 0.65              |
| 12:1L:357:ARG:NH1  | 39:1n:28:SER:OG    | 2.30                     | 0.65              |
| 3:1C:119:SER:OG    | 3:1C:144:ASN:O     | 2.14                     | 0.65              |
| 6:1F:14:SER:H      | 6:1F:282:LYS:HE3   | 1.61                     | 0.65              |
| 7:1G:594:ARG:HD2   | 22:1W:126:HIS:HB3  | 1.78                     | 0.65              |
| 8:1H:195:ARG:HD3   | 8:1H:196:ALA:H     | 1.59                     | 0.65              |
| 9:1I:8:ARG:HH22    | 43:1r:111:TYR:HB2  | 1.61                     | 0.65              |
| 16:1P:312:LEU:HD22 | 16:1P:313:LYS:HD3  | 1.79                     | 0.65              |
| 34:1i:27:LEU:HB2   | 34:1i:31:GLU:HB2   | 1.77                     | 0.65              |
| 20:1T:72:CYS:H     | 20:1T:75:GLU:HB2   | 1.61                     | 0.65              |
| 35:1j:5:VAL:HG23   | 35:1j:7:ILE:H      | 1.60                     | 0.65              |
| 36:1k:35:LEU:HB2   | 36:1k:40:LEU:HB2   | 1.79                     | 0.65              |
| 25:1Z:127:LEU:HD13 | 30:1e:97:HIS:CE1   | 2.32                     | 0.65              |
| 3:1C:166:PHE:HE1   | 3:1C:170:GLY:HA2   | 1.62                     | 0.65              |
| 13:1M:272:THR:HA   | 13:1M:275:ILE:HD12 | 1.79                     | 0.65              |
| 23:1X:89:ASP:OD1   | 26:1a:37:ARG:NH2   | 2.30                     | 0.65              |
| 34:1i:76:ILE:HD12  | 34:1i:77:PRO:CD    | 2.23                     | 0.65              |
| 10:1J:113:VAL:HG23 | 10:1J:119:PHE:HB2  | 1.79                     | 0.65              |
| 11:1K:5:TYR:HE1    | 11:1K:46:LEU:HB3   | 1.61                     | 0.65              |
| 14:1N:17:THR:HG23  | 14:1N:137:ALA:HB2  | 1.78                     | 0.65              |
| 4:1D:115:GLU:HB3   | 4:1D:194:ILE:HB    | 1.79                     | 0.64              |
| 5:1E:105:THR:HA    | 6:1F:349:ARG:HG3   | 1.77                     | 0.64              |
| 5:1E:124:LEU:HD13  | 5:1E:126:ILE:HG12  | 1.78                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:1J:28:TYR:HA    | 10:1J:31:LEU:HD12  | 1.79                     | 0.64              |
| 13:1M:44:GLN:HG3   | 13:1M:60:SER:HA    | 1.77                     | 0.64              |
| 21:1V:27:TYR:HE2   | 21:1V:54:LYS:HB3   | 1.60                     | 0.64              |
| 3:1C:131:GLU:OE2   | 3:1C:145:HIS:NE2   | 2.30                     | 0.64              |
| 50:1M:502:PC1:H2B1 | 32:1g:70:LEU:HD12  | 1.78                     | 0.64              |
| 17:1Q:70:MET:HG2   | 17:1Q:70:MET:O     | 1.97                     | 0.64              |
| 20:1T:36:PHE:HB2   | 20:1T:37:MET:HE3   | 1.78                     | 0.64              |
| 24:1Y:114:CYS:O    | 24:1Y:118:GLY:N    | 2.30                     | 0.64              |
| 3:1C:61:LEU:HB3    | 3:1C:123:VAL:HG21  | 1.78                     | 0.64              |
| 4:1D:20:TYR:OH     | 14:1N:295:ARG:NH2  | 2.31                     | 0.64              |
| 13:1M:14:MET:HE1   | 13:1M:30:HIS:ND1   | 2.13                     | 0.64              |
| 20:1T:45:LEU:HD11  | 22:1W:36:TYR:CE2   | 2.32                     | 0.64              |
| 3:1C:199:LEU:HD13  | 4:1D:385:ARG:HD3   | 1.80                     | 0.64              |
| 4:1D:238:ARG:NH1   | 8:1H:279:ARG:O     | 2.28                     | 0.64              |
| 5:1E:69:VAL:HA     | 5:1E:72:ILE:HG22   | 1.79                     | 0.64              |
| 7:1G:290:LEU:H     | 42:1q:143:PRO:CA   | 2.11                     | 0.64              |
| 7:1G:379:LEU:HB2   | 7:1G:408:LEU:HD13  | 1.79                     | 0.64              |
| 27:1b:78:GLU:OE1   | 27:1b:78:GLU:N     | 2.28                     | 0.64              |
| 3:1C:127:ALA:O     | 3:1C:130:TYR:N     | 2.29                     | 0.64              |
| 6:1F:49:LEU:O      | 6:1F:127:ARG:NE    | 2.26                     | 0.64              |
| 8:1H:138:GLN:HA    | 8:1H:286:MET:HE1   | 1.79                     | 0.64              |
| 9:1I:64:GLU:O      | 9:1I:134:GLY:N     | 2.30                     | 0.64              |
| 12:1L:250:SER:HB2  | 12:1L:333:ALA:HA   | 1.80                     | 0.64              |
| 13:1M:433:GLU:O    | 13:1M:437:MET:HG3  | 1.98                     | 0.64              |
| 16:1P:182:PHE:HB2  | 16:1P:245:ILE:HD13 | 1.78                     | 0.64              |
| 34:1i:71:VAL:HA    | 34:1i:75:LEU:HD12  | 1.78                     | 0.64              |
| 7:1G:192:MET:N     | 7:1G:192:MET:SD    | 2.68                     | 0.64              |
| 7:1G:284:ILE:O     | 7:1G:292:THR:OG1   | 2.10                     | 0.64              |
| 7:1G:365:ASN:HB2   | 7:1G:488:LYS:HD2   | 1.80                     | 0.64              |
| 12:1L:73:THR:O     | 41:1p:106:GLN:NE2  | 2.31                     | 0.64              |
| 15:1O:182:ARG:HG3  | 15:1O:185:LYS:HD2  | 1.80                     | 0.64              |
| 6:1F:360:GLY:HA2   | 6:1F:366:ARG:HB2   | 1.79                     | 0.64              |
| 7:1G:284:ILE:HG22  | 7:1G:285:ARG:H     | 1.63                     | 0.64              |
| 7:1G:290:LEU:N     | 42:1q:143:PRO:HA   | 2.11                     | 0.64              |
| 9:1I:172:ASP:OD2   | 9:1I:176:ARG:NH2   | 2.30                     | 0.64              |
| 12:1L:599:MET:O    | 12:1L:605:HIS:ND1  | 2.30                     | 0.64              |
| 16:1P:319:ARG:NH1  | 16:1P:327:LEU:O    | 2.30                     | 0.64              |
| 3:1C:94:TYR:HB2    | 3:1C:107:VAL:HG22  | 1.79                     | 0.64              |
| 5:1E:37:ASN:O      | 44:1s:65:GLN:NE2   | 2.30                     | 0.64              |
| 16:1P:228:PHE:HA   | 16:1P:298:PRO:HG2  | 1.78                     | 0.64              |
| 25:1Z:121:MET:HE1  | 25:1Z:137:THR:HA   | 1.79                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1B:96:MET:HE2    | 2:1B:96:MET:HA     | 1.80                     | 0.64              |
| 4:1D:157:HIS:HD2   | 4:1D:419:GLY:HA3   | 1.62                     | 0.64              |
| 7:1G:382:THR:HB    | 7:1G:454:GLY:HA3   | 1.80                     | 0.64              |
| 3:1C:132:ARG:HH21  | 3:1C:151:ILE:HG21  | 1.63                     | 0.64              |
| 12:1L:7:LEU:HD11   | 12:1L:49:VAL:HB    | 1.80                     | 0.64              |
| 12:1L:364:LYS:NZ   | 36:1k:58:ASN:O     | 2.31                     | 0.64              |
| 15:1O:199:LEU:O    | 15:1O:202:ILE:HG13 | 1.98                     | 0.64              |
| 7:1G:136:ALA:O     | 18:1R:74:ASN:ND2   | 2.31                     | 0.63              |
| 7:1G:470:VAL:HA    | 7:1G:473:ILE:HG12  | 1.79                     | 0.63              |
| 13:1M:36:LEU:HD21  | 50:1f:101:PC1:H371 | 1.79                     | 0.63              |
| 7:1G:227:SER:O     | 7:1G:253:ARG:NH2   | 2.31                     | 0.63              |
| 13:1M:72:LEU:HD23  | 13:1M:75:LEU:HD12  | 1.80                     | 0.63              |
| 32:1g:85:MET:H     | 32:1g:85:MET:HE2   | 1.63                     | 0.63              |
| 42:1q:27:LEU:O     | 42:1q:31:ASN:ND2   | 2.32                     | 0.63              |
| 8:1H:203:GLY:O     | 8:1H:208:VAL:N     | 2.31                     | 0.63              |
| 9:1I:89:ALA:O      | 9:1I:115:LYS:NZ    | 2.26                     | 0.63              |
| 9:1I:133:GLU:N     | 9:1I:133:GLU:OE1   | 2.32                     | 0.63              |
| 15:1O:76:ASN:OD1   | 15:1O:95:ARG:NE    | 2.32                     | 0.63              |
| 16:1P:166:ILE:HG22 | 16:1P:168:PRO:HD3  | 1.80                     | 0.63              |
| 1:1A:84:LEU:HD21   | 27:1b:45:ASN:HD22  | 1.62                     | 0.63              |
| 15:1O:141:GLN:NE2  | 15:1O:201:ASP:OD2  | 2.24                     | 0.63              |
| 34:1i:65:ARG:HH11  | 34:1i:65:ARG:HG2   | 1.63                     | 0.63              |
| 7:1G:381:GLY:O     | 7:1G:456:SER:OG    | 2.16                     | 0.63              |
| 52:1M:501:PGT:O4P  | 52:1M:501:PGT:O6   | 2.15                     | 0.63              |
| 7:1G:46:LEU:HD11   | 7:1G:161:ARG:HB2   | 1.80                     | 0.63              |
| 21:1V:66:LYS:C     | 21:1V:70:GLN:HE21  | 2.06                     | 0.63              |
| 37:1l:80:ASP:HB3   | 37:1l:83:MET:SD    | 2.39                     | 0.63              |
| 5:1E:72:ILE:HG23   | 5:1E:73:LEU:HD22   | 1.80                     | 0.63              |
| 5:1E:106:THR:OG1   | 6:1F:346:ALA:O     | 2.16                     | 0.63              |
| 15:1O:130:SER:O    | 15:1O:133:VAL:HG22 | 1.98                     | 0.63              |
| 31:1f:53:GLU:HG2   | 31:1f:54:VAL:HG23  | 1.80                     | 0.63              |
| 37:1l:129:GLY:HA2  | 40:1o:21:MET:HE1   | 1.81                     | 0.63              |
| 1:1A:7:LEU:HD23    | 8:1H:84:THR:HG21   | 1.81                     | 0.63              |
| 4:1D:169:TRP:CH2   | 9:1I:36:MET:HE1    | 2.34                     | 0.63              |
| 14:1N:120:GLN:HA   | 14:1N:176:ARG:HE   | 1.63                     | 0.63              |
| 14:1N:318:GLU:OE1  | 29:1d:50:ARG:NH1   | 2.31                     | 0.63              |
| 20:1U:22:TYR:OH    | 20:1U:46:ASP:OD2   | 2.16                     | 0.63              |
| 33:1h:34:ILE:HG13  | 33:1h:35:PRO:HD3   | 1.80                     | 0.63              |
| 11:1K:91:GLN:OE1   | 11:1K:91:GLN:N     | 2.23                     | 0.62              |
| 12:1L:486:MET:O    | 12:1L:489:THR:OG1  | 2.17                     | 0.62              |
| 13:1M:108:MET:HB3  | 13:1M:121:LEU:HD13 | 1.80                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:1N:339:MET:HG3  | 29:1d:34:MET:HE3  | 1.81                     | 0.62              |
| 20:1T:52:MET:HE1   | 22:1W:37:ARG:HA   | 1.81                     | 0.62              |
| 7:1G:138:GLU:HB3   | 18:1R:77:LYS:HG3  | 1.81                     | 0.62              |
| 7:1G:444:LYS:HA    | 7:1G:477:ILE:HD13 | 1.81                     | 0.62              |
| 20:1T:66:ASP:OD1   | 20:1T:66:ASP:N    | 2.30                     | 0.62              |
| 5:1E:194:GLU:OE1   | 6:1F:26:TYR:OH    | 2.16                     | 0.62              |
| 25:1Z:21:TYR:O     | 25:1Z:21:TYR:HD2  | 1.81                     | 0.62              |
| 38:1m:122:GLN:HB2  | 38:1m:125:ASN:HB3 | 1.81                     | 0.62              |
| 9:1I:113:MET:HE1   | 9:1I:118:TYR:CE2  | 2.34                     | 0.62              |
| 16:1P:98:GLU:O     | 16:1P:145:TYR:OH  | 2.15                     | 0.62              |
| 21:1V:74:GLY:HA2   | 43:1r:102:ARG:NH1 | 2.14                     | 0.62              |
| 5:1E:35:VAL:HG23   | 5:1E:43:LYS:HB2   | 1.81                     | 0.62              |
| 20:1U:45:LEU:HD21  | 39:1n:44:ARG:HD2  | 1.81                     | 0.62              |
| 23:1X:134:ARG:O    | 27:1b:57:ARG:NH2  | 2.32                     | 0.62              |
| 43:1r:1:ALA:O      | 43:1r:2:SER:N     | 2.33                     | 0.62              |
| 3:1C:97:LEU:HD23   | 3:1C:104:GLN:HG3  | 1.79                     | 0.62              |
| 4:1D:228:MET:O     | 4:1D:232:ASN:ND2  | 2.31                     | 0.62              |
| 7:1G:266:LYS:NZ    | 7:1G:671:PHE:O    | 2.32                     | 0.62              |
| 14:1N:36:ASN:OD1   | 14:1N:134:GLN:NE2 | 2.32                     | 0.62              |
| 18:1R:79:THR:OG1   | 18:1R:80:LYS:N    | 2.18                     | 0.62              |
| 30:1e:80:ARG:NH1   | 30:1e:83:ASP:OD2  | 2.32                     | 0.62              |
| 3:1C:72:PHE:O      | 3:1C:124:TYR:OH   | 2.14                     | 0.62              |
| 3:1C:131:GLU:HA    | 3:1C:134:ILE:HG22 | 1.81                     | 0.62              |
| 3:1C:193:GLU:OE1   | 3:1C:193:GLU:N    | 2.22                     | 0.62              |
| 3:1C:204:GLU:HA    | 17:1Q:50:ASN:ND2  | 2.13                     | 0.62              |
| 15:1O:133:VAL:HG21 | 15:1O:206:TYR:CE1 | 2.34                     | 0.62              |
| 7:1G:288:LYS:H     | 42:1q:143:PRO:CD  | 2.11                     | 0.62              |
| 12:1L:210:ASN:HB3  | 12:1L:211:MET:HE2 | 1.82                     | 0.62              |
| 16:1P:46:ILE:HD13  | 18:1R:26:VAL:HG21 | 1.80                     | 0.62              |
| 3:1C:185:ALA:HB2   | 22:1W:105:ARG:HE  | 1.64                     | 0.62              |
| 6:1F:298:ILE:HB    | 6:1F:335:ILE:HB   | 1.82                     | 0.62              |
| 6:1F:410:GLY:HA2   | 6:1F:413:TRP:CZ3  | 2.34                     | 0.62              |
| 13:1M:235:LEU:HA   | 13:1M:238:LEU:HB3 | 1.82                     | 0.62              |
| 29:1d:104:LYS:NZ   | 41:1p:78:GLU:OE2  | 2.33                     | 0.62              |
| 5:1E:31:ILE:HG22   | 5:1E:50:VAL:HG23  | 1.82                     | 0.62              |
| 6:1F:258:ILE:HD11  | 6:1F:262:VAL:HG21 | 1.82                     | 0.62              |
| 15:1O:230:ASP:OD2  | 15:1O:233:LYS:N   | 2.32                     | 0.62              |
| 17:1Q:91:ASP:OD1   | 17:1Q:91:ASP:N    | 2.33                     | 0.62              |
| 37:1l:50:LEU:HD11  | 37:1l:76:PRO:HB2  | 1.82                     | 0.62              |
| 3:1C:58:ILE:HD11   | 3:1C:118:GLU:HB2  | 1.81                     | 0.61              |
| 5:1E:145:LEU:O     | 5:1E:160:TYR:OH   | 2.17                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:243:ALA:HA    | 6:1F:251:SER:HB2   | 1.81                     | 0.61              |
| 10:1J:125:TRP:HB2  | 25:1Z:137:THR:HG21 | 1.81                     | 0.61              |
| 15:1O:170:VAL:HG13 | 15:1O:223:TYR:HD2  | 1.64                     | 0.61              |
| 19:1S:72:GLN:HG2   | 19:1S:74:LYS:HE2   | 1.81                     | 0.61              |
| 39:1n:123:GLN:OE1  | 39:1n:126:ARG:NH2  | 2.33                     | 0.61              |
| 2:1B:125:TYR:CE1   | 9:1I:88:PRO:HB2    | 2.26                     | 0.61              |
| 4:1D:239:THR:O     | 4:1D:294:TYR:N     | 2.32                     | 0.61              |
| 10:1J:55:MET:HE1   | 10:1J:59:ILE:HD13  | 1.80                     | 0.61              |
| 14:1N:66:ALA:HB2   | 14:1N:104:MET:HG2  | 1.82                     | 0.61              |
| 7:1G:460:ARG:NE    | 7:1G:462:ASP:OD1   | 2.33                     | 0.61              |
| 7:1G:503:LEU:HD12  | 7:1G:509:PRO:HB3   | 1.81                     | 0.61              |
| 8:1H:183:MET:HE3   | 50:1H:401:PC1:H372 | 1.81                     | 0.61              |
| 12:1L:407:TRP:NE1  | 37:1l:112:MET:SD   | 2.72                     | 0.61              |
| 18:1R:93:GLN:HG3   | 18:1R:95:HIS:H     | 1.64                     | 0.61              |
| 25:1Z:58:ARG:NH2   | 27:1b:48:THR:OG1   | 2.33                     | 0.61              |
| 8:1H:207:LEU:HD23  | 8:1H:210:GLY:HA2   | 1.82                     | 0.61              |
| 9:1I:136:ASN:HD22  | 9:1I:161:TRP:HZ2   | 1.47                     | 0.61              |
| 26:1a:39:ALA:HA    | 26:1a:44:GLN:HB2   | 1.82                     | 0.61              |
| 14:1N:170:LEU:HD21 | 14:1N:291:TYR:HB3  | 1.82                     | 0.61              |
| 16:1P:22:THR:HG23  | 16:1P:46:ILE:HB    | 1.82                     | 0.61              |
| 16:1P:143:SER:OG   | 16:1P:282:ASP:OD1  | 2.17                     | 0.61              |
| 29:1d:119:VAL:HG21 | 41:1p:146:GLY:HA2  | 1.82                     | 0.61              |
| 37:1l:63:ASP:O     | 38:1m:43:LYS:NZ    | 2.33                     | 0.61              |
| 4:1D:111:MET:N     | 4:1D:111:MET:SD    | 2.73                     | 0.61              |
| 7:1G:155:GLN:NE2   | 7:1G:181:MET:O     | 2.34                     | 0.61              |
| 12:1L:340:PHE:O    | 12:1L:344:GLY:N    | 2.33                     | 0.61              |
| 16:1P:263:TYR:HD1  | 16:1P:284:VAL:HB   | 1.66                     | 0.61              |
| 29:1d:46:ASN:HD21  | 29:1d:61:GLN:HE21  | 1.49                     | 0.61              |
| 38:1m:16:THR:HG23  | 38:1m:17:LEU:HD12  | 1.82                     | 0.61              |
| 42:1q:60:ARG:NH2   | 42:1q:95:ASP:OD1   | 2.33                     | 0.61              |
| 6:1F:162:ILE:HB    | 6:1F:174:ASP:HA    | 1.82                     | 0.61              |
| 13:1M:22:MET:O     | 13:1M:26:ASN:ND2   | 2.33                     | 0.61              |
| 16:1P:208:VAL:HG22 | 16:1P:212:LYS:HE2  | 1.82                     | 0.61              |
| 16:1P:263:TYR:CD1  | 16:1P:284:VAL:HB   | 2.36                     | 0.61              |
| 6:1F:112:ARG:HB3   | 6:1F:145:GLU:HG3   | 1.82                     | 0.61              |
| 6:1F:301:GLY:H     | 6:1F:333:ALA:HB3   | 1.65                     | 0.61              |
| 7:1G:213:TYR:O     | 7:1G:216:THR:OG1   | 2.18                     | 0.61              |
| 7:1G:672:TYR:HB3   | 7:1G:684:MET:SD    | 2.41                     | 0.61              |
| 9:1I:44:GLU:OE1    | 9:1I:44:GLU:N      | 2.34                     | 0.61              |
| 20:1T:18:VAL:HG21  | 20:1T:57:GLU:HG2   | 1.83                     | 0.61              |
| 23:1X:124:LEU:HD21 | 25:1Z:70:ALA:HB2   | 1.83                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:337:MET:HE1   | 6:1F:343:ILE:HA    | 1.81                     | 0.61              |
| 13:1M:72:LEU:HA    | 13:1M:75:LEU:HD12  | 1.81                     | 0.61              |
| 16:1P:258:LEU:HD12 | 16:1P:263:TYR:CD2  | 2.35                     | 0.61              |
| 19:1S:81:PHE:CE1   | 19:1S:85:GLN:HG2   | 2.35                     | 0.61              |
| 4:1D:87:THR:OG1    | 4:1D:88:GLU:OE1    | 2.19                     | 0.61              |
| 7:1G:314:ASP:HB2   | 7:1G:520:LYS:HB2   | 1.83                     | 0.61              |
| 7:1G:481:SER:O     | 7:1G:484:THR:OG1   | 2.15                     | 0.61              |
| 12:1L:434:LYS:NZ   | 36:1k:56:PHE:O     | 2.31                     | 0.61              |
| 19:1S:57:CYS:SG    | 19:1S:58:SER:N     | 2.74                     | 0.61              |
| 3:1C:199:LEU:HD23  | 4:1D:354:GLU:HA    | 1.82                     | 0.60              |
| 4:1D:322:GLU:HG2   | 43:1r:43:GLY:HA2   | 1.83                     | 0.60              |
| 12:1L:159:HIS:HE1  | 13:1M:349:GLN:HB3  | 1.64                     | 0.60              |
| 16:1P:258:LEU:HD12 | 16:1P:263:TYR:HD2  | 1.66                     | 0.60              |
| 17:1Q:40:PRO:HD3   | 17:1Q:56:LYS:HD2   | 1.83                     | 0.60              |
| 3:1C:113:GLU:OE1   | 3:1C:113:GLU:N     | 2.30                     | 0.60              |
| 4:1D:270:ARG:HG2   | 4:1D:278:TYR:CE2   | 2.37                     | 0.60              |
| 7:1G:272:ASP:HB2   | 7:1G:681:SER:HB2   | 1.83                     | 0.60              |
| 10:1J:64:MET:HE1   | 11:1K:68:ALA:HA    | 1.82                     | 0.60              |
| 16:1P:107:GLU:OE1  | 16:1P:112:LYS:NZ   | 2.34                     | 0.60              |
| 19:1S:38:LYS:O     | 19:1S:38:LYS:NZ    | 2.32                     | 0.60              |
| 19:1S:44:LYS:NZ    | 19:1S:50:LEU:O     | 2.34                     | 0.60              |
| 3:1C:117:ILE:O     | 3:1C:143:ALA:N     | 2.30                     | 0.60              |
| 8:1H:284:GLN:HA    | 8:1H:287:HIS:HB3   | 1.83                     | 0.60              |
| 13:1M:60:SER:HB3   | 13:1M:457:PRO:HA   | 1.83                     | 0.60              |
| 13:1M:447:LEU:HD21 | 13:1M:454:ILE:HD13 | 1.84                     | 0.60              |
| 17:1Q:127:ARG:HD3  | 44:1s:70:ARG:HH22  | 1.66                     | 0.60              |
| 23:1X:47:TRP:CH2   | 33:1h:141:PRO:HD3  | 2.36                     | 0.60              |
| 1:1A:10:ASN:ND2    | 8:1H:10:ILE:HD11   | 2.17                     | 0.60              |
| 4:1D:326:ASP:HB2   | 43:1r:44:PRO:HD2   | 1.84                     | 0.60              |
| 5:1E:111:ARG:NH1   | 6:1F:260:GLY:O     | 2.33                     | 0.60              |
| 7:1G:282:PRO:O     | 7:1G:294:THR:OG1   | 2.15                     | 0.60              |
| 7:1G:437:HIS:NE2   | 7:1G:439:PHE:HB3   | 2.16                     | 0.60              |
| 12:1L:574:SER:OG   | 14:1N:167:TRP:O    | 2.17                     | 0.60              |
| 13:1M:153:THR:HA   | 13:1M:205:VAL:HG11 | 1.83                     | 0.60              |
| 38:1m:54:ASN:OD1   | 39:1n:129:ARG:NH2  | 2.33                     | 0.60              |
| 4:1D:246:THR:HA    | 21:1V:11:VAL:HG13  | 1.82                     | 0.60              |
| 8:1H:149:ILE:HG21  | 8:1H:185:TRP:HB2   | 1.82                     | 0.60              |
| 21:1V:43:TYR:HB2   | 21:1V:99:TRP:HZ2   | 1.65                     | 0.60              |
| 40:1o:61:TYR:CD2   | 40:1o:89:CYS:HB2   | 2.36                     | 0.60              |
| 2:1B:165:ARG:NH1   | 42:1q:78:ASP:OD1   | 2.34                     | 0.60              |
| 5:1E:27:ASN:HA     | 5:1E:30:ARG:HD2    | 1.82                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:587:TYR:O    | 12:1L:590:SER:OG   | 2.19                     | 0.60              |
| 13:1M:115:LEU:HB3  | 13:1M:164:LEU:HD23 | 1.83                     | 0.60              |
| 34:1i:18:ARG:NH1   | 39:1n:172:ARG:O    | 2.34                     | 0.60              |
| 1:1A:9:THR:HG21    | 8:1H:6:ILE:HG21    | 1.83                     | 0.60              |
| 7:1G:347:GLU:OE1   | 7:1G:459:GLN:NE2   | 2.35                     | 0.60              |
| 12:1L:97:THR:HG21  | 12:1L:125:LEU:HD11 | 1.84                     | 0.60              |
| 14:1N:62:THR:HG21  | 14:1N:114:TRP:CD1  | 2.37                     | 0.60              |
| 17:1Q:15:GLU:HG2   | 22:1W:74:THR:HG23  | 1.83                     | 0.60              |
| 32:1g:66:PHE:HA    | 32:1g:70:LEU:HB3   | 1.83                     | 0.60              |
| 4:1D:169:TRP:NE1   | 8:1H:32:GLN:HA     | 2.17                     | 0.60              |
| 5:1E:100:ILE:HA    | 5:1E:156:ILE:HG22  | 1.83                     | 0.60              |
| 7:1G:169:VAL:HG21  | 7:1G:191:PHE:HE1   | 1.66                     | 0.60              |
| 13:1M:237:LYS:HE3  | 13:1M:319:HIS:HD1  | 1.67                     | 0.60              |
| 7:1G:283:MET:HB3   | 7:1G:291:LEU:HD12  | 1.83                     | 0.60              |
| 7:1G:295:THR:OG1   | 7:1G:297:GLU:OE1   | 2.20                     | 0.60              |
| 7:1G:348:VAL:N     | 7:1G:459:GLN:OE1   | 2.34                     | 0.60              |
| 9:1I:123:GLN:NE2   | 9:1I:132:VAL:HG12  | 2.17                     | 0.60              |
| 17:1Q:90:GLU:OE1   | 17:1Q:90:GLU:N     | 2.25                     | 0.60              |
| 19:1S:26:SER:O     | 19:1S:33:ARG:NH2   | 2.35                     | 0.60              |
| 27:1b:27:LEU:HB3   | 27:1b:31:LEU:HD11  | 1.83                     | 0.60              |
| 1:1A:21:ALA:HB1    | 8:1H:218:GLY:HA2   | 1.83                     | 0.60              |
| 6:1F:276:LEU:HD23  | 6:1F:317:MET:HG2   | 1.83                     | 0.60              |
| 13:1M:47:GLU:HB3   | 41:1p:92:ARG:HE    | 1.67                     | 0.60              |
| 20:1U:21:LEU:O     | 36:1k:46:ARG:NH2   | 2.35                     | 0.60              |
| 21:1V:27:TYR:HB3   | 21:1V:55:LEU:HD22  | 1.83                     | 0.60              |
| 21:1V:37:ILE:O     | 21:1V:44:ARG:NH1   | 2.35                     | 0.60              |
| 24:1Y:80:ARG:NH1   | 24:1Y:88:ASN:OD1   | 2.35                     | 0.60              |
| 44:1s:63:MET:HE3   | 44:1s:64:PRO:HD3   | 1.84                     | 0.60              |
| 5:1E:27:ASN:OD1    | 5:1E:30:ARG:NH1    | 2.33                     | 0.59              |
| 12:1L:324:LEU:HG   | 12:1L:476:THR:HG21 | 1.84                     | 0.59              |
| 13:1M:106:LEU:HD13 | 13:1M:234:VAL:HG11 | 1.84                     | 0.59              |
| 18:1R:57:ILE:HG12  | 18:1R:75:LEU:HD12  | 1.84                     | 0.59              |
| 33:1h:17:TYR:HE1   | 39:1n:107:HIS:HB2  | 1.67                     | 0.59              |
| 7:1G:6:SER:OG      | 7:1G:7:ASN:N       | 2.35                     | 0.59              |
| 9:1I:99:ARG:NH2    | 9:1I:101:ASP:OD2   | 2.34                     | 0.59              |
| 13:1M:257:MET:HE3  | 13:1M:260:PRO:HG2  | 1.82                     | 0.59              |
| 16:1P:168:PRO:HA   | 16:1P:230:PHE:HB2  | 1.83                     | 0.59              |
| 36:1k:23:ILE:HG12  | 36:1k:32:GLN:HG3   | 1.82                     | 0.59              |
| 1:1A:10:ASN:HD22   | 8:1H:10:ILE:HD11   | 1.68                     | 0.59              |
| 3:1C:116:PRO:HB2   | 3:1C:143:ALA:HB2   | 1.85                     | 0.59              |
| 4:1D:332:PRO:HB3   | 4:1D:352:TYR:HE1   | 1.66                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:1G:10:GLU:O     | 7:1G:75:LYS:NZ     | 2.32                     | 0.59              |
| 12:1L:425:ARG:NH2 | 45:1L:704:3PE:O13  | 2.35                     | 0.59              |
| 16:1P:230:PHE:HD2 | 16:1P:300:LEU:HD12 | 1.67                     | 0.59              |
| 20:1T:22:TYR:HD2  | 20:1T:23:ASP:H     | 1.51                     | 0.59              |
| 25:1Z:56:GLU:HA   | 25:1Z:59:ARG:HD3   | 1.82                     | 0.59              |
| 37:1l:34:TYR:OH   | 37:1l:46:ASP:O     | 2.19                     | 0.59              |
| 41:1p:88:GLU:OE2  | 41:1p:150:SER:OG   | 2.18                     | 0.59              |
| 6:1F:95:VAL:HG22  | 6:1F:228:VAL:HG21  | 1.84                     | 0.59              |
| 6:1F:309:LYS:HA   | 6:1F:312:CYS:HB2   | 1.84                     | 0.59              |
| 9:1I:113:MET:HB2  | 9:1I:147:LEU:O     | 2.03                     | 0.59              |
| 12:1L:14:ILE:H    | 12:1L:14:ILE:HD12  | 1.67                     | 0.59              |
| 14:1N:5:ILE:HA    | 14:1N:8:THR:HG22   | 1.84                     | 0.59              |
| 20:1U:48:VAL:HG21 | 39:1n:16:LEU:HB3   | 1.84                     | 0.59              |
| 34:1i:71:VAL:O    | 34:1i:76:ILE:HG13  | 2.02                     | 0.59              |
| 34:1i:107:ASP:H   | 40:1o:67:LYS:HZ1   | 1.50                     | 0.59              |
| 39:1n:167:TRP:O   | 39:1n:171:THR:OG1  | 2.16                     | 0.59              |
| 5:1E:22:ASP:OD1   | 5:1E:23:PHE:N      | 2.35                     | 0.59              |
| 6:1F:137:TYR:CE1  | 6:1F:180:GLY:HA2   | 2.37                     | 0.59              |
| 20:1T:40:LEU:HB3  | 20:1T:42:LEU:HG    | 1.84                     | 0.59              |
| 2:1B:81:ARG:HD2   | 8:1H:61:LEU:HD21   | 1.85                     | 0.59              |
| 4:1D:295:ASP:OD1  | 9:1I:6:ASN:ND2     | 2.33                     | 0.59              |
| 6:1F:365:CYS:HB2  | 46:1F:502:SF4:S2   | 2.43                     | 0.59              |
| 12:1L:310:LEU:HA  | 12:1L:313:MET:HG3  | 1.84                     | 0.59              |
| 32:1g:112:CYS:SG  | 32:1g:113:PHE:N    | 2.76                     | 0.59              |
| 34:1i:102:ARG:HB2 | 40:1o:49:GLN:HG2   | 1.84                     | 0.59              |
| 1:1A:106:TRP:NE1  | 45:1A:201:3PE:O12  | 2.24                     | 0.59              |
| 6:1F:199:LYS:HE3  | 17:1Q:132:THR:HA   | 1.84                     | 0.59              |
| 10:1J:125:TRP:HH2 | 25:1Z:126:GLY:HA2  | 1.67                     | 0.59              |
| 45:1L:703:3PE:O14 | 24:1Y:58:TYR:OH    | 2.15                     | 0.59              |
| 13:1M:6:ILE:HD12  | 31:1f:23:GLY:HA2   | 1.83                     | 0.59              |
| 13:1M:338:HIS:NE2 | 32:1g:34:ASP:OD2   | 2.35                     | 0.59              |
| 14:1N:344:SER:HB2 | 29:1d:82:MET:HB3   | 1.84                     | 0.59              |
| 31:1f:42:LEU:HD23 | 31:1f:42:LEU:H     | 1.67                     | 0.59              |
| 1:1A:54:LYS:NZ    | 4:1D:71:GLU:OE1    | 2.23                     | 0.59              |
| 4:1D:111:MET:HE3  | 4:1D:189:MET:HG3   | 1.85                     | 0.59              |
| 4:1D:300:ARG:NH2  | 4:1D:422:ASP:OD2   | 2.35                     | 0.59              |
| 4:1D:305:ARG:NH1  | 25:1Z:22:LYS:O     | 2.36                     | 0.59              |
| 10:1J:68:PHE:HZ   | 11:1K:30:LEU:HB3   | 1.67                     | 0.59              |
| 14:1N:319:HIS:HD2 | 14:1N:321:LYS:H    | 1.50                     | 0.59              |
| 25:1Z:138:TYR:HB3 | 25:1Z:142:TRP:CD1  | 2.38                     | 0.59              |
| 3:1C:158:GLU:OE2  | 3:1C:158:GLU:N     | 2.31                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:285:ARG:HH11  | 7:1G:291:LEU:HD22  | 1.67                     | 0.59              |
| 8:1H:207:LEU:O     | 8:1H:209:SER:N     | 2.35                     | 0.59              |
| 12:1L:132:VAL:HG23 | 12:1L:258:PHE:CZ   | 2.38                     | 0.59              |
| 3:1C:127:ALA:HA    | 3:1C:130:TYR:HD1   | 1.68                     | 0.59              |
| 4:1D:220:PHE:HD2   | 43:1r:17:ARG:HH21  | 1.49                     | 0.59              |
| 7:1G:632:ARG:NH2   | 19:1S:59:ASP:OD1   | 2.34                     | 0.59              |
| 8:1H:168:THR:OG1   | 25:1Z:57:ARG:NH1   | 2.35                     | 0.59              |
| 12:1L:81:LYS:C     | 12:1L:82:MET:HE2   | 2.28                     | 0.59              |
| 23:1X:126:LYS:HD2  | 27:1b:66:PRO:HG3   | 1.85                     | 0.59              |
| 25:1Z:28:ARG:NH2   | 43:1r:13:TRP:O     | 2.31                     | 0.59              |
| 29:1d:10:PRO:HG3   | 30:1e:4:ASP:HB3    | 1.84                     | 0.59              |
| 4:1D:289:SER:OG    | 4:1D:290:ARG:N     | 2.26                     | 0.58              |
| 42:1q:2:GLU:HA     | 42:1q:5:GLN:HE22   | 1.68                     | 0.58              |
| 3:1C:50:ILE:HD13   | 3:1C:52:ILE:HG23   | 1.84                     | 0.58              |
| 12:1L:359:MET:N    | 12:1L:359:MET:SD   | 2.76                     | 0.58              |
| 12:1L:482:MET:HB3  | 12:1L:486:MET:SD   | 2.43                     | 0.58              |
| 7:1G:433:ALA:O     | 7:1G:476:ASN:ND2   | 2.37                     | 0.58              |
| 7:1G:693:GLU:N     | 7:1G:693:GLU:OE2   | 2.35                     | 0.58              |
| 12:1L:526:LEU:HD23 | 12:1L:530:PRO:HG2  | 1.86                     | 0.58              |
| 20:1T:31:SER:N     | 20:1T:34:SER:OG    | 2.36                     | 0.58              |
| 20:1T:34:SER:H     | 20:1T:73:PRO:HD2   | 1.69                     | 0.58              |
| 6:1F:264:HIS:ND1   | 6:1F:284:ALA:O     | 2.31                     | 0.58              |
| 7:1G:283:MET:HG3   | 7:1G:291:LEU:HB3   | 1.85                     | 0.58              |
| 7:1G:673:MET:HA    | 7:1G:673:MET:HE3   | 1.85                     | 0.58              |
| 12:1L:12:LEU:HD11  | 12:1L:129:MET:HB2  | 1.85                     | 0.58              |
| 12:1L:132:VAL:O    | 12:1L:262:ARG:NH2  | 2.25                     | 0.58              |
| 12:1L:295:GLN:O    | 12:1L:425:ARG:NH1  | 2.37                     | 0.58              |
| 16:1P:236:TYR:HB3  | 16:1P:240:ASP:HB3  | 1.83                     | 0.58              |
| 23:1X:95:LEU:HD13  | 23:1X:97:ARG:HG3   | 1.85                     | 0.58              |
| 4:1D:66:MET:HE2    | 4:1D:73:VAL:HG21   | 1.84                     | 0.58              |
| 7:1G:108:CYS:O     | 7:1G:218:ARG:NH1   | 2.22                     | 0.58              |
| 9:1I:76:ARG:NH1    | 9:1I:129:ASP:OD1   | 2.34                     | 0.58              |
| 12:1L:346:ILE:HD11 | 12:1L:359:MET:HG2  | 1.85                     | 0.58              |
| 17:1Q:55:TRP:O     | 17:1Q:86:PHE:N     | 2.35                     | 0.58              |
| 23:1X:11:ASP:N     | 23:1X:11:ASP:OD1   | 2.33                     | 0.58              |
| 25:1Z:59:ARG:NH2   | 27:1b:81:LYS:O     | 2.37                     | 0.58              |
| 2:1B:109:GLU:OE2   | 2:1B:111:ARG:NE    | 2.37                     | 0.58              |
| 3:1C:32:ILE:HG22   | 3:1C:33:LEU:HD12   | 1.85                     | 0.58              |
| 4:1D:51:PHE:HB3    | 4:1D:64:LEU:HB3    | 1.86                     | 0.58              |
| 16:1P:200:THR:O    | 16:1P:238:LEU:N    | 2.37                     | 0.58              |
| 16:1P:236:TYR:HB2  | 16:1P:241:LEU:HD23 | 1.84                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1T:51:ILE:HB    | 20:1T:62:ILE:HD11  | 1.85                     | 0.58              |
| 35:1j:33:TRP:O     | 35:1j:37:LEU:HD12  | 2.03                     | 0.58              |
| 6:1F:259:SER:N     | 6:1F:334:VAL:O     | 2.31                     | 0.58              |
| 11:1K:2:PRO:HD3    | 30:1e:72:MET:HE1   | 1.84                     | 0.58              |
| 13:1M:204:MET:HA   | 13:1M:207:MET:HB2  | 1.85                     | 0.58              |
| 34:1i:4:THR:OG1    | 34:1i:6:ASP:OD1    | 2.16                     | 0.58              |
| 7:1G:667:THR:HG22  | 7:1G:668:ILE:H     | 1.68                     | 0.58              |
| 12:1L:293:ILE:HD12 | 12:1L:294:THR:HG23 | 1.86                     | 0.58              |
| 20:1T:14:ARG:HA    | 20:1T:17:TYR:CD1   | 2.39                     | 0.58              |
| 37:1l:59:ASP:O     | 37:1l:64:TRP:NE1   | 2.34                     | 0.58              |
| 38:1m:52:ASP:OD1   | 38:1m:54:ASN:ND2   | 2.34                     | 0.58              |
| 1:1A:110:GLY:HA2   | 10:1J:169:MET:HE2  | 1.86                     | 0.58              |
| 3:1C:116:PRO:HG3   | 22:1W:20:ILE:HG23  | 1.86                     | 0.58              |
| 7:1G:283:MET:HB3   | 7:1G:560:ILE:HB    | 1.85                     | 0.58              |
| 8:1H:29:GLY:O      | 8:1H:34:ARG:N      | 2.37                     | 0.58              |
| 13:1M:70:THR:HA    | 13:1M:103:GLN:HE21 | 1.68                     | 0.58              |
| 7:1G:632:ARG:HB3   | 7:1G:635:ASP:HB2   | 1.85                     | 0.58              |
| 13:1M:261:PHE:HB2  | 13:1M:302:MET:HE1  | 1.86                     | 0.58              |
| 14:1N:292:PHE:HA   | 14:1N:295:ARG:HB3  | 1.84                     | 0.58              |
| 16:1P:153:GLU:OE1  | 16:1P:165:ILE:HG12 | 2.03                     | 0.58              |
| 20:1T:13:ASP:OD1   | 20:1T:14:ARG:N     | 2.37                     | 0.58              |
| 33:1h:114:MET:HG2  | 33:1h:122:TRP:CD1  | 2.38                     | 0.58              |
| 4:1D:200:HIS:NE2   | 9:1I:124:GLU:OE2   | 2.37                     | 0.57              |
| 4:1D:430:ARG:HH11  | 4:1D:430:ARG:H     | 1.50                     | 0.57              |
| 7:1G:549:HIS:HB2   | 7:1G:676:SER:HB2   | 1.85                     | 0.57              |
| 8:1H:65:THR:HA     | 16:1P:324:TYR:HB3  | 1.86                     | 0.57              |
| 8:1H:235:ASN:CG    | 8:1H:266:LEU:HB3   | 2.29                     | 0.57              |
| 8:1H:269:THR:HA    | 8:1H:272:TRP:HB3   | 1.86                     | 0.57              |
| 9:1I:119:CYS:HB2   | 9:1I:121:PHE:H     | 1.68                     | 0.57              |
| 20:1T:11:ILE:HG23  | 20:1T:80:ILE:HG22  | 1.85                     | 0.57              |
| 22:1W:34:GLU:HA    | 22:1W:37:ARG:HG2   | 1.86                     | 0.57              |
| 22:1W:99:GLN:H     | 22:1W:102:HIS:HD2  | 1.52                     | 0.57              |
| 36:1k:49:ALA:O     | 36:1k:53:SER:OG    | 2.18                     | 0.57              |
| 37:1l:94:THR:HG22  | 37:1l:96:VAL:H     | 1.69                     | 0.57              |
| 2:1B:61:HIS:HA     | 4:1D:171:PHE:HZ    | 1.69                     | 0.57              |
| 2:1B:81:ARG:HG3    | 8:1H:216:ALA:HB2   | 1.87                     | 0.57              |
| 4:1D:238:ARG:HD2   | 8:1H:281:ARG:HG2   | 1.85                     | 0.57              |
| 7:1G:138:GLU:N     | 7:1G:138:GLU:OE1   | 2.35                     | 0.57              |
| 12:1L:417:SER:HB2  | 12:1L:493:VAL:HB   | 1.85                     | 0.57              |
| 12:1L:502:LEU:O    | 12:1L:506:ASN:ND2  | 2.37                     | 0.57              |
| 17:1Q:13:VAL:HG12  | 17:1Q:15:GLU:HB2   | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1U:8:LEU:HD12   | 20:1U:9:GLU:OE1    | 2.03                     | 0.57              |
| 21:1V:44:ARG:O     | 21:1V:48:GLU:HG3   | 2.04                     | 0.57              |
| 50:1f:101:PC1:H3A1 | 32:1g:72:LEU:HD11  | 1.84                     | 0.57              |
| 4:1D:157:HIS:CD2   | 4:1D:419:GLY:HA3   | 2.40                     | 0.57              |
| 5:1E:154:VAL:HG12  | 5:1E:161:TYR:HB2   | 1.85                     | 0.57              |
| 14:1N:320:THR:OG1  | 15:1O:265:ASN:ND2  | 2.37                     | 0.57              |
| 15:1O:311:ASP:OD1  | 15:1O:312:VAL:N    | 2.36                     | 0.57              |
| 17:1Q:89:LYS:O     | 17:1Q:93:VAL:HG12  | 2.04                     | 0.57              |
| 21:1V:85:ASN:O     | 21:1V:89:LEU:N     | 2.35                     | 0.57              |
| 4:1D:405:MET:HE3   | 4:1D:417:ILE:HD12  | 1.85                     | 0.57              |
| 13:1M:13:PRO:HB3   | 45:1N:401:3PE:H2C1 | 1.86                     | 0.57              |
| 13:1M:216:LEU:HD13 | 13:1M:220:HIS:NE2  | 2.20                     | 0.57              |
| 52:1M:501:PGT:H131 | 52:1M:501:PGT:H361 | 1.85                     | 0.57              |
| 20:1T:34:SER:HB2   | 20:1T:73:PRO:HG2   | 1.86                     | 0.57              |
| 22:1W:87:LYS:O     | 22:1W:87:LYS:HD3   | 2.04                     | 0.57              |
| 33:1h:130:LYS:O    | 33:1h:133:ILE:HG13 | 2.04                     | 0.57              |
| 37:1l:65:ASP:HB3   | 38:1m:46:TYR:HE2   | 1.69                     | 0.57              |
| 5:1E:48:LEU:HB3    | 5:1E:49:PRO:HD3    | 1.86                     | 0.57              |
| 7:1G:704:CYS:SG    | 9:1I:103:SER:HA    | 2.44                     | 0.57              |
| 13:1M:183:SER:O    | 41:1p:152:ARG:NH2  | 2.36                     | 0.57              |
| 32:1g:66:PHE:HB2   | 33:1h:28:TYR:CE2   | 2.39                     | 0.57              |
| 36:1k:12:LYS:HA    | 36:1k:12:LYS:HE3   | 1.86                     | 0.57              |
| 7:1G:362:TYR:OH    | 7:1G:504:ASP:OD1   | 2.19                     | 0.57              |
| 9:1I:72:SER:O      | 42:1q:107:LYS:NZ   | 2.36                     | 0.57              |
| 50:1I:203:PC1:H11  | 25:1Z:29:GLY:HA3   | 1.86                     | 0.57              |
| 15:1O:78:SER:O     | 15:1O:92:ASN:ND2   | 2.36                     | 0.57              |
| 42:1q:5:GLN:HA     | 42:1q:8:ARG:HB3    | 1.86                     | 0.57              |
| 4:1D:303:GLU:O     | 4:1D:307:SER:OG    | 2.21                     | 0.57              |
| 7:1G:60:GLU:HG2    | 7:1G:61:LYS:HG3    | 1.85                     | 0.57              |
| 8:1H:35:LYS:HB2    | 9:1I:47:THR:HG21   | 1.84                     | 0.57              |
| 9:1I:164:GLU:OE2   | 42:1q:87:HIS:ND1   | 2.36                     | 0.57              |
| 14:1N:103:ALA:O    | 14:1N:107:GLY:N    | 2.35                     | 0.57              |
| 3:1C:95:ASN:HD21   | 3:1C:106:ARG:HH11  | 1.52                     | 0.57              |
| 3:1C:202:PRO:HG3   | 17:1Q:46:GLN:OE1   | 2.05                     | 0.57              |
| 9:1I:39:SER:OG     | 9:1I:43:ARG:NH2    | 2.38                     | 0.57              |
| 9:1I:70:TYR:CD1    | 9:1I:76:ARG:HG2    | 2.40                     | 0.57              |
| 12:1L:102:GLU:HB2  | 12:1L:453:SER:HB3  | 1.87                     | 0.57              |
| 14:1N:5:ILE:H      | 14:1N:5:ILE:HD12   | 1.70                     | 0.57              |
| 33:1h:7:ARG:CZ     | 34:1i:27:LEU:HG    | 2.34                     | 0.57              |
| 39:1n:19:TYR:HB2   | 39:1n:47:PHE:HE2   | 1.69                     | 0.57              |
| 40:1o:61:TYR:CE2   | 40:1o:89:CYS:HB2   | 2.39                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:1N:102:LEU:HD21 | 14:1N:141:VAL:HB  | 1.87                     | 0.57              |
| 15:1O:47:GLY:O     | 15:1O:120:GLN:NE2 | 2.38                     | 0.57              |
| 22:1W:37:ARG:O     | 22:1W:41:ARG:NH1  | 2.37                     | 0.57              |
| 27:1b:14:LYS:HA    | 27:1b:14:LYS:HE3  | 1.86                     | 0.57              |
| 35:1j:55:ASP:OD2   | 35:1j:58:GLN:N    | 2.35                     | 0.57              |
| 39:1n:96:TYR:HB2   | 39:1n:177:PRO:HG2 | 1.85                     | 0.57              |
| 39:1n:176:ARG:HG3  | 39:1n:178:MET:SD  | 2.45                     | 0.57              |
| 9:1I:74:GLU:HG2    | 18:1R:44:ILE:HD13 | 1.86                     | 0.57              |
| 9:1I:153:LYS:HD2   | 9:1I:157:ASN:HD21 | 1.68                     | 0.57              |
| 12:1L:407:TRP:CD2  | 37:1l:115:MET:HE2 | 2.39                     | 0.57              |
| 15:1O:270:LEU:O    | 15:1O:273:THR:OG1 | 2.20                     | 0.57              |
| 16:1P:311:GLU:OE2  | 16:1P:311:GLU:N   | 2.27                     | 0.57              |
| 29:1d:34:MET:HE2   | 29:1d:34:MET:HA   | 1.87                     | 0.57              |
| 32:1g:113:PHE:O    | 41:1p:158:GLN:NE2 | 2.33                     | 0.57              |
| 40:1o:68:CYS:O     | 40:1o:72:SER:OG   | 2.19                     | 0.57              |
| 8:1H:77:LEU:HD13   | 8:1H:118:TRP:HZ3  | 1.70                     | 0.56              |
| 8:1H:215:TYR:CE2   | 8:1H:219:PRO:HB2  | 2.40                     | 0.56              |
| 13:1M:281:ASP:HB3  | 13:1M:284:SER:HB3 | 1.85                     | 0.56              |
| 32:1g:23:THR:C     | 32:1g:25:ARG:H    | 2.11                     | 0.56              |
| 33:1h:114:MET:HG2  | 33:1h:122:TRP:NE1 | 2.20                     | 0.56              |
| 6:1F:184:TYR:CE2   | 48:1F:501:FMN:H6  | 2.40                     | 0.56              |
| 6:1F:205:LEU:HB2   | 17:1Q:118:TYR:CZ  | 2.40                     | 0.56              |
| 7:1G:367:THR:OG1   | 7:1G:577:GLU:OE1  | 2.19                     | 0.56              |
| 16:1P:29:PHE:HZ    | 16:1P:173:GLY:HA3 | 1.69                     | 0.56              |
| 24:1Y:40:ILE:HD12  | 24:1Y:45:PRO:HG3  | 1.87                     | 0.56              |
| 44:1s:71:GLN:HE21  | 44:1s:75:HIS:HD2  | 1.51                     | 0.56              |
| 3:1C:32:ILE:HD11   | 21:1V:46:TYR:HD2  | 1.70                     | 0.56              |
| 4:1D:281:VAL:HG21  | 4:1D:310:ILE:HG23 | 1.87                     | 0.56              |
| 4:1D:326:ASP:OD1   | 7:1G:127:ARG:NH2  | 2.38                     | 0.56              |
| 4:1D:375:GLY:O     | 4:1D:392:LYS:N    | 2.30                     | 0.56              |
| 7:1G:107:ILE:HD13  | 9:1I:78:ILE:HG23  | 1.86                     | 0.56              |
| 7:1G:538:PRO:HB2   | 7:1G:541:CYS:SG   | 2.44                     | 0.56              |
| 7:1G:599:ILE:HG22  | 22:1W:122:PHE:HE1 | 1.71                     | 0.56              |
| 13:1M:424:ASN:OD1  | 38:1m:55:ARG:NH1  | 2.38                     | 0.56              |
| 17:1Q:30:ILE:HD12  | 17:1Q:101:TRP:CD1 | 2.40                     | 0.56              |
| 20:1U:35:HIS:HE2   | 20:1U:71:MET:HE3  | 1.71                     | 0.56              |
| 35:1j:10:ARG:NH1   | 35:1j:16:GLN:OE1  | 2.38                     | 0.56              |
| 39:1n:71:TRP:O     | 39:1n:74:GLN:NE2  | 2.36                     | 0.56              |
| 43:1r:29:GLU:N     | 43:1r:29:GLU:OE2  | 2.38                     | 0.56              |
| 5:1E:148:CYS:HA    | 5:1E:153:MET:HE2  | 1.87                     | 0.56              |
| 7:1G:165:GLU:HA    | 7:1G:396:ARG:HH21 | 1.71                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:1G:389:PRO:HD2  | 7:1G:390:LEU:N     | 2.08                     | 0.56              |
| 20:1U:35:HIS:NE2  | 20:1U:71:MET:HE3   | 2.21                     | 0.56              |
| 21:1V:67:LEU:HA   | 21:1V:70:GLN:HG2   | 1.87                     | 0.56              |
| 5:1E:82:GLU:OE2   | 7:1G:174:THR:N     | 2.37                     | 0.56              |
| 11:1K:42:ILE:O    | 11:1K:45:THR:OG1   | 2.23                     | 0.56              |
| 14:1N:49:ASN:OD1  | 14:1N:52:ALA:N     | 2.38                     | 0.56              |
| 16:1P:147:ARG:O   | 16:1P:151:VAL:HG22 | 2.05                     | 0.56              |
| 19:1S:61:GLN:HB2  | 19:1S:79:ASN:HD22  | 1.70                     | 0.56              |
| 30:1e:66:LEU:HD12 | 30:1e:67:LEU:HD22  | 1.88                     | 0.56              |
| 41:1p:139:GLN:HA  | 41:1p:143:SER:HB3  | 1.86                     | 0.56              |
| 6:1F:16:LYS:HB2   | 6:1F:19:ASP:HB2    | 1.87                     | 0.56              |
| 6:1F:305:PRO:HG3  | 6:1F:413:TRP:HB3   | 1.88                     | 0.56              |
| 15:1O:207:LYS:HA  | 15:1O:211:LEU:HD23 | 1.86                     | 0.56              |
| 16:1P:198:LYS:HE3 | 16:1P:239:PHE:CD2  | 2.41                     | 0.56              |
| 20:1U:20:LYS:HE3  | 20:1U:27:PRO:HB3   | 1.87                     | 0.56              |
| 42:1q:111:THR:OG1 | 42:1q:112:ASN:OD1  | 2.21                     | 0.56              |
| 44:1s:71:GLN:HE21 | 44:1s:75:HIS:CD2   | 2.23                     | 0.56              |
| 8:1H:134:ARG:HH22 | 8:1H:207:LEU:HD21  | 1.69                     | 0.56              |
| 9:1I:70:TYR:CE2   | 18:1R:87:CYS:HA    | 2.32                     | 0.56              |
| 21:1V:54:LYS:HD2  | 21:1V:71:LEU:HB3   | 1.88                     | 0.56              |
| 4:1D:259:MET:HE1  | 4:1D:296:ARG:CZ    | 2.35                     | 0.56              |
| 7:1G:249:ARG:HH11 | 7:1G:251:LEU:HD21  | 1.69                     | 0.56              |
| 15:1O:192:MET:N   | 15:1O:192:MET:SD   | 2.78                     | 0.56              |
| 41:1p:4:TRP:O     | 41:1p:6:LYS:NZ     | 2.38                     | 0.56              |
| 1:1A:108:GLN:O    | 1:1A:110:GLY:N     | 2.39                     | 0.56              |
| 4:1D:145:THR:HG1  | 4:1D:181:TYR:HH    | 1.54                     | 0.56              |
| 6:1F:140:GLY:HA2  | 6:1F:179:ARG:HG3   | 1.87                     | 0.56              |
| 6:1F:295:LEU:HD22 | 6:1F:339:ARG:HG3   | 1.88                     | 0.56              |
| 7:1G:252:PRO:HB3  | 7:1G:263:ILE:HG23  | 1.88                     | 0.56              |
| 13:1M:44:GLN:HB2  | 32:1g:83:TYR:HE1   | 1.71                     | 0.56              |
| 15:1O:260:ARG:HA  | 15:1O:263:VAL:HG22 | 1.87                     | 0.56              |
| 16:1P:97:ARG:H    | 16:1P:109:VAL:HG21 | 1.70                     | 0.56              |
| 34:1i:14:LEU:HD13 | 39:1n:169:ILE:HG21 | 1.88                     | 0.56              |
| 34:1i:77:PRO:O    | 34:1i:81:ILE:HG12  | 2.06                     | 0.56              |
| 6:1F:194:GLU:OE2  | 6:1F:202:LYS:N     | 2.35                     | 0.56              |
| 7:1G:243:ARG:HD2  | 7:1G:244:THR:HB    | 1.88                     | 0.56              |
| 7:1G:257:ASP:OD1  | 7:1G:257:ASP:N     | 2.39                     | 0.56              |
| 13:1M:50:LEU:N    | 13:1M:58:SER:O     | 2.38                     | 0.56              |
| 21:1V:18:THR:O    | 21:1V:18:THR:OG1   | 2.24                     | 0.56              |
| 21:1V:76:ILE:HA   | 21:1V:79:VAL:HG22  | 1.88                     | 0.56              |
| 22:1W:49:LEU:O    | 22:1W:51:GLN:NE2   | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:99:ALA:HA     | 4:1D:102:TYR:HD2   | 1.70                     | 0.55              |
| 4:1D:237:ASN:HA    | 4:1D:240:VAL:HG12  | 1.88                     | 0.55              |
| 6:1F:197:GLU:OE2   | 6:1F:204:ARG:NH2   | 2.39                     | 0.55              |
| 8:1H:233:MET:O     | 8:1H:236:ALA:N     | 2.39                     | 0.55              |
| 13:1M:176:PHE:HE2  | 13:1M:245:ARG:HB3  | 1.71                     | 0.55              |
| 19:1S:17:GLU:HB3   | 19:1S:67:ARG:HG2   | 1.89                     | 0.55              |
| 20:1T:80:ILE:O     | 20:1T:83:LYS:HE3   | 2.05                     | 0.55              |
| 27:1b:23:ALA:O     | 27:1b:27:LEU:HD12  | 2.06                     | 0.55              |
| 30:1e:6:GLN:OE1    | 30:1e:15:ARG:NH1   | 2.39                     | 0.55              |
| 9:1I:14:MET:HE1    | 27:1b:9:LYS:HG2    | 1.88                     | 0.55              |
| 14:1N:263:LYS:O    | 14:1N:267:ILE:HG12 | 2.05                     | 0.55              |
| 16:1P:250:TYR:HE2  | 16:1P:322:ARG:HD2  | 1.71                     | 0.55              |
| 20:1T:14:ARG:HA    | 20:1T:17:TYR:HD1   | 1.72                     | 0.55              |
| 3:1C:38:GLN:NE2    | 3:1C:110:TYR:OH    | 2.40                     | 0.55              |
| 6:1F:272:MET:SD    | 6:1F:273:SER:OG    | 2.58                     | 0.55              |
| 10:1J:172:THR:HA   | 11:1K:80:MET:HE2   | 1.87                     | 0.55              |
| 12:1L:359:MET:HB2  | 12:1L:430:ALA:HA   | 1.88                     | 0.55              |
| 12:1L:501:ALA:O    | 12:1L:505:ASN:ND2  | 2.38                     | 0.55              |
| 12:1L:535:ARG:NH2  | 37:1I:92:SER:OG    | 2.39                     | 0.55              |
| 15:1O:24:VAL:HB    | 15:1O:166:PRO:HA   | 1.89                     | 0.55              |
| 16:1P:30:LEU:HA    | 16:1P:207:ILE:HD11 | 1.89                     | 0.55              |
| 21:1V:22:ARG:HH12  | 21:1V:26:LEU:HB2   | 1.70                     | 0.55              |
| 28:1c:27:LEU:HD11  | 29:1d:70:PHE:CG    | 2.42                     | 0.55              |
| 5:1E:76:PRO:HG3    | 7:1G:170:ASP:OD2   | 2.06                     | 0.55              |
| 5:1E:129:GLY:N     | 5:1E:139:LEU:O     | 2.21                     | 0.55              |
| 12:1L:561:ILE:HG23 | 12:1L:562:LEU:H    | 1.72                     | 0.55              |
| 16:1P:176:ASP:CG   | 16:1P:179:LEU:H    | 2.15                     | 0.55              |
| 16:1P:201:VAL:N    | 16:1P:290:SER:OG   | 2.38                     | 0.55              |
| 16:1P:250:TYR:OH   | 16:1P:322:ARG:NH1  | 2.40                     | 0.55              |
| 17:1Q:59:PHE:HD2   | 17:1Q:79:LEU:HB3   | 1.70                     | 0.55              |
| 22:1W:68:MET:N     | 22:1W:68:MET:SD    | 2.79                     | 0.55              |
| 26:1a:51:ASP:HA    | 26:1a:54:ILE:HG22  | 1.87                     | 0.55              |
| 40:1o:117:ARG:O    | 40:1o:117:ARG:NH1  | 2.30                     | 0.55              |
| 1:1A:90:MET:HE3    | 10:1J:151:THR:HA   | 1.89                     | 0.55              |
| 14:1N:72:MET:HA    | 14:1N:75:ILE:HB    | 1.88                     | 0.55              |
| 17:1Q:59:PHE:CD2   | 17:1Q:79:LEU:HB3   | 2.42                     | 0.55              |
| 20:1T:45:LEU:HD11  | 22:1W:36:TYR:CZ    | 2.41                     | 0.55              |
| 1:1A:113:TRP:HH2   | 8:1H:287:HIS:HB2   | 1.72                     | 0.55              |
| 7:1G:501:ALA:HB2   | 7:1G:574:VAL:HB    | 1.87                     | 0.55              |
| 7:1G:624:GLU:OE1   | 7:1G:628:PRO:HA    | 2.07                     | 0.55              |
| 7:1G:672:TYR:O     | 7:1G:678:SER:HB2   | 2.07                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:1L:577:VAL:HA  | 45:1L:703:3PE:H331 | 1.87                     | 0.55              |
| 17:1Q:35:VAL:HG22 | 17:1Q:59:PHE:CE1   | 2.41                     | 0.55              |
| 25:1Z:97:ILE:HG23 | 25:1Z:98:MET:SD    | 2.47                     | 0.55              |
| 34:1i:101:PRO:HG2 | 41:1p:16:THR:HG22  | 1.89                     | 0.55              |
| 42:1q:29:ARG:NH1  | 42:1q:64:TYR:O     | 2.40                     | 0.55              |
| 7:1G:359:ARG:CZ   | 7:1G:359:ARG:HA    | 2.36                     | 0.55              |
| 7:1G:611:LEU:HD13 | 7:1G:612:PRO:HD2   | 1.86                     | 0.55              |
| 8:1H:179:TRP:NE1  | 25:1Z:43:LEU:HG    | 2.21                     | 0.55              |
| 12:1L:524:ASN:OD1 | 39:1n:77:GLN:HG3   | 2.06                     | 0.55              |
| 14:1N:44:LEU:HG   | 14:1N:122:ILE:HG21 | 1.88                     | 0.55              |
| 32:1g:64:PHE:HA   | 32:1g:68:ILE:HB    | 1.88                     | 0.55              |
| 3:1C:86:ARG:NH2   | 21:1V:113:TRP:HB2  | 2.20                     | 0.55              |
| 8:1H:150:LEU:O    | 8:1H:154:LEU:HD12  | 2.07                     | 0.55              |
| 9:1I:92:ILE:HG12  | 9:1I:111:ILE:HG12  | 1.89                     | 0.55              |
| 16:1P:283:LYS:HA  | 16:1P:286:ARG:HG2  | 1.89                     | 0.55              |
| 31:1f:28:ARG:HH12 | 50:1f:101:PC1:H112 | 1.72                     | 0.55              |
| 33:1h:34:ILE:O    | 33:1h:38:ILE:HG12  | 2.07                     | 0.55              |
| 1:1A:67:LEU:HD12  | 11:1K:65:VAL:HG22  | 1.88                     | 0.55              |
| 3:1C:90:PHE:HE1   | 3:1C:113:GLU:HG3   | 1.72                     | 0.55              |
| 7:1G:118:ASP:OD2  | 17:1Q:46:GLN:NE2   | 2.40                     | 0.55              |
| 7:1G:306:MET:N    | 7:1G:306:MET:SD    | 2.80                     | 0.55              |
| 12:1L:76:LEU:HD21 | 12:1L:196:TRP:HE3  | 1.71                     | 0.55              |
| 13:1M:355:MET:HA  | 13:1M:355:MET:HE3  | 1.88                     | 0.55              |
| 16:1P:294:LEU:HB2 | 16:1P:296:HIS:CE1  | 2.41                     | 0.55              |
| 37:1l:98:TRP:O    | 37:1l:101:MET:HB2  | 2.07                     | 0.55              |
| 43:1r:47:LYS:N    | 43:1r:47:LYS:HD3   | 2.22                     | 0.55              |
| 1:1A:54:LYS:NZ    | 4:1D:71:GLU:HB3    | 2.22                     | 0.55              |
| 4:1D:158:ALA:HA   | 4:1D:161:ILE:HG22  | 1.88                     | 0.55              |
| 4:1D:283:PHE:HA   | 4:1D:309:ARG:NH2   | 2.22                     | 0.55              |
| 4:1D:284:ASP:OD2  | 4:1D:309:ARG:NH2   | 2.35                     | 0.55              |
| 13:1M:355:MET:HE1 | 13:1M:437:MET:SD   | 2.47                     | 0.55              |
| 17:1Q:56:LYS:HE2  | 17:1Q:58:GLU:OE2   | 2.06                     | 0.55              |
| 19:1S:39:ARG:HH22 | 19:1S:86:VAL:HG13  | 1.72                     | 0.55              |
| 20:1U:52:MET:HA   | 20:1U:55:GLU:HB2   | 1.89                     | 0.55              |
| 2:1B:81:ARG:HD3   | 8:1H:214:GLU:HG3   | 1.88                     | 0.54              |
| 4:1D:184:VAL:O    | 9:1I:60:ARG:NH1    | 2.40                     | 0.54              |
| 4:1D:204:PRO:HG2  | 4:1D:207:LEU:HB2   | 1.89                     | 0.54              |
| 6:1F:138:ILE:O    | 6:1F:180:GLY:N     | 2.37                     | 0.54              |
| 6:1F:163:GLY:N    | 6:1F:173:PHE:O     | 2.39                     | 0.54              |
| 7:1G:359:ARG:HG3  | 19:1S:56:GLU:HB3   | 1.89                     | 0.54              |
| 11:1K:71:ALA:O    | 11:1K:75:LEU:HD12  | 2.08                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:597:ILE:CD1  | 12:1L:601:LEU:HB3  | 2.36                     | 0.54              |
| 13:1M:285:LEU:HD13 | 13:1M:342:MET:HE1  | 1.88                     | 0.54              |
| 14:1N:312:LYS:HD2  | 15:1O:75:GLY:H     | 1.72                     | 0.54              |
| 15:1O:32:CYS:N     | 54:1O:401:GTP:O1A  | 2.31                     | 0.54              |
| 15:1O:214:MET:HA   | 15:1O:217:LYS:HD3  | 1.87                     | 0.54              |
| 19:1S:13:LEU:HD22  | 19:1S:72:GLN:OE1   | 2.06                     | 0.54              |
| 33:1h:134:ASP:OD1  | 33:1h:136:SER:OG   | 2.24                     | 0.54              |
| 6:1F:160:GLY:O     | 6:1F:167:CYS:N     | 2.39                     | 0.54              |
| 7:1G:504:ASP:O     | 19:1S:55:ARG:NH1   | 2.40                     | 0.54              |
| 8:1H:283:ASP:OD1   | 8:1H:283:ASP:N     | 2.39                     | 0.54              |
| 14:1N:120:GLN:HB2  | 14:1N:177:LYS:HD3  | 1.88                     | 0.54              |
| 16:1P:145:TYR:O    | 16:1P:149:LYS:HG2  | 2.07                     | 0.54              |
| 19:1S:18:ILE:HG23  | 19:1S:52:ILE:HG23  | 1.90                     | 0.54              |
| 20:1T:83:LYS:HD2   | 20:1T:84:LYS:N     | 2.23                     | 0.54              |
| 23:1X:41:GLU:N     | 23:1X:41:GLU:OE1   | 2.41                     | 0.54              |
| 29:1d:99:GLU:OE1   | 29:1d:99:GLU:N     | 2.40                     | 0.54              |
| 39:1n:30:CYS:O     | 39:1n:32:HIS:N     | 2.38                     | 0.54              |
| 3:1C:137:MET:HB3   | 3:1C:162:PHE:CG    | 2.42                     | 0.54              |
| 7:1G:126:ASP:OD2   | 7:1G:127:ARG:NH2   | 2.40                     | 0.54              |
| 7:1G:255:HIS:CD2   | 7:1G:255:HIS:O     | 2.61                     | 0.54              |
| 14:1N:73:ALA:HB1   | 14:1N:98:MET:HB2   | 1.88                     | 0.54              |
| 22:1W:62:LYS:HD3   | 22:1W:107:PHE:CE2  | 2.42                     | 0.54              |
| 32:1g:66:PHE:O     | 32:1g:71:VAL:N     | 2.40                     | 0.54              |
| 1:1A:22:PHE:HA     | 8:1H:60:PRO:HG2    | 1.89                     | 0.54              |
| 2:1B:111:ARG:N     | 16:1P:54:TYR:OH    | 2.28                     | 0.54              |
| 4:1D:219:SER:HA    | 4:1D:222:ILE:HG12  | 1.88                     | 0.54              |
| 4:1D:390:LYS:HE2   | 4:1D:430:ARG:HD2   | 1.88                     | 0.54              |
| 5:1E:89:MET:SD     | 5:1E:89:MET:N      | 2.65                     | 0.54              |
| 6:1F:137:TYR:HE2   | 6:1F:195:SER:HB2   | 1.72                     | 0.54              |
| 7:1G:276:ARG:HA    | 42:1q:135:GLN:HB2  | 1.89                     | 0.54              |
| 8:1H:209:SER:HB3   | 8:1H:213:VAL:HA    | 1.89                     | 0.54              |
| 12:1L:584:ILE:HD11 | 14:1N:58:LYS:HG2   | 1.89                     | 0.54              |
| 13:1M:258:ALA:HA   | 13:1M:302:MET:HE3  | 1.89                     | 0.54              |
| 14:1N:7:THR:HG21   | 53:1N:402:CDL:H352 | 1.89                     | 0.54              |
| 20:1T:47:GLN:NE2   | 20:1T:67:ALA:O     | 2.40                     | 0.54              |
| 21:1V:21:GLU:O     | 21:1V:25:ILE:HG12  | 2.06                     | 0.54              |
| 50:1f:101:PC1:H282 | 50:1f:101:PC1:H351 | 1.89                     | 0.54              |
| 40:1o:7:ARG:NH2    | 40:1o:15:GLU:O     | 2.39                     | 0.54              |
| 2:1B:144:ILE:HG13  | 2:1B:163:LEU:HB2   | 1.89                     | 0.54              |
| 11:1K:2:PRO:HG2    | 11:1K:5:TYR:CD2    | 2.42                     | 0.54              |
| 12:1L:258:PHE:HA   | 12:1L:261:ILE:HD12 | 1.90                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:1V:113:TRP:CG   | 21:1V:113:TRP:O    | 2.61                     | 0.54              |
| 44:1s:71:GLN:NE2   | 44:1s:75:HIS:HD2   | 2.04                     | 0.54              |
| 2:1B:90:GLY:HA2    | 46:1B:201:SF4:S2   | 2.47                     | 0.54              |
| 4:1D:379:VAL:HG13  | 4:1D:387:TYR:HB3   | 1.89                     | 0.54              |
| 7:1G:286:ASN:C     | 42:1q:143:PRO:HB2  | 2.33                     | 0.54              |
| 14:1N:267:ILE:HD12 | 14:1N:279:PRO:HB3  | 1.88                     | 0.54              |
| 16:1P:281:ARG:O    | 16:1P:284:VAL:HG22 | 2.08                     | 0.54              |
| 29:1d:17:GLU:N     | 29:1d:17:GLU:OE2   | 2.41                     | 0.54              |
| 35:1j:56:PRO:HA    | 35:1j:59:TRP:CE3   | 2.42                     | 0.54              |
| 2:1B:126:TYR:HE1   | 4:1D:85:ARG:NE     | 2.06                     | 0.54              |
| 4:1D:371:LYS:HZ3   | 4:1D:424:VAL:HG21  | 1.73                     | 0.54              |
| 6:1F:280:ILE:HD12  | 6:1F:280:ILE:H     | 1.72                     | 0.54              |
| 7:1G:375:ASP:OD2   | 7:1G:448:LYS:N     | 2.40                     | 0.54              |
| 11:1K:44:SER:O     | 11:1K:48:ILE:HG13  | 2.07                     | 0.54              |
| 12:1L:126:ILE:HD12 | 12:1L:127:THR:N    | 2.22                     | 0.54              |
| 3:1C:132:ARG:HD2   | 3:1C:149:ARG:H     | 1.72                     | 0.54              |
| 6:1F:82:MET:HG3    | 6:1F:129:MET:HB3   | 1.89                     | 0.54              |
| 6:1F:156:ALA:HA    | 6:1F:161:LEU:HD12  | 1.89                     | 0.54              |
| 9:1I:113:MET:HE3   | 9:1I:113:MET:O     | 2.07                     | 0.54              |
| 12:1L:54:PHE:O     | 12:1L:58:GLY:N     | 2.41                     | 0.54              |
| 15:1O:46:LEU:HB2   | 15:1O:48:LEU:HD11  | 1.89                     | 0.54              |
| 16:1P:139:ILE:HG13 | 16:1P:150:ALA:HB3  | 1.89                     | 0.54              |
| 20:1U:35:HIS:CE1   | 20:1U:38:LYS:HD3   | 2.43                     | 0.54              |
| 20:1U:74:GLN:NE2   | 20:1U:78:ASP:OD2   | 2.41                     | 0.54              |
| 33:1h:47:ILE:HA    | 41:1p:58:ASN:HD21  | 1.72                     | 0.54              |
| 41:1p:162:MET:HA   | 41:1p:165:GLU:HG2  | 1.89                     | 0.54              |
| 2:1B:125:TYR:CD1   | 9:1I:117:ILE:HD13  | 2.43                     | 0.54              |
| 5:1E:99:HIS:HA     | 5:1E:138:THR:OG1   | 2.07                     | 0.54              |
| 6:1F:307:ILE:HA    | 6:1F:421:HIS:ND1   | 2.23                     | 0.54              |
| 7:1G:314:ASP:O     | 7:1G:520:LYS:N     | 2.41                     | 0.54              |
| 7:1G:378:LEU:HD21  | 7:1G:439:PHE:CZ    | 2.41                     | 0.54              |
| 7:1G:591:GLY:HA2   | 16:1P:6:ILE:HG21   | 1.90                     | 0.54              |
| 12:1L:136:ASN:OD1  | 12:1L:139:GLN:N    | 2.38                     | 0.54              |
| 13:1M:309:PHE:HB2  | 13:1M:458:LEU:HD12 | 1.90                     | 0.54              |
| 14:1N:251:MET:HB3  | 14:1N:293:TYR:CE2  | 2.43                     | 0.54              |
| 15:1O:134:PHE:O    | 15:1O:138:MET:HG3  | 2.08                     | 0.54              |
| 16:1P:315:ILE:H    | 16:1P:331:MET:HE1  | 1.72                     | 0.54              |
| 21:1V:91:ARG:NH1   | 21:1V:91:ARG:HB2   | 2.23                     | 0.54              |
| 39:1n:9:LEU:O      | 39:1n:14:LYS:NZ    | 2.36                     | 0.54              |
| 1:1A:63:LEU:HD22   | 11:1K:72:ALA:HB2   | 1.90                     | 0.54              |
| 5:1E:103:CYS:HB3   | 5:1E:153:MET:SD    | 2.48                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:58:GLU:HG2    | 7:1G:85:LYS:HB3    | 1.90                     | 0.54              |
| 7:1G:628:PRO:HD3   | 19:1S:21:HIS:CE1   | 2.43                     | 0.54              |
| 14:1N:320:THR:HG21 | 15:1O:265:ASN:HA   | 1.90                     | 0.54              |
| 16:1P:144:ARG:H    | 16:1P:144:ARG:HD2  | 1.73                     | 0.54              |
| 22:1W:51:GLN:HB2   | 22:1W:100:ARG:HH21 | 1.73                     | 0.54              |
| 37:1I:72:ASN:ND2   | 37:1I:75:GLU:OE2   | 2.39                     | 0.54              |
| 38:1m:2:PHE:CD2    | 38:1m:3:PRO:HD2    | 2.41                     | 0.54              |
| 3:1C:28:TYR:O      | 3:1C:32:ILE:HG12   | 2.08                     | 0.53              |
| 12:1L:272:LEU:O    | 12:1L:275:THR:OG1  | 2.24                     | 0.53              |
| 14:1N:192:ALA:HB1  | 14:1N:270:MET:HE1  | 1.90                     | 0.53              |
| 23:1X:51:ASP:OD2   | 23:1X:54:ARG:N     | 2.39                     | 0.53              |
| 40:1o:27:ASP:N     | 40:1o:27:ASP:OD1   | 2.39                     | 0.53              |
| 2:1B:62:MET:HE2    | 2:1B:156:LEU:HD11  | 1.90                     | 0.53              |
| 2:1B:84:ASP:OD2    | 8:1H:54:LYS:NZ     | 2.18                     | 0.53              |
| 3:1C:22:LEU:HD12   | 3:1C:48:LEU:HB2    | 1.90                     | 0.53              |
| 4:1D:404:LYS:HA    | 4:1D:407:LYS:HE2   | 1.89                     | 0.53              |
| 7:1G:546:GLN:HG3   | 7:1G:599:ILE:HD11  | 1.90                     | 0.53              |
| 13:1M:5:ILE:O      | 13:1M:9:THR:HG23   | 2.07                     | 0.53              |
| 16:1P:306:GLN:NE2  | 16:1P:307:ALA:O    | 2.42                     | 0.53              |
| 17:1Q:62:ARG:HG3   | 17:1Q:63:GLU:H     | 1.73                     | 0.53              |
| 25:1Z:21:TYR:O     | 25:1Z:21:TYR:CD2   | 2.61                     | 0.53              |
| 26:1a:22:ALA:O     | 26:1a:26:ILE:HD12  | 2.09                     | 0.53              |
| 34:1i:10:ARG:NH2   | 39:1n:154:PRO:O    | 2.36                     | 0.53              |
| 5:1E:159:ASN:OD1   | 5:1E:184:PRO:HB3   | 2.08                     | 0.53              |
| 6:1F:125:GLY:O     | 6:1F:129:MET:HG2   | 2.08                     | 0.53              |
| 8:1H:51:ASP:OD1    | 8:1H:52:ALA:N      | 2.42                     | 0.53              |
| 9:1I:138:GLU:OE1   | 9:1I:138:GLU:N     | 2.42                     | 0.53              |
| 13:1M:325:MET:HG3  | 13:1M:440:HIS:HB3  | 1.90                     | 0.53              |
| 20:1U:35:HIS:CE1   | 20:1U:71:MET:HE3   | 2.43                     | 0.53              |
| 4:1D:116:GLN:HE22  | 4:1D:138:ARG:HG2   | 1.72                     | 0.53              |
| 5:1E:156:ILE:HD11  | 5:1E:161:TYR:CE2   | 2.44                     | 0.53              |
| 6:1F:136:ILE:HD11  | 6:1F:177:VAL:HA    | 1.89                     | 0.53              |
| 6:1F:137:TYR:HE1   | 6:1F:180:GLY:HA2   | 1.74                     | 0.53              |
| 7:1G:308:GLN:NE2   | 7:1G:607:ALA:O     | 2.42                     | 0.53              |
| 8:1H:120:GLY:HA3   | 8:1H:132:ALA:HB2   | 1.90                     | 0.53              |
| 15:1O:175:PRO:HD2  | 15:1O:175:PRO:O    | 2.08                     | 0.53              |
| 15:1O:175:PRO:HD2  | 15:1O:178:GLU:HB3  | 1.89                     | 0.53              |
| 1:1A:61:THR:O      | 1:1A:65:PHE:HB2    | 2.09                     | 0.53              |
| 7:1G:94:MET:HE3    | 7:1G:120:SER:HA    | 1.89                     | 0.53              |
| 7:1G:278:ARG:NH1   | 7:1G:279:LEU:O     | 2.42                     | 0.53              |
| 7:1G:331:LEU:HD12  | 7:1G:525:LEU:HD12  | 1.89                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:1H:264:LEU:HD12  | 26:1a:13:ALA:HB2  | 1.90                     | 0.53              |
| 13:1M:42:LEU:HD21  | 13:1M:67:VAL:HG11 | 1.91                     | 0.53              |
| 14:1N:109:SER:O    | 14:1N:111:PHE:N   | 2.41                     | 0.53              |
| 19:1S:23:CYS:HB2   | 19:1S:60:VAL:H    | 1.73                     | 0.53              |
| 23:1X:121:LEU:HD13 | 25:1Z:62:ILE:HD11 | 1.91                     | 0.53              |
| 43:1r:57:ASP:O     | 43:1r:61:GLU:HG2  | 2.07                     | 0.53              |
| 3:1C:118:GLU:CD    | 3:1C:118:GLU:H    | 2.15                     | 0.53              |
| 3:1C:155:TYR:OH    | 4:1D:79:HIS:ND1   | 2.41                     | 0.53              |
| 4:1D:228:MET:HB3   | 9:1I:36:MET:HE2   | 1.91                     | 0.53              |
| 6:1F:272:MET:SD    | 6:1F:273:SER:N    | 2.82                     | 0.53              |
| 7:1G:359:ARG:NH1   | 7:1G:362:TYR:OH   | 2.40                     | 0.53              |
| 7:1G:432:ILE:HD11  | 7:1G:437:HIS:HD2  | 1.73                     | 0.53              |
| 9:1I:75:GLU:OE2    | 9:1I:151:LYS:NZ   | 2.33                     | 0.53              |
| 12:1L:1:FME:HE1    | 34:1i:86:LYS:HA   | 1.91                     | 0.53              |
| 12:1L:591:PHE:CZ   | 14:1N:111:PHE:HA  | 2.44                     | 0.53              |
| 13:1M:119:TYR:CZ   | 13:1M:161:LEU:HB2 | 2.44                     | 0.53              |
| 14:1N:339:MET:HE2  | 14:1N:339:MET:HA  | 1.90                     | 0.53              |
| 16:1P:166:ILE:HD12 | 16:1P:230:PHE:CE1 | 2.44                     | 0.53              |
| 23:1X:17:VAL:HG21  | 25:1Z:74:LEU:HD21 | 1.91                     | 0.53              |
| 25:1Z:72:MET:HE2   | 27:1b:52:TYR:HD2  | 1.73                     | 0.53              |
| 32:1g:77:VAL:HA    | 32:1g:80:LEU:HG   | 1.90                     | 0.53              |
| 34:1i:50:LEU:HD13  | 34:1i:57:LYS:HG3  | 1.90                     | 0.53              |
| 35:1j:71:GLU:O     | 40:1o:114:ARG:NH1 | 2.41                     | 0.53              |
| 38:1m:69:TYR:CZ    | 38:1m:74:ASN:HB2  | 2.44                     | 0.53              |
| 42:1q:85:GLU:OE2   | 42:1q:85:GLU:N    | 2.27                     | 0.53              |
| 2:1B:101:ARG:NH1   | 2:1B:139:ILE:O    | 2.40                     | 0.53              |
| 3:1C:40:VAL:HG22   | 43:1r:69:MET:HE3  | 1.91                     | 0.53              |
| 4:1D:100:LEU:HD12  | 4:1D:118:TYR:HD2  | 1.73                     | 0.53              |
| 4:1D:378:LEU:HD23  | 4:1D:378:LEU:H    | 1.74                     | 0.53              |
| 5:1E:101:GLN:HB2   | 5:1E:155:GLN:HB3  | 1.89                     | 0.53              |
| 52:1M:501:PGT:H242 | 14:1N:284:MET:HG3 | 1.91                     | 0.53              |
| 14:1N:97:MET:HA    | 14:1N:97:MET:HE2  | 1.91                     | 0.53              |
| 19:1S:78:LEU:HA    | 19:1S:81:PHE:CD2  | 2.43                     | 0.53              |
| 27:1b:27:LEU:O     | 27:1b:31:LEU:HD12 | 2.09                     | 0.53              |
| 36:1k:71:LYS:H     | 36:1k:71:LYS:HD3  | 1.74                     | 0.53              |
| 5:1E:99:HIS:O      | 5:1E:157:ASN:N    | 2.40                     | 0.53              |
| 7:1G:256:GLU:O     | 7:1G:394:ARG:NH1  | 2.42                     | 0.53              |
| 7:1G:380:VAL:HG21  | 7:1G:429:LEU:HD11 | 1.91                     | 0.53              |
| 9:1I:69:ARG:HD3    | 42:1q:108:TYR:CD1 | 2.44                     | 0.53              |
| 12:1L:370:THR:HA   | 12:1L:431:PHE:CE2 | 2.44                     | 0.53              |
| 13:1M:279:GLN:OE1  | 13:1M:284:SER:OG  | 2.26                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:112:HIS:HB2  | 14:1N:184:ILE:HD13 | 1.90                     | 0.53              |
| 14:1N:272:LYS:HE3  | 33:1h:108:LEU:HD21 | 1.90                     | 0.53              |
| 16:1P:166:ILE:HG23 | 16:1P:230:PHE:CE1  | 2.44                     | 0.53              |
| 21:1V:92:LYS:HA    | 21:1V:95:ARG:HH21  | 1.74                     | 0.53              |
| 33:1h:94:LEU:HD12  | 41:1p:81:ILE:HG12  | 1.91                     | 0.53              |
| 1:1A:113:TRP:CZ2   | 8:1H:286:MET:HB3   | 2.44                     | 0.53              |
| 4:1D:195:ARG:HG3   | 4:1D:200:HIS:HB2   | 1.90                     | 0.53              |
| 4:1D:234:ILE:HG21  | 8:1H:280:PHE:CE1   | 2.43                     | 0.53              |
| 7:1G:588:THR:HG22  | 22:1W:126:HIS:NE2  | 2.23                     | 0.53              |
| 12:1L:312:LEU:O    | 12:1L:316:THR:HG23 | 2.09                     | 0.53              |
| 13:1M:160:LEU:HG   | 13:1M:164:LEU:HD11 | 1.91                     | 0.53              |
| 20:1U:26:ASP:OD1   | 20:1U:29:LYS:HD2   | 2.09                     | 0.53              |
| 21:1V:111:TRP:O    | 21:1V:112:LYS:HG2  | 2.09                     | 0.53              |
| 23:1X:142:HIS:ND1  | 25:1Z:114:THR:OG1  | 2.37                     | 0.53              |
| 28:1c:13:ASP:O     | 28:1c:17:VAL:HG12  | 2.08                     | 0.53              |
| 38:1m:14:PRO:HB2   | 38:1m:16:THR:HG22  | 1.90                     | 0.53              |
| 43:1r:104:GLU:N    | 43:1r:104:GLU:OE2  | 2.40                     | 0.53              |
| 8:1H:220:PHE:CZ    | 8:1H:224:PHE:HD2   | 2.27                     | 0.53              |
| 11:1K:94:ASN:HD22  | 12:1L:583:LEU:HD21 | 1.74                     | 0.53              |
| 14:1N:230:LEU:HD23 | 14:1N:296:LEU:HD11 | 1.90                     | 0.53              |
| 22:1W:84:ILE:O     | 22:1W:88:MET:N     | 2.42                     | 0.53              |
| 23:1X:129:LYS:HD3  | 27:1b:65:VAL:HG13  | 1.90                     | 0.53              |
| 40:1o:36:ARG:NH2   | 40:1o:93:ASP:OD1   | 2.42                     | 0.53              |
| 1:1A:6:THR:HG21    | 8:1H:87:VAL:HG11   | 1.91                     | 0.52              |
| 4:1D:155:THR:HB    | 4:1D:167:PHE:CB    | 2.39                     | 0.52              |
| 5:1E:151:ALA:HB1   | 5:1E:152:PRO:HD2   | 1.91                     | 0.52              |
| 7:1G:24:THR:HG23   | 7:1G:28:GLN:HB3    | 1.91                     | 0.52              |
| 7:1G:357:ASP:N     | 7:1G:357:ASP:OD1   | 2.42                     | 0.52              |
| 7:1G:572:THR:OG1   | 7:1G:633:TYR:OH    | 2.22                     | 0.52              |
| 9:1I:114:THR:HG21  | 9:1I:144:HIS:CE1   | 2.44                     | 0.52              |
| 25:1Z:120:MET:O    | 25:1Z:123:GLU:HG2  | 2.09                     | 0.52              |
| 30:1e:14:ASP:O     | 30:1e:18:THR:OG1   | 2.26                     | 0.52              |
| 41:1p:5:ASP:HB3    | 41:1p:8:VAL:HB     | 1.91                     | 0.52              |
| 3:1C:203:TRP:CG    | 7:1G:119:GLN:HE22  | 2.27                     | 0.52              |
| 4:1D:352:TYR:CD2   | 9:1I:86:VAL:HG21   | 2.44                     | 0.52              |
| 5:1E:54:ALA:O      | 5:1E:58:ASN:ND2    | 2.42                     | 0.52              |
| 6:1F:29:HIS:NE2    | 44:1s:35:ASN:OD1   | 2.42                     | 0.52              |
| 6:1F:137:TYR:CD2   | 6:1F:192:LEU:HG    | 2.43                     | 0.52              |
| 7:1G:551:ASP:OD2   | 7:1G:679:ARG:NE    | 2.38                     | 0.52              |
| 11:1K:89:TYR:O     | 11:1K:92:ASN:ND2   | 2.42                     | 0.52              |
| 13:1M:204:MET:HE3  | 13:1M:209:LEU:HD22 | 1.90                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:206:LEU:HD12 | 14:1N:346:LEU:HD21 | 1.91                     | 0.52              |
| 17:1Q:12:ALA:HA    | 22:1W:16:SER:HA    | 1.90                     | 0.52              |
| 37:1l:132:GLN:HB2  | 40:1o:57:TYR:CE1   | 2.44                     | 0.52              |
| 39:1n:116:ASP:OD1  | 39:1n:117:TYR:N    | 2.43                     | 0.52              |
| 42:1q:115:PHE:HD1  | 42:1q:115:PHE:H    | 1.55                     | 0.52              |
| 13:1M:26:ASN:OD1   | 31:1f:13:HIS:NE2   | 2.42                     | 0.52              |
| 13:1M:82:SER:OG    | 13:1M:432:ARG:NH2  | 2.42                     | 0.52              |
| 16:1P:141:SER:O    | 16:1P:147:ARG:NH2  | 2.43                     | 0.52              |
| 31:1f:49:ARG:HB2   | 31:1f:52:GLU:OE1   | 2.09                     | 0.52              |
| 35:1j:9:PRO:HD2    | 36:1k:13:MET:HE1   | 1.91                     | 0.52              |
| 40:1o:55:ARG:NH2   | 41:1p:119:SER:HB2  | 2.25                     | 0.52              |
| 1:1A:60:ILE:H      | 1:1A:60:ILE:HD12   | 1.73                     | 0.52              |
| 6:1F:215:VAL:HG22  | 6:1F:220:THR:OG1   | 2.09                     | 0.52              |
| 6:1F:259:SER:HA    | 6:1F:265:PRO:HB3   | 1.91                     | 0.52              |
| 6:1F:274:VAL:O     | 6:1F:317:MET:HG3   | 2.08                     | 0.52              |
| 11:1K:25:HIS:HD2   | 11:1K:27:MET:HB2   | 1.75                     | 0.52              |
| 12:1L:159:HIS:NE2  | 13:1M:416:ARG:HA   | 2.25                     | 0.52              |
| 12:1L:274:GLN:O    | 12:1L:277:THR:OG1  | 2.23                     | 0.52              |
| 14:1N:28:LEU:HA    | 14:1N:31:ILE:HB    | 1.91                     | 0.52              |
| 14:1N:78:LEU:HD12  | 14:1N:82:GLY:HA2   | 1.90                     | 0.52              |
| 32:1g:80:LEU:HD22  | 32:1g:81:PRO:HD2   | 1.90                     | 0.52              |
| 43:1r:92:LYS:HE2   | 43:1r:92:LYS:N     | 2.25                     | 0.52              |
| 3:1C:39:GLN:O      | 3:1C:51:PHE:N      | 2.38                     | 0.52              |
| 8:1H:130:ILE:HD12  | 8:1H:131:GLY:N     | 2.25                     | 0.52              |
| 10:1J:25:SER:N     | 10:1J:81:GLU:OE1   | 2.39                     | 0.52              |
| 10:1J:119:PHE:CD1  | 11:1K:6:MET:HB2    | 2.44                     | 0.52              |
| 12:1L:197:ASP:HB2  | 41:1p:110:LYS:HE2  | 1.92                     | 0.52              |
| 12:1L:557:TRP:HA   | 12:1L:560:THR:HG22 | 1.91                     | 0.52              |
| 13:1M:116:ILE:HG12 | 13:1M:174:LEU:HD12 | 1.90                     | 0.52              |
| 13:1M:326:LEU:HA   | 13:1M:329:LEU:HD13 | 1.92                     | 0.52              |
| 16:1P:280:THR:O    | 16:1P:284:VAL:HG13 | 2.09                     | 0.52              |
| 35:1j:41:TRP:HB2   | 36:1k:77:PHE:HZ    | 1.75                     | 0.52              |
| 2:1B:54:CYS:CA     | 4:1D:108:TYR:HB2   | 2.40                     | 0.52              |
| 7:1G:190:MET:HE3   | 7:1G:695:ILE:HD13  | 1.92                     | 0.52              |
| 7:1G:252:PRO:HG2   | 17:1Q:44:ASN:HD22  | 1.73                     | 0.52              |
| 11:1K:26:LEU:HD23  | 11:1K:88:ASP:HB2   | 1.90                     | 0.52              |
| 12:1L:10:THR:O     | 12:1L:13:ILE:HG22  | 2.10                     | 0.52              |
| 12:1L:306:THR:O    | 12:1L:310:LEU:N    | 2.32                     | 0.52              |
| 16:1P:136:ASN:O    | 16:1P:146:LEU:HB3  | 2.09                     | 0.52              |
| 2:1B:54:CYS:SG     | 4:1D:190:HIS:NE2   | 2.75                     | 0.52              |
| 3:1C:10:THR:O      | 4:1D:129:GLN:N     | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:71:GLU:HG2    | 4:1D:72:MET:HB2    | 1.91                     | 0.52              |
| 4:1D:428:VAL:O     | 4:1D:430:ARG:NH1   | 2.43                     | 0.52              |
| 5:1E:95:VAL:O      | 5:1E:135:LYS:NZ    | 2.41                     | 0.52              |
| 6:1F:246:GLY:HA3   | 6:1F:251:SER:HA    | 1.92                     | 0.52              |
| 7:1G:255:HIS:NE2   | 7:1G:258:ILE:HD13  | 2.23                     | 0.52              |
| 7:1G:460:ARG:NH1   | 7:1G:659:ASP:O     | 2.43                     | 0.52              |
| 8:1H:195:ARG:HD3   | 8:1H:196:ALA:N     | 2.25                     | 0.52              |
| 8:1H:263:THR:O     | 8:1H:267:THR:OG1   | 2.28                     | 0.52              |
| 12:1L:542:LEU:HD11 | 37:1l:88:ARG:HD2   | 1.91                     | 0.52              |
| 13:1M:139:GLN:O    | 13:1M:142:ARG:NH1  | 2.43                     | 0.52              |
| 13:1M:201:MET:HG2  | 52:1M:501:PGT:H441 | 1.91                     | 0.52              |
| 15:1O:13:ARG:O     | 15:1O:17:LYS:NZ    | 2.30                     | 0.52              |
| 37:1l:33:ASP:OD1   | 37:1l:33:ASP:N     | 2.37                     | 0.52              |
| 37:1l:54:SER:N     | 37:1l:57:GLU:OE1   | 2.43                     | 0.52              |
| 43:1r:46:HIS:C     | 43:1r:47:LYS:HD3   | 2.35                     | 0.52              |
| 6:1F:189:GLU:HA    | 6:1F:222:VAL:HG11  | 1.90                     | 0.52              |
| 6:1F:207:PRO:HA    | 6:1F:208:PRO:C     | 2.35                     | 0.52              |
| 7:1G:37:ILE:H      | 7:1G:37:ILE:HD12   | 1.73                     | 0.52              |
| 7:1G:165:GLU:O     | 7:1G:167:ALA:N     | 2.43                     | 0.52              |
| 7:1G:289:GLY:N     | 42:1q:143:PRO:C    | 2.64                     | 0.52              |
| 7:1G:313:ASN:O     | 7:1G:517:ASN:ND2   | 2.42                     | 0.52              |
| 10:1J:60:TYR:CD2   | 10:1J:64:MET:HG3   | 2.45                     | 0.52              |
| 12:1L:452:ASN:HB3  | 12:1L:456:ARG:HH12 | 1.74                     | 0.52              |
| 21:1V:87:LEU:HD23  | 21:1V:91:ARG:HH12  | 1.74                     | 0.52              |
| 2:1B:86:MET:HE1    | 2:1B:104:TYR:HB2   | 1.92                     | 0.52              |
| 4:1D:369:ALA:HB2   | 4:1D:374:PHE:HB2   | 1.91                     | 0.52              |
| 5:1E:121:GLN:NE2   | 5:1E:126:ILE:O     | 2.40                     | 0.52              |
| 7:1G:172:LEU:HB3   | 7:1G:185:THR:HG23  | 1.92                     | 0.52              |
| 7:1G:494:HIS:CE1   | 7:1G:499:GLN:HG3   | 2.45                     | 0.52              |
| 10:1J:126:VAL:HB   | 25:1Z:120:MET:HE2  | 1.91                     | 0.52              |
| 15:1O:138:MET:HB3  | 15:1O:143:PHE:HB2  | 1.91                     | 0.52              |
| 15:1O:201:ASP:HA   | 15:1O:204:ASN:HD21 | 1.75                     | 0.52              |
| 19:1S:24:GLN:HB2   | 19:1S:25:ARG:NH1   | 2.25                     | 0.52              |
| 22:1W:18:LYS:HA    | 22:1W:18:LYS:HE3   | 1.92                     | 0.52              |
| 34:1i:107:ASP:N    | 40:1o:67:LYS:HZ1   | 2.08                     | 0.52              |
| 2:1B:127:HIS:CE1   | 2:1B:134:ARG:HG2   | 2.45                     | 0.52              |
| 6:1F:306:LEU:O     | 6:1F:421:HIS:ND1   | 2.43                     | 0.52              |
| 7:1G:135:ARG:NH1   | 7:1G:179:ASN:OD1   | 2.43                     | 0.52              |
| 12:1L:597:ILE:HG13 | 12:1L:602:PHE:CZ   | 2.45                     | 0.52              |
| 13:1M:403:THR:HA   | 13:1M:406:TYR:CE2  | 2.44                     | 0.52              |
| 13:1M:422:HIS:HB2  | 38:1m:59:ILE:HD12  | 1.92                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:1Q:27:GLU:N    | 17:1Q:27:GLU:OE1   | 2.43                     | 0.52              |
| 23:1X:126:LYS:HD3 | 27:1b:74:GLY:HA3   | 1.92                     | 0.52              |
| 23:1X:146:ARG:NH1 | 30:1e:38:GLU:OE1   | 2.42                     | 0.52              |
| 34:1i:64:TYR:O    | 34:1i:68:ILE:HG22  | 2.10                     | 0.52              |
| 43:1r:90:GLU:O    | 43:1r:92:LYS:NZ    | 2.29                     | 0.52              |
| 2:1B:58:GLU:OE1   | 2:1B:61:HIS:ND1    | 2.43                     | 0.51              |
| 5:1E:156:ILE:HD12 | 5:1E:156:ILE:O     | 2.10                     | 0.51              |
| 7:1G:318:ILE:HD13 | 7:1G:344:CYS:SG    | 2.50                     | 0.51              |
| 7:1G:455:SER:OG   | 7:1G:493:LEU:O     | 2.20                     | 0.51              |
| 9:1I:67:LEU:HD21  | 9:1I:77:CYS:HB2    | 1.92                     | 0.51              |
| 9:1I:119:CYS:HB3  | 9:1I:121:PHE:CD2   | 2.45                     | 0.51              |
| 24:1Y:94:CYS:HB3  | 24:1Y:98:LEU:HD23  | 1.93                     | 0.51              |
| 35:1j:64:LEU:HD11 | 40:1o:102:GLU:HG3  | 1.92                     | 0.51              |
| 43:1r:8:GLN:HG2   | 43:1r:11:ARG:HH21  | 1.75                     | 0.51              |
| 6:1F:247:ARG:HH11 | 6:1F:316:LEU:HD23  | 1.75                     | 0.51              |
| 14:1N:150:ASN:HB3 | 14:1N:153:LEU:HB3  | 1.91                     | 0.51              |
| 14:1N:214:ALA:HB1 | 14:1N:330:ILE:HD13 | 1.93                     | 0.51              |
| 16:1P:168:PRO:HB2 | 16:1P:171:ILE:HD11 | 1.90                     | 0.51              |
| 16:1P:197:GLY:HA2 | 16:1P:288:HIS:HE1  | 1.76                     | 0.51              |
| 20:1T:81:ALA:O    | 20:1T:84:LYS:NZ    | 2.41                     | 0.51              |
| 22:1W:54:ILE:HG21 | 22:1W:107:PHE:CE1  | 2.43                     | 0.51              |
| 25:1Z:140:PHE:HB2 | 26:1a:45:TRP:CD1   | 2.45                     | 0.51              |
| 36:1k:38:ARG:N    | 36:1k:38:ARG:HD2   | 2.24                     | 0.51              |
| 1:1A:56:PHE:CZ    | 1:1A:60:ILE:HD11   | 2.46                     | 0.51              |
| 2:1B:126:TYR:CD1  | 4:1D:85:ARG:HD2    | 2.46                     | 0.51              |
| 6:1F:17:ASP:HA    | 6:1F:20:ARG:HG3    | 1.91                     | 0.51              |
| 7:1G:74:MET:HE3   | 7:1G:77:TRP:CZ3    | 2.46                     | 0.51              |
| 9:1I:68:ARG:HH12  | 9:1I:76:ARG:NH1    | 2.09                     | 0.51              |
| 15:1O:153:ASN:HA  | 15:1O:156:LYS:HB3  | 1.91                     | 0.51              |
| 27:1b:56:LEU:HD11 | 27:1b:62:MET:HG3   | 1.91                     | 0.51              |
| 41:1p:119:SER:OG  | 41:1p:119:SER:O    | 2.29                     | 0.51              |
| 4:1D:161:ILE:HD13 | 4:1D:235:TRP:CE3   | 2.45                     | 0.51              |
| 4:1D:403:ASP:OD1  | 4:1D:407:LYS:NZ    | 2.41                     | 0.51              |
| 7:1G:42:TYR:HD1   | 7:1G:48:VAL:HG12   | 1.75                     | 0.51              |
| 12:1L:83:ASP:CG   | 12:1L:262:ARG:HH12 | 2.18                     | 0.51              |
| 13:1M:61:LEU:HB2  | 13:1M:457:PRO:HD3  | 1.92                     | 0.51              |
| 14:1N:207:ILE:O   | 14:1N:210:THR:OG1  | 2.28                     | 0.51              |
| 40:1o:57:TYR:O    | 40:1o:60:HIS:ND1   | 2.42                     | 0.51              |
| 5:1E:100:ILE:HD11 | 5:1E:137:PHE:HD2   | 1.75                     | 0.51              |
| 6:1F:287:VAL:HG21 | 6:1F:294:LEU:HD12  | 1.91                     | 0.51              |
| 7:1G:110:GLN:HB3  | 7:1G:114:CYS:HB2   | 1.91                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:1G:288:LYS:N    | 42:1q:143:PRO:HD2  | 2.16                     | 0.51              |
| 7:1G:442:ILE:O    | 7:1G:446:ALA:N     | 2.43                     | 0.51              |
| 9:1I:52:PHE:CZ    | 42:1q:30:ALA:HA    | 2.45                     | 0.51              |
| 10:1J:33:LEU:O    | 10:1J:37:GLY:N     | 2.37                     | 0.51              |
| 14:1N:1:FME:HG2   | 14:1N:6:TYR:HB2    | 1.93                     | 0.51              |
| 14:1N:200:MET:HE1 | 14:1N:343:LEU:HD13 | 1.93                     | 0.51              |
| 14:1N:245:MET:HE2 | 45:1N:401:3PE:H3A2 | 1.92                     | 0.51              |
| 15:1O:141:GLN:NE2 | 15:1O:198:TYR:HA   | 2.25                     | 0.51              |
| 16:1P:171:ILE:HB  | 56:1P:501:NDP:N7N  | 2.25                     | 0.51              |
| 20:1T:70:LEU:HD12 | 20:1T:76:ILE:HG13  | 1.93                     | 0.51              |
| 28:1c:37:GLU:OE1  | 28:1c:37:GLU:N     | 2.41                     | 0.51              |
| 1:1A:70:ALA:HB2   | 10:1J:59:ILE:HG21  | 1.92                     | 0.51              |
| 3:1C:183:VAL:O    | 22:1W:101:THR:OG1  | 2.26                     | 0.51              |
| 3:1C:189:GLU:OE2  | 16:1P:14:SER:N     | 2.44                     | 0.51              |
| 4:1D:48:THR:HA    | 4:1D:67:GLU:HA     | 1.92                     | 0.51              |
| 5:1E:10:ARG:NH2   | 18:1R:76:ASP:O     | 2.44                     | 0.51              |
| 7:1G:670:ASP:CG   | 7:1G:671:PHE:H     | 2.19                     | 0.51              |
| 8:1H:210:GLY:O    | 8:1H:213:VAL:HG13  | 2.10                     | 0.51              |
| 10:1J:18:VAL:HA   | 11:1K:14:ILE:HD13  | 1.92                     | 0.51              |
| 12:1L:397:GLU:OE2 | 12:1L:482:MET:HG2  | 2.10                     | 0.51              |
| 13:1M:297:VAL:O   | 13:1M:301:ILE:HG12 | 2.11                     | 0.51              |
| 13:1M:300:ALA:O   | 13:1M:308:SER:OG   | 2.21                     | 0.51              |
| 13:1M:442:LEU:N   | 13:1M:443:PRO:HD2  | 2.26                     | 0.51              |
| 14:1N:267:ILE:O   | 14:1N:271:THR:OG1  | 2.25                     | 0.51              |
| 32:1g:48:ASP:OD1  | 32:1g:49:LYS:N     | 2.44                     | 0.51              |
| 3:1C:78:LEU:HG    | 3:1C:130:TYR:HB3   | 1.93                     | 0.51              |
| 4:1D:202:ASP:HB2  | 4:1D:323:ILE:HD13  | 1.92                     | 0.51              |
| 7:1G:59:ILE:HG13  | 7:1G:77:TRP:CD1    | 2.46                     | 0.51              |
| 9:1I:120:GLY:HA2  | 9:1I:133:GLU:OE2   | 2.11                     | 0.51              |
| 10:1J:110:GLU:HG2 | 10:1J:112:GLU:HG2  | 1.93                     | 0.51              |
| 39:1n:133:GLU:OE2 | 39:1n:133:GLU:N    | 2.25                     | 0.51              |
| 41:1p:50:PHE:O    | 41:1p:53:GLN:NE2   | 2.44                     | 0.51              |
| 4:1D:167:PHE:O    | 4:1D:171:PHE:HB3   | 2.11                     | 0.51              |
| 12:1L:35:TYR:OH   | 34:1i:73:HIS:NE2   | 2.31                     | 0.51              |
| 12:1L:570:GLN:OE1 | 14:1N:167:TRP:NE1  | 2.43                     | 0.51              |
| 19:1S:39:ARG:NH2  | 19:1S:86:VAL:HG13  | 2.26                     | 0.51              |
| 20:1U:12:LYS:NZ   | 20:1U:13:ASP:OD1   | 2.44                     | 0.51              |
| 28:1c:43:LYS:HD3  | 28:1c:48:LEU:HD22  | 1.93                     | 0.51              |
| 33:1h:17:TYR:CE1  | 39:1n:107:HIS:HB2  | 2.45                     | 0.51              |
| 3:1C:210:ARG:HH12 | 3:1C:212:PRO:HA    | 1.75                     | 0.51              |
| 6:1F:22:PHE:HE2   | 6:1F:255:LEU:HD11  | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:1F:116:HIS:O    | 6:1F:120:GLU:HG2  | 2.11                     | 0.51              |
| 6:1F:297:VAL:HG23 | 6:1F:336:VAL:HA   | 1.93                     | 0.51              |
| 7:1G:38:PRO:HG3   | 7:1G:123:PHE:CD2  | 2.45                     | 0.51              |
| 7:1G:546:GLN:NE2  | 7:1G:596:ASP:OD1  | 2.43                     | 0.51              |
| 16:1P:64:ASP:HB3  | 16:1P:67:GLN:HG2  | 1.93                     | 0.51              |
| 24:1Y:123:LEU:HA  | 24:1Y:126:MET:HG3 | 1.91                     | 0.51              |
| 26:1a:26:ILE:HD12 | 26:1a:26:ILE:H    | 1.76                     | 0.51              |
| 32:1g:71:VAL:O    | 32:1g:74:SER:OG   | 2.19                     | 0.51              |
| 32:1g:93:ALA:O    | 32:1g:97:VAL:HG23 | 2.11                     | 0.51              |
| 38:1m:49:GLN:HG3  | 38:1m:59:ILE:HG12 | 1.92                     | 0.51              |
| 2:1B:78:ALA:HB1   | 8:1H:208:VAL:HG13 | 1.93                     | 0.51              |
| 2:1B:81:ARG:HE    | 8:1H:216:ALA:N    | 2.09                     | 0.51              |
| 4:1D:160:ASP:O    | 8:1H:279:ARG:NH1  | 2.41                     | 0.51              |
| 7:1G:46:LEU:HD11  | 7:1G:161:ARG:CB   | 2.41                     | 0.51              |
| 8:1H:296:LEU:HD13 | 8:1H:300:LEU:HD23 | 1.91                     | 0.51              |
| 9:1I:48:ILE:HG23  | 9:1I:53:GLU:HB2   | 1.93                     | 0.51              |
| 9:1I:73:GLY:HA2   | 42:1q:108:TYR:CE1 | 2.45                     | 0.51              |
| 9:1I:113:MET:HE1  | 9:1I:118:TYR:HE2  | 1.75                     | 0.51              |
| 10:1J:160:SER:O   | 10:1J:164:GLY:N   | 2.44                     | 0.51              |
| 12:1L:1:FME:HE1   | 34:1i:86:LYS:HG3  | 1.94                     | 0.51              |
| 12:1L:560:THR:HA  | 12:1L:564:LYS:HB2 | 1.91                     | 0.51              |
| 13:1M:46:GLY:HA2  | 32:1g:84:ARG:HA   | 1.91                     | 0.51              |
| 16:1P:240:ASP:OD1 | 16:1P:338:LYS:HB3 | 2.10                     | 0.51              |
| 22:1W:108:HIS:HB3 | 22:1W:111:GLU:CD  | 2.36                     | 0.51              |
| 30:1e:44:HIS:ND1  | 33:1h:130:LYS:HD3 | 2.26                     | 0.51              |
| 4:1D:83:LEU:O     | 4:1D:85:ARG:HG3   | 2.11                     | 0.50              |
| 5:1E:149:VAL:HB   | 6:1F:105:CYS:HB2  | 1.92                     | 0.50              |
| 6:1F:141:GLU:OE1  | 6:1F:141:GLU:N    | 2.42                     | 0.50              |
| 7:1G:115:ASP:O    | 7:1G:119:GLN:HG2  | 2.11                     | 0.50              |
| 7:1G:450:MET:HG2  | 7:1G:487:TRP:HZ2  | 1.76                     | 0.50              |
| 8:1H:268:ILE:O    | 8:1H:272:TRP:N    | 2.38                     | 0.50              |
| 10:1J:159:TRP:HE1 | 14:1N:12:THR:HG22 | 1.76                     | 0.50              |
| 11:1K:23:ARG:HG3  | 11:1K:24:SER:H    | 1.76                     | 0.50              |
| 13:1M:403:THR:O   | 13:1M:407:SER:OG  | 2.19                     | 0.50              |
| 17:1Q:114:LYS:HD3 | 17:1Q:114:LYS:N   | 2.26                     | 0.50              |
| 42:1q:67:GLU:OE2  | 42:1q:68:MET:N    | 2.43                     | 0.50              |
| 4:1D:87:THR:OG1   | 4:1D:88:GLU:N     | 2.42                     | 0.50              |
| 4:1D:139:VAL:HG23 | 4:1D:278:TYR:CE1  | 2.45                     | 0.50              |
| 4:1D:157:HIS:HE1  | 4:1D:239:THR:HG22 | 1.76                     | 0.50              |
| 8:1H:224:PHE:HE1  | 8:1H:228:TYR:CZ   | 2.29                     | 0.50              |
| 11:1K:97:GLN:NE2  | 12:1L:581:LYS:O   | 2.44                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1U:76:ILE:O     | 20:1U:80:ILE:HG12  | 2.10                     | 0.50              |
| 22:1W:75:ASP:HB3   | 22:1W:78:VAL:HG12  | 1.92                     | 0.50              |
| 27:1b:17:VAL:HG13  | 27:1b:18:LEU:HD22  | 1.93                     | 0.50              |
| 50:1f:101:PC1:H361 | 32:1g:76:PHE:CE2   | 2.47                     | 0.50              |
| 40:1o:55:ARG:HH22  | 41:1p:119:SER:HB2  | 1.75                     | 0.50              |
| 3:1C:129:TRP:CE3   | 4:1D:400:ALA:HA    | 2.46                     | 0.50              |
| 3:1C:137:MET:HB3   | 3:1C:162:PHE:HB2   | 1.93                     | 0.50              |
| 3:1C:206:PHE:HB3   | 43:1r:60:ARG:HD3   | 1.92                     | 0.50              |
| 4:1D:143:GLU:HA    | 4:1D:146:ARG:HB3   | 1.93                     | 0.50              |
| 4:1D:147:LEU:HD22  | 4:1D:218:PHE:HE2   | 1.76                     | 0.50              |
| 4:1D:357:GLN:OE1   | 43:1r:59:ARG:NH2   | 2.44                     | 0.50              |
| 5:1E:147:ALA:HB3   | 5:1E:153:MET:HG3   | 1.92                     | 0.50              |
| 7:1G:344:CYS:HA    | 7:1G:508:LYS:HB2   | 1.93                     | 0.50              |
| 9:1I:89:ALA:HB1    | 9:1I:115:LYS:HE2   | 1.93                     | 0.50              |
| 16:1P:97:ARG:HD2   | 16:1P:99:TRP:CE2   | 2.46                     | 0.50              |
| 40:1o:75:ASN:HD22  | 41:1p:25:LEU:HD21  | 1.77                     | 0.50              |
| 3:1C:8:ARG:HD3     | 3:1C:11:ILE:HD11   | 1.93                     | 0.50              |
| 3:1C:133:GLU:HA    | 3:1C:136:ASP:HB2   | 1.92                     | 0.50              |
| 5:1E:200:THR:HG21  | 6:1F:283:HIS:HA    | 1.93                     | 0.50              |
| 6:1F:433:PHE:HA    | 6:1F:436:GLN:HE21  | 1.77                     | 0.50              |
| 7:1G:524:LEU:HB3   | 7:1G:545:TYR:HA    | 1.93                     | 0.50              |
| 50:1H:401:PC1:H382 | 9:1I:25:LEU:HD12   | 1.93                     | 0.50              |
| 9:1I:116:CYS:HB2   | 46:1I:201:SF4:S1   | 2.52                     | 0.50              |
| 12:1L:132:VAL:HG13 | 12:1L:133:THR:HG23 | 1.93                     | 0.50              |
| 45:1L:703:3PE:H371 | 45:1L:703:3PE:H231 | 1.93                     | 0.50              |
| 13:1M:354:LEU:HD22 | 33:1h:18:ASP:OD1   | 2.11                     | 0.50              |
| 19:1S:24:GLN:HE22  | 19:1S:58:SER:HB2   | 1.76                     | 0.50              |
| 20:1U:37:MET:HB3   | 20:1U:42:LEU:HB3   | 1.94                     | 0.50              |
| 21:1V:93:MET:HG2   | 21:1V:96:TRP:HD1   | 1.76                     | 0.50              |
| 31:1f:37:PHE:HA    | 31:1f:40:LYS:HG3   | 1.94                     | 0.50              |
| 32:1g:100:ARG:NE   | 32:1g:107:LEU:O    | 2.44                     | 0.50              |
| 34:1i:120:LYS:HE3  | 34:1i:121:GLU:OE1  | 2.11                     | 0.50              |
| 6:1F:122:CYS:HB3   | 6:1F:173:PHE:HE2   | 1.76                     | 0.50              |
| 7:1G:285:ARG:HG2   | 7:1G:290:LEU:O     | 2.11                     | 0.50              |
| 7:1G:626:VAL:HA    | 19:1S:19:ARG:HH21  | 1.77                     | 0.50              |
| 12:1L:51:LEU:HB3   | 12:1L:55:MET:HE1   | 1.93                     | 0.50              |
| 12:1L:319:ILE:HG21 | 12:1L:404:THR:HG22 | 1.93                     | 0.50              |
| 13:1M:278:ARG:CZ   | 37:1l:83:MET:HE3   | 2.42                     | 0.50              |
| 13:1M:422:HIS:HD2  | 38:1m:59:ILE:HB    | 1.77                     | 0.50              |
| 15:1O:90:ASP:O     | 32:1g:27:GLN:NE2   | 2.35                     | 0.50              |
| 18:1R:56:VAL:C     | 18:1R:57:ILE:HD13  | 2.36                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:1S:19:ARG:CZ    | 19:1S:65:TRP:HB3   | 2.42                     | 0.50              |
| 23:1X:137:PRO:HG2  | 23:1X:140:PRO:HG3  | 1.94                     | 0.50              |
| 32:1g:85:MET:HE2   | 32:1g:85:MET:N     | 2.27                     | 0.50              |
| 33:1h:129:ASP:OD1  | 33:1h:129:ASP:N    | 2.45                     | 0.50              |
| 37:1l:90:ASP:OD1   | 37:1l:90:ASP:N     | 2.44                     | 0.50              |
| 41:1p:28:PRO:O     | 41:1p:32:LEU:HG    | 2.12                     | 0.50              |
| 4:1D:328:ALA:HB3   | 7:1G:126:ASP:HB2   | 1.94                     | 0.50              |
| 5:1E:111:ARG:HB3   | 5:1E:152:PRO:HD3   | 1.93                     | 0.50              |
| 5:1E:150:ASN:ND2   | 5:1E:163:ASP:OD2   | 2.34                     | 0.50              |
| 6:1F:118:LEU:HD12  | 6:1F:225:VAL:HG13  | 1.93                     | 0.50              |
| 7:1G:155:GLN:HG2   | 7:1G:181:MET:HG2   | 1.92                     | 0.50              |
| 13:1M:351:LEU:HD11 | 13:1M:419:TYR:HB2  | 1.94                     | 0.50              |
| 21:1V:82:GLN:HA    | 21:1V:85:ASN:HD21  | 1.75                     | 0.50              |
| 34:1i:120:LYS:HB3  | 40:1o:39:VAL:HG22  | 1.94                     | 0.50              |
| 39:1n:139:LEU:O    | 39:1n:143:THR:OG1  | 2.22                     | 0.50              |
| 1:1A:4:MET:HE2     | 25:1Z:142:TRP:CZ3  | 2.46                     | 0.50              |
| 3:1C:12:ARG:HA     | 4:1D:129:GLN:HB3   | 1.94                     | 0.50              |
| 7:1G:296:TRP:O     | 7:1G:300:LEU:HD12  | 2.12                     | 0.50              |
| 7:1G:319:ALA:HB3   | 7:1G:345:THR:HA    | 1.94                     | 0.50              |
| 7:1G:440:SER:HA    | 7:1G:443:LEU:HD13  | 1.93                     | 0.50              |
| 9:1I:149:TYR:HD2   | 9:1I:154:LEU:HD22  | 1.77                     | 0.50              |
| 12:1L:324:LEU:HB3  | 12:1L:395:ILE:HD11 | 1.94                     | 0.50              |
| 15:1O:86:PRO:HB2   | 15:1O:87:LYS:HD3   | 1.94                     | 0.50              |
| 18:1R:7:THR:O      | 18:1R:7:THR:HG22   | 2.12                     | 0.50              |
| 22:1W:64:ARG:O     | 22:1W:68:MET:HE2   | 2.11                     | 0.50              |
| 22:1W:115:PRO:O    | 22:1W:121:LYS:HE3  | 2.12                     | 0.50              |
| 26:1a:1:MET:HA     | 26:1a:1:MET:HE3    | 1.93                     | 0.50              |
| 32:1g:67:SER:HA    | 32:1g:71:VAL:HB    | 1.93                     | 0.50              |
| 40:1o:57:TYR:H     | 40:1o:57:TYR:HD1   | 1.60                     | 0.50              |
| 5:1E:23:PHE:HB3    | 5:1E:27:ASN:HB2    | 1.94                     | 0.50              |
| 13:1M:231:LEU:HA   | 13:1M:235:LEU:HG   | 1.92                     | 0.50              |
| 20:1T:52:MET:HA    | 20:1T:55:GLU:OE1   | 2.11                     | 0.50              |
| 31:1f:24:CYS:O     | 31:1f:28:ARG:NE    | 2.45                     | 0.50              |
| 31:1f:54:VAL:HG12  | 31:1f:55:THR:O     | 2.11                     | 0.50              |
| 32:1g:91:ARG:HG2   | 32:1g:91:ARG:HH11  | 1.77                     | 0.50              |
| 39:1n:144:PRO:HG2  | 39:1n:148:PRO:HA   | 1.93                     | 0.50              |
| 3:1C:50:ILE:HD12   | 3:1C:50:ILE:O      | 2.11                     | 0.50              |
| 4:1D:161:ILE:HD11  | 4:1D:238:ARG:HB2   | 1.94                     | 0.50              |
| 7:1G:140:LYS:H     | 7:1G:148:THR:HG21  | 1.76                     | 0.50              |
| 10:1J:141:MET:HA   | 10:1J:141:MET:HE2  | 1.93                     | 0.50              |
| 12:1L:160:GLY:HA3  | 39:1n:94:GLU:OE1   | 2.11                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:244:MET:O    | 14:1N:248:LEU:HB2  | 2.11                     | 0.50              |
| 16:1P:174:ARG:HB3  | 16:1P:175:GLU:OE2  | 2.11                     | 0.50              |
| 17:1Q:65:TRP:CE2   | 17:1Q:74:SER:HB3   | 2.47                     | 0.50              |
| 22:1W:42:GLU:OE1   | 22:1W:42:GLU:N     | 2.45                     | 0.50              |
| 30:1e:85:LEU:HB3   | 30:1e:90:LYS:HB2   | 1.93                     | 0.50              |
| 34:1i:71:VAL:HA    | 34:1i:75:LEU:HB2   | 1.93                     | 0.50              |
| 37:1l:30:ARG:CZ    | 38:1m:34:GLU:HG3   | 2.42                     | 0.50              |
| 41:1p:55:HIS:HB3   | 41:1p:59:ARG:HH12  | 1.77                     | 0.50              |
| 2:1B:147:PRO:HD3   | 9:1I:140:SER:HA    | 1.94                     | 0.49              |
| 3:1C:193:GLU:OE2   | 17:1Q:73:SER:OG    | 2.29                     | 0.49              |
| 6:1F:184:TYR:HB3   | 6:1F:357:GLU:CG    | 2.42                     | 0.49              |
| 6:1F:327:THR:OG1   | 6:1F:328:GLY:N     | 2.45                     | 0.49              |
| 7:1G:282:PRO:HG3   | 7:1G:296:TRP:CD2   | 2.47                     | 0.49              |
| 7:1G:460:ARG:HH21  | 7:1G:657:LEU:HB3   | 1.76                     | 0.49              |
| 8:1H:32:GLN:OE1    | 8:1H:34:ARG:NE     | 2.44                     | 0.49              |
| 12:1L:413:LEU:HD12 | 12:1L:493:VAL:HG11 | 1.94                     | 0.49              |
| 15:1O:294:GLN:O    | 15:1O:297:THR:OG1  | 2.29                     | 0.49              |
| 16:1P:258:LEU:HD11 | 16:1P:262:ALA:HB3  | 1.94                     | 0.49              |
| 21:1V:63:ASP:HB3   | 21:1V:66:LYS:HE3   | 1.93                     | 0.49              |
| 23:1X:18:LYS:CA    | 26:1a:54:ILE:HD11  | 2.40                     | 0.49              |
| 23:1X:76:HIS:ND1   | 23:1X:113:LYS:HE2  | 2.27                     | 0.49              |
| 32:1g:87:GLU:OE2   | 32:1g:91:ARG:NH1   | 2.45                     | 0.49              |
| 37:1l:66:HIS:O     | 37:1l:70:ARG:N     | 2.43                     | 0.49              |
| 37:1l:97:SER:HB3   | 38:1m:6:LYS:HG3    | 1.93                     | 0.49              |
| 37:1l:115:MET:HA   | 37:1l:118:VAL:HG22 | 1.94                     | 0.49              |
| 37:1l:157:GLU:HG2  | 40:1o:34:LYS:O     | 2.11                     | 0.49              |
| 44:1s:38:TYR:CZ    | 44:1s:40:ASN:HB3   | 2.47                     | 0.49              |
| 2:1B:45:LEU:N      | 2:1B:74:VAL:HG12   | 2.27                     | 0.49              |
| 5:1E:191:PHE:HD2   | 6:1F:28:ARG:HH22   | 1.60                     | 0.49              |
| 6:1F:264:HIS:HB2   | 6:1F:284:ALA:HA    | 1.95                     | 0.49              |
| 7:1G:25:THR:O      | 7:1G:29:ALA:N      | 2.43                     | 0.49              |
| 7:1G:704:CYS:HB3   | 18:1R:85:GLY:HA3   | 1.94                     | 0.49              |
| 12:1L:598:SER:HA   | 12:1L:602:PHE:CD2  | 2.47                     | 0.49              |
| 16:1P:300:LEU:HB3  | 16:1P:305:ILE:O    | 2.12                     | 0.49              |
| 32:1g:56:TRP:O     | 32:1g:60:VAL:HG22  | 2.12                     | 0.49              |
| 33:1h:63:HIS:NE2   | 33:1h:76:ALA:O     | 2.44                     | 0.49              |
| 35:1j:32:MET:O     | 35:1j:36:ILE:HG12  | 2.12                     | 0.49              |
| 6:1F:60:VAL:HG13   | 6:1F:76:GLY:HA2    | 1.93                     | 0.49              |
| 6:1F:93:LEU:HD23   | 6:1F:94:VAL:N      | 2.28                     | 0.49              |
| 9:1I:86:VAL:CG1    | 9:1I:121:PHE:HB3   | 2.42                     | 0.49              |
| 13:1M:331:ASN:ND2  | 13:1M:335:GLU:OE2  | 2.43                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:1N:261:MET:SD   | 14:1N:340:THR:OG1  | 2.68                     | 0.49              |
| 16:1P:108:ASP:HA   | 16:1P:112:LYS:HG3  | 1.93                     | 0.49              |
| 23:1X:157:LEU:HG   | 29:1d:21:LEU:HD21  | 1.94                     | 0.49              |
| 9:1I:27:TRP:HB3    | 9:1I:30:LEU:HB2    | 1.93                     | 0.49              |
| 9:1I:65:HIS:HB3    | 9:1I:131:ILE:HD11  | 1.93                     | 0.49              |
| 9:1I:101:ASP:OD1   | 9:1I:101:ASP:N     | 2.41                     | 0.49              |
| 13:1M:150:LEU:HD11 | 14:1N:254:LEU:HD21 | 1.92                     | 0.49              |
| 14:1N:2:ASN:HB2    | 15:1O:254:ARG:HD2  | 1.95                     | 0.49              |
| 14:1N:112:HIS:NE2  | 14:1N:164:ILE:HG21 | 2.28                     | 0.49              |
| 14:1N:163:LEU:HD12 | 14:1N:167:TRP:CZ3  | 2.48                     | 0.49              |
| 15:1O:252:ASP:N    | 15:1O:252:ASP:OD1  | 2.43                     | 0.49              |
| 16:1P:314:ALA:HB3  | 16:1P:331:MET:HE1  | 1.94                     | 0.49              |
| 21:1V:5:LYS:HB3    | 21:1V:15:VAL:HG11  | 1.95                     | 0.49              |
| 21:1V:10:LEU:HD12  | 21:1V:10:LEU:H     | 1.77                     | 0.49              |
| 32:1g:88:TRP:NE1   | 41:1p:65:ARG:O     | 2.40                     | 0.49              |
| 39:1n:133:GLU:H    | 39:1n:133:GLU:CD   | 2.15                     | 0.49              |
| 39:1n:178:MET:SD   | 39:1n:178:MET:N    | 2.85                     | 0.49              |
| 2:1B:126:TYR:CE1   | 4:1D:85:ARG:NE     | 2.81                     | 0.49              |
| 4:1D:350:LYS:HD3   | 7:1G:117:GLN:HB3   | 1.95                     | 0.49              |
| 9:1I:119:CYS:N     | 46:1I:201:SF4:S2   | 2.85                     | 0.49              |
| 10:1J:115:ILE:HG12 | 10:1J:116:ILE:HG12 | 1.95                     | 0.49              |
| 12:1L:339:LEU:HD21 | 12:1L:376:GLY:HA3  | 1.93                     | 0.49              |
| 14:1N:272:LYS:HG2  | 33:1h:108:LEU:HD21 | 1.92                     | 0.49              |
| 17:1Q:106:GLU:OE1  | 17:1Q:107:GLU:N    | 2.46                     | 0.49              |
| 34:1i:125:GLN:HB3  | 40:1o:88:TYR:HE2   | 1.76                     | 0.49              |
| 37:1l:10:PRO:HD3   | 38:1m:66:ARG:HG2   | 1.95                     | 0.49              |
| 40:1o:46:ASN:HA    | 40:1o:55:ARG:HH22  | 1.78                     | 0.49              |
| 2:1B:54:CYS:HA     | 4:1D:108:TYR:HB2   | 1.94                     | 0.49              |
| 2:1B:69:MET:SD     | 2:1B:74:VAL:HG23   | 2.53                     | 0.49              |
| 2:1B:126:TYR:HD1   | 4:1D:85:ARG:HD2    | 1.77                     | 0.49              |
| 4:1D:3:GLN:NE2     | 4:1D:5:GLN:OE1     | 2.42                     | 0.49              |
| 4:1D:165:THR:HB    | 4:1D:169:TRP:CH2   | 2.47                     | 0.49              |
| 5:1E:127:LYS:HG2   | 5:1E:130:GLU:HG2   | 1.94                     | 0.49              |
| 6:1F:101:GLU:O     | 6:1F:104:THR:OG1   | 2.26                     | 0.49              |
| 6:1F:321:ALA:O     | 6:1F:322:LEU:HD22  | 2.12                     | 0.49              |
| 7:1G:500:VAL:HG21  | 7:1G:576:THR:HA    | 1.94                     | 0.49              |
| 8:1H:142:TYR:CE1   | 8:1H:289:LEU:HB2   | 2.47                     | 0.49              |
| 10:1J:40:GLY:HA2   | 10:1J:43:ILE:HD12  | 1.95                     | 0.49              |
| 12:1L:62:ILE:O     | 34:1i:96:VAL:HA    | 2.13                     | 0.49              |
| 13:1M:175:ASN:HB3  | 13:1M:178:ILE:HG22 | 1.94                     | 0.49              |
| 14:1N:238:PRO:HB2  | 45:1N:401:3PE:O32  | 2.13                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:1W:52:LEU:HD21  | 22:1W:104:MET:SD   | 2.53                     | 0.49              |
| 26:1a:27:HIS:HD2   | 26:1a:36:LYS:HB2   | 1.76                     | 0.49              |
| 28:1c:27:LEU:HD11  | 29:1d:70:PHE:CD2   | 2.47                     | 0.49              |
| 35:1j:10:ARG:HD2   | 35:1j:15:PRO:HA    | 1.94                     | 0.49              |
| 42:1q:56:PHE:HZ    | 43:1r:33:ARG:HD3   | 1.78                     | 0.49              |
| 4:1D:329:LYS:NZ    | 7:1G:125:SER:O     | 2.41                     | 0.49              |
| 5:1E:78:MET:O      | 5:1E:82:GLU:HG2    | 2.13                     | 0.49              |
| 6:1F:33:LEU:HD22   | 6:1F:155:GLU:HG2   | 1.93                     | 0.49              |
| 7:1G:285:ARG:CZ    | 42:1q:144:TYR:HA   | 2.43                     | 0.49              |
| 11:1K:27:MET:HE3   | 11:1K:27:MET:HA    | 1.95                     | 0.49              |
| 12:1L:184:LEU:HD13 | 13:1M:393:ILE:HG21 | 1.94                     | 0.49              |
| 12:1L:500:LEU:HD12 | 12:1L:501:ALA:N    | 2.27                     | 0.49              |
| 13:1M:237:LYS:HE2  | 13:1M:316:MET:O    | 2.13                     | 0.49              |
| 15:1O:93:SER:OG    | 15:1O:94:TYR:N     | 2.46                     | 0.49              |
| 16:1P:235:ARG:HG2  | 16:1P:341:ASN:HA   | 1.94                     | 0.49              |
| 16:1P:248:VAL:HG13 | 16:1P:318:LEU:HD13 | 1.94                     | 0.49              |
| 19:1S:22:LEU:HD23  | 19:1S:22:LEU:H     | 1.77                     | 0.49              |
| 23:1X:21:SER:HA    | 23:1X:24:LEU:HD23  | 1.94                     | 0.49              |
| 31:1f:42:LEU:HG    | 41:1p:70:VAL:HG12  | 1.95                     | 0.49              |
| 34:1i:74:VAL:C     | 34:1i:77:PRO:HD2   | 2.37                     | 0.49              |
| 38:1m:82:THR:HG23  | 38:1m:85:THR:H     | 1.78                     | 0.49              |
| 41:1p:55:HIS:HB3   | 41:1p:59:ARG:NH1   | 2.26                     | 0.49              |
| 2:1B:45:LEU:H      | 2:1B:74:VAL:HG12   | 1.76                     | 0.49              |
| 2:1B:162:GLN:NE2   | 9:1I:140:SER:OG    | 2.46                     | 0.49              |
| 4:1D:101:PRO:HB3   | 4:1D:105:ARG:HH21  | 1.77                     | 0.49              |
| 4:1D:133:ARG:O     | 4:1D:137:ILE:HD12  | 2.13                     | 0.49              |
| 4:1D:168:PHE:HB2   | 8:1H:32:GLN:HB2    | 1.95                     | 0.49              |
| 6:1F:45:THR:HA     | 6:1F:48:ILE:HG22   | 1.95                     | 0.49              |
| 8:1H:63:PRO:HB2    | 8:1H:66:SER:HB3    | 1.94                     | 0.49              |
| 9:1I:4:PHE:HB2     | 43:1r:111:TYR:HD1  | 1.78                     | 0.49              |
| 9:1I:84:GLU:OE1    | 9:1I:92:ILE:HB     | 2.12                     | 0.49              |
| 9:1I:153:LYS:O     | 9:1I:157:ASN:ND2   | 2.38                     | 0.49              |
| 12:1L:463:PHE:O    | 12:1L:465:GLY:N    | 2.46                     | 0.49              |
| 13:1M:40:SER:O     | 33:1h:80:TYR:OH    | 2.21                     | 0.49              |
| 20:1T:14:ARG:HD3   | 20:1T:58:PHE:CE2   | 2.47                     | 0.49              |
| 21:1V:93:MET:HG2   | 21:1V:96:TRP:CD1   | 2.48                     | 0.49              |
| 30:1e:76:SER:O     | 30:1e:80:ARG:HG2   | 2.13                     | 0.49              |
| 32:1g:67:SER:N     | 33:1h:28:TYR:OH    | 2.34                     | 0.49              |
| 2:1B:71:ARG:NH2    | 9:1I:50:TYR:H      | 2.10                     | 0.49              |
| 6:1F:56:ILE:H      | 6:1F:56:ILE:HD12   | 1.78                     | 0.49              |
| 6:1F:307:ILE:HG22  | 6:1F:421:HIS:HE1   | 1.78                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:343:ILE:HD12  | 6:1F:344:VAL:N     | 2.28                     | 0.49              |
| 8:1H:85:MET:HG2    | 8:1H:233:MET:SD    | 2.52                     | 0.49              |
| 13:1M:354:LEU:HG   | 13:1M:358:TRP:NE1  | 2.27                     | 0.49              |
| 15:1O:111:ALA:HB1  | 15:1O:122:VAL:HG21 | 1.93                     | 0.49              |
| 30:1e:64:GLU:OE2   | 30:1e:70:LYS:N     | 2.46                     | 0.49              |
| 39:1n:15:VAL:HG22  | 39:1n:63:LEU:HD21  | 1.95                     | 0.49              |
| 43:1r:3:ALA:O      | 43:1r:8:GLN:NE2    | 2.44                     | 0.49              |
| 3:1C:79:THR:HB     | 4:1D:390:LYS:HG2   | 1.95                     | 0.49              |
| 4:1D:296:ARG:HD2   | 4:1D:420:THR:OG1   | 2.13                     | 0.49              |
| 4:1D:423:ILE:HG23  | 4:1D:428:VAL:HG21  | 1.94                     | 0.49              |
| 5:1E:87:TYR:HB3    | 6:1F:181:ALA:O     | 2.13                     | 0.49              |
| 14:1N:200:MET:HE3  | 14:1N:269:GLU:OE1  | 2.13                     | 0.49              |
| 14:1N:211:MET:SD   | 14:1N:211:MET:N    | 2.85                     | 0.49              |
| 14:1N:226:THR:HG23 | 14:1N:229:SER:H    | 1.78                     | 0.49              |
| 15:1O:139:TYR:HD2  | 15:1O:140:ARG:HH12 | 1.59                     | 0.49              |
| 20:1T:84:LYS:HG3   | 20:1T:86:VAL:HB    | 1.93                     | 0.49              |
| 31:1f:31:ASP:OD1   | 31:1f:32:GLU:N     | 2.46                     | 0.49              |
| 33:1h:95:GLN:HB2   | 41:1p:82:LEU:HD11  | 1.94                     | 0.49              |
| 41:1p:91:TRP:HH2   | 41:1p:149:TYR:HB2  | 1.78                     | 0.49              |
| 7:1G:53:ARG:NH2    | 7:1G:56:LEU:HD21   | 2.28                     | 0.48              |
| 7:1G:465:ALA:HB2   | 7:1G:654:GLN:HB2   | 1.95                     | 0.48              |
| 8:1H:235:ASN:OD1   | 8:1H:267:THR:N     | 2.46                     | 0.48              |
| 12:1L:313:MET:O    | 12:1L:316:THR:OG1  | 2.26                     | 0.48              |
| 13:1M:201:MET:HE1  | 13:1M:261:PHE:CE1  | 2.48                     | 0.48              |
| 14:1N:106:LEU:HB3  | 14:1N:108:LEU:HD11 | 1.95                     | 0.48              |
| 15:1O:21:THR:O     | 15:1O:121:GLY:N    | 2.46                     | 0.48              |
| 16:1P:81:ILE:O     | 16:1P:85:VAL:HG22  | 2.12                     | 0.48              |
| 16:1P:259:PRO:HB2  | 16:1P:261:PHE:HD1  | 1.78                     | 0.48              |
| 20:1T:18:VAL:HA    | 20:1T:21:LEU:HD23  | 1.94                     | 0.48              |
| 33:1h:114:MET:HG2  | 33:1h:122:TRP:HE1  | 1.78                     | 0.48              |
| 40:1o:41:THR:O     | 40:1o:45:MET:HE1   | 2.13                     | 0.48              |
| 4:1D:178:PHE:CE2   | 4:1D:189:MET:HB2   | 2.48                     | 0.48              |
| 4:1D:261:ARG:NH2   | 4:1D:368:GLU:OE1   | 2.44                     | 0.48              |
| 5:1E:131:THR:HG22  | 5:1E:132:THR:O     | 2.12                     | 0.48              |
| 6:1F:292:ASP:O     | 6:1F:339:ARG:NH2   | 2.38                     | 0.48              |
| 7:1G:333:ASP:HB3   | 7:1G:611:LEU:HD11  | 1.95                     | 0.48              |
| 7:1G:363:LEU:N     | 7:1G:492:ILE:HG12  | 2.29                     | 0.48              |
| 7:1G:670:ASP:CG    | 7:1G:671:PHE:N     | 2.72                     | 0.48              |
| 8:1H:201:THR:O     | 8:1H:210:GLY:HA3   | 2.13                     | 0.48              |
| 9:1I:106:THR:O     | 9:1I:151:LYS:HE3   | 2.13                     | 0.48              |
| 10:1J:146:LEU:CA   | 11:1K:58:MET:HE1   | 2.42                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:1K:11:ALA:O    | 11:1K:14:ILE:HG13  | 2.13                     | 0.48              |
| 12:1L:86:SER:O    | 12:1L:90:ILE:HG12  | 2.13                     | 0.48              |
| 12:1L:550:SER:HB2 | 13:1M:275:ILE:HG23 | 1.94                     | 0.48              |
| 13:1M:388:TRP:HD1 | 29:1d:120:ARG:C    | 2.21                     | 0.48              |
| 14:1N:108:LEU:HB3 | 14:1N:161:SER:HB2  | 1.94                     | 0.48              |
| 21:1V:92:LYS:HA   | 21:1V:95:ARG:NH2   | 2.28                     | 0.48              |
| 26:1a:1:MET:HB2   | 26:1a:3:PHE:CZ     | 2.48                     | 0.48              |
| 34:1i:16:GLU:HA   | 34:1i:19:ARG:HB3   | 1.95                     | 0.48              |
| 36:1k:29:GLU:OE1  | 36:1k:30:THR:N     | 2.45                     | 0.48              |
| 5:1E:10:ARG:NH2   | 18:1R:76:ASP:OD1   | 2.46                     | 0.48              |
| 6:1F:136:ILE:HD12 | 6:1F:136:ILE:O     | 2.13                     | 0.48              |
| 7:1G:194:GLU:OE1  | 7:1G:194:GLU:N     | 2.44                     | 0.48              |
| 7:1G:383:ASN:O    | 7:1G:387:GLU:HG2   | 2.13                     | 0.48              |
| 9:1I:145:GLU:OE2  | 16:1P:66:GLY:N     | 2.40                     | 0.48              |
| 11:1K:70:GLU:O    | 11:1K:74:GLY:N     | 2.45                     | 0.48              |
| 11:1K:94:ASN:HB3  | 12:1L:583:LEU:HD23 | 1.96                     | 0.48              |
| 12:1L:51:LEU:HD23 | 12:1L:87:VAL:HG22  | 1.95                     | 0.48              |
| 12:1L:541:ASN:C   | 12:1L:541:ASN:HD22 | 2.21                     | 0.48              |
| 12:1L:548:SER:O   | 12:1L:550:SER:N    | 2.46                     | 0.48              |
| 12:1L:571:MET:HE2 | 12:1L:571:MET:HA   | 1.95                     | 0.48              |
| 13:1M:10:MET:O    | 13:1M:13:PRO:HD2   | 2.13                     | 0.48              |
| 14:1N:273:ASN:OD1 | 24:1Y:139:LYS:N    | 2.39                     | 0.48              |
| 16:1P:210:VAL:O   | 16:1P:214:ILE:HG12 | 2.13                     | 0.48              |
| 21:1V:27:TYR:HA   | 21:1V:30:ILE:HG12  | 1.95                     | 0.48              |
| 23:1X:132:THR:HB  | 27:1b:57:ARG:HH21  | 1.78                     | 0.48              |
| 34:1i:42:MET:SD   | 34:1i:43:GLU:N     | 2.86                     | 0.48              |
| 37:1l:82:ASP:O    | 37:1l:88:ARG:NH1   | 2.38                     | 0.48              |
| 1:1A:94:LEU:HD21  | 10:1J:154:VAL:HG22 | 1.95                     | 0.48              |
| 5:1E:98:TYR:CE2   | 5:1E:176:LEU:HD22  | 2.48                     | 0.48              |
| 7:1G:357:ASP:O    | 19:1S:54:ILE:N     | 2.43                     | 0.48              |
| 8:1H:86:TRP:CD1   | 8:1H:233:MET:HE3   | 2.49                     | 0.48              |
| 16:1P:17:SER:OG   | 16:1P:42:GLY:O     | 2.25                     | 0.48              |
| 16:1P:318:LEU:HG  | 16:1P:321:HIS:HD2  | 1.77                     | 0.48              |
| 18:1R:10:LYS:O    | 18:1R:33:LYS:NZ    | 2.34                     | 0.48              |
| 19:1S:21:HIS:O    | 19:1S:62:PRO:HA    | 2.13                     | 0.48              |
| 20:1U:42:LEU:HD11 | 20:1U:47:GLN:HB2   | 1.94                     | 0.48              |
| 23:1X:156:ASP:N   | 23:1X:156:ASP:OD1  | 2.44                     | 0.48              |
| 33:1h:7:ARG:NH2   | 34:1i:27:LEU:HG    | 2.28                     | 0.48              |
| 2:1B:41:ARG:HA    | 8:1H:54:LYS:HE2    | 1.96                     | 0.48              |
| 3:1C:40:VAL:HG23  | 43:1r:68:VAL:HG23  | 1.94                     | 0.48              |
| 6:1F:314:THR:O    | 6:1F:314:THR:OG1   | 2.29                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:378:ARG:NE    | 6:1F:383:ASP:O     | 2.45                     | 0.48              |
| 7:1G:279:LEU:HD21  | 7:1G:550:GLY:HA3   | 1.95                     | 0.48              |
| 13:1M:71:TRP:CH2   | 13:1M:439:LEU:HG   | 2.49                     | 0.48              |
| 13:1M:367:LEU:HD21 | 13:1M:408:LEU:HG   | 1.94                     | 0.48              |
| 16:1P:203:GLN:HE21 | 16:1P:235:ARG:NE   | 2.11                     | 0.48              |
| 19:1S:24:GLN:O     | 19:1S:33:ARG:NE    | 2.47                     | 0.48              |
| 23:1X:141:TYR:HA   | 25:1Z:115:ARG:HD3  | 1.94                     | 0.48              |
| 13:1M:295:ALA:HA   | 13:1M:298:ILE:HD12 | 1.96                     | 0.48              |
| 16:1P:144:ARG:HD2  | 16:1P:144:ARG:N    | 2.29                     | 0.48              |
| 16:1P:173:GLY:H    | 16:1P:176:ASP:HB3  | 1.79                     | 0.48              |
| 22:1W:111:GLU:N    | 22:1W:111:GLU:OE1  | 2.47                     | 0.48              |
| 28:1c:39:VAL:O     | 28:1c:43:LYS:HG2   | 2.13                     | 0.48              |
| 3:1C:71:GLN:HE21   | 3:1C:100:ARG:HB3   | 1.78                     | 0.48              |
| 3:1C:85:THR:OG1    | 17:1Q:86:PHE:HA    | 2.14                     | 0.48              |
| 4:1D:4:TRP:CD1     | 13:1M:140:THR:HA   | 2.49                     | 0.48              |
| 4:1D:352:TYR:O     | 9:1I:86:VAL:HG23   | 2.14                     | 0.48              |
| 5:1E:109:MET:HA    | 5:1E:113:SER:H     | 1.78                     | 0.48              |
| 6:1F:42:TRP:N      | 6:1F:120:GLU:OE1   | 2.47                     | 0.48              |
| 7:1G:409:ILE:HD13  | 7:1G:429:LEU:HD21  | 1.96                     | 0.48              |
| 7:1G:545:TYR:HB3   | 7:1G:560:ILE:HD13  | 1.94                     | 0.48              |
| 9:1I:141:THR:OG1   | 9:1I:142:GLU:N     | 2.46                     | 0.48              |
| 12:1L:401:MET:HG3  | 12:1L:482:MET:HG3  | 1.95                     | 0.48              |
| 45:1L:702:3PE:H112 | 45:1L:702:3PE:H11  | 1.94                     | 0.48              |
| 13:1M:220:HIS:CE1  | 13:1M:232:ALA:HB2  | 2.49                     | 0.48              |
| 15:1O:22:SER:OG    | 15:1O:119:GLY:O    | 2.28                     | 0.48              |
| 15:1O:78:SER:N     | 15:1O:92:ASN:OD1   | 2.43                     | 0.48              |
| 19:1S:20:ILE:HA    | 19:1S:64:LEU:HA    | 1.95                     | 0.48              |
| 20:1T:17:TYR:O     | 20:1T:20:LYS:HG3   | 2.14                     | 0.48              |
| 21:1V:82:GLN:HA    | 21:1V:85:ASN:ND2   | 2.28                     | 0.48              |
| 33:1h:23:LYS:HG2   | 33:1h:26:ARG:HH22  | 1.77                     | 0.48              |
| 3:1C:43:SER:HA     | 43:1r:65:PRO:HB3   | 1.95                     | 0.48              |
| 6:1F:247:ARG:HD3   | 6:1F:273:SER:HB3   | 1.95                     | 0.48              |
| 6:1F:270:GLU:OE1   | 6:1F:283:HIS:NE2   | 2.40                     | 0.48              |
| 7:1G:611:LEU:HD12  | 7:1G:613:TYR:CZ    | 2.49                     | 0.48              |
| 14:1N:172:GLN:OE1  | 14:1N:177:LYS:NZ   | 2.26                     | 0.48              |
| 14:1N:182:SER:O    | 14:1N:186:HIS:ND1  | 2.44                     | 0.48              |
| 15:1O:167:HIS:HE2  | 15:1O:248:TRP:HB3  | 1.79                     | 0.48              |
| 16:1P:35:VAL:O     | 16:1P:39:GLY:N     | 2.33                     | 0.48              |
| 20:1U:47:GLN:NE2   | 20:1U:70:LEU:O     | 2.47                     | 0.48              |
| 22:1W:80:ASP:O     | 22:1W:84:ILE:HG23  | 2.14                     | 0.48              |
| 25:1Z:77:ALA:HB1   | 25:1Z:81:ARG:HH22  | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:1e:6:GLN:HG2    | 30:1e:13:LEU:HB2   | 1.96                     | 0.48              |
| 34:1i:122:PHE:CE2  | 40:1o:61:TYR:CE1   | 3.02                     | 0.48              |
| 40:1o:7:ARG:HH12   | 40:1o:17:ASP:HA    | 1.79                     | 0.48              |
| 3:1C:33:LEU:O      | 3:1C:37:VAL:HG22   | 2.13                     | 0.48              |
| 4:1D:83:LEU:HD23   | 4:1D:426:GLY:HA2   | 1.95                     | 0.48              |
| 6:1F:118:LEU:HD21  | 6:1F:136:ILE:HG21  | 1.96                     | 0.48              |
| 7:1G:55:CYS:SG     | 7:1G:68:ALA:N      | 2.86                     | 0.48              |
| 7:1G:439:PHE:HD1   | 7:1G:442:ILE:HD11  | 1.79                     | 0.48              |
| 7:1G:591:GLY:HA2   | 16:1P:6:ILE:HD13   | 1.95                     | 0.48              |
| 12:1L:63:ILE:O     | 12:1L:65:ASN:ND2   | 2.36                     | 0.48              |
| 15:1O:43:ALA:HB2   | 15:1O:123:VAL:HG11 | 1.95                     | 0.48              |
| 16:1P:120:VAL:HA   | 16:1P:123:GLU:HB2  | 1.96                     | 0.48              |
| 16:1P:243:GLN:OE1  | 16:1P:243:GLN:HA   | 2.14                     | 0.48              |
| 22:1W:102:HIS:HA   | 22:1W:105:ARG:HH12 | 1.78                     | 0.48              |
| 25:1Z:94:GLU:HA    | 25:1Z:97:ILE:HG22  | 1.94                     | 0.48              |
| 32:1g:68:ILE:O     | 32:1g:72:LEU:HB3   | 2.13                     | 0.48              |
| 45:1A:201:3PE:H2G2 | 27:1b:22:PHE:HD1   | 1.79                     | 0.48              |
| 2:1B:66:ARG:HD3    | 9:1I:48:ILE:HG12   | 1.95                     | 0.48              |
| 2:1B:68:ASP:HB3    | 2:1B:71:ARG:HB3    | 1.96                     | 0.48              |
| 3:1C:136:ASP:HB3   | 3:1C:137:MET:HE2   | 1.96                     | 0.48              |
| 4:1D:115:GLU:OE2   | 4:1D:192:ALA:HA    | 2.14                     | 0.48              |
| 4:1D:169:TRP:CZ3   | 9:1I:36:MET:HE1    | 2.49                     | 0.48              |
| 6:1F:254:LYS:HB3   | 6:1F:256:PHE:CZ    | 2.49                     | 0.48              |
| 6:1F:391:SER:OG    | 43:1r:48:LEU:O     | 2.32                     | 0.48              |
| 10:1J:150:GLY:HA2  | 30:1e:16:TRP:CH2   | 2.49                     | 0.48              |
| 12:1L:375:ILE:HD11 | 35:1j:32:MET:HG2   | 1.95                     | 0.48              |
| 13:1M:76:MET:HB3   | 13:1M:226:ALA:HB1  | 1.96                     | 0.48              |
| 15:1O:174:VAL:HG22 | 15:1O:225:ALA:HB2  | 1.96                     | 0.48              |
| 16:1P:318:LEU:HD23 | 16:1P:321:HIS:HB2  | 1.95                     | 0.48              |
| 20:1T:27:PRO:HA    | 20:1T:30:LEU:HB3   | 1.96                     | 0.48              |
| 21:1V:21:GLU:HA    | 21:1V:24:LYS:HD2   | 1.96                     | 0.48              |
| 37:1l:27:TYR:CE2   | 37:1l:48:PRO:HD3   | 2.49                     | 0.48              |
| 1:1A:60:ILE:HD12   | 1:1A:60:ILE:N      | 2.29                     | 0.47              |
| 3:1C:55:ASP:OD1    | 3:1C:55:ASP:N      | 2.46                     | 0.47              |
| 3:1C:74:SER:OG     | 3:1C:97:LEU:HB3    | 2.13                     | 0.47              |
| 5:1E:103:CYS:SG    | 5:1E:144:CYS:HA    | 2.54                     | 0.47              |
| 6:1F:30:ASP:OD1    | 6:1F:35:GLY:N      | 2.39                     | 0.47              |
| 6:1F:216:PHE:HA    | 17:1Q:129:ARG:NH2  | 2.29                     | 0.47              |
| 7:1G:54:MET:HE1    | 7:1G:94:MET:HE2    | 1.95                     | 0.47              |
| 7:1G:240:VAL:HG22  | 7:1G:250:ILE:HD12  | 1.94                     | 0.47              |
| 7:1G:248:MET:N     | 7:1G:248:MET:SD    | 2.87                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:339:ASP:OD1   | 19:1S:70:PHE:N     | 2.46                     | 0.47              |
| 7:1G:615:THR:OG1   | 7:1G:618:GLN:NE2   | 2.43                     | 0.47              |
| 10:1J:33:LEU:HD12  | 10:1J:34:ILE:N     | 2.29                     | 0.47              |
| 12:1L:10:THR:O     | 12:1L:14:ILE:HD12  | 2.13                     | 0.47              |
| 12:1L:489:THR:HA   | 12:1L:492:ILE:HG22 | 1.96                     | 0.47              |
| 12:1L:561:ILE:HG23 | 12:1L:562:LEU:HD12 | 1.95                     | 0.47              |
| 17:1Q:54:LYS:HE3   | 17:1Q:87:SER:HA    | 1.96                     | 0.47              |
| 20:1U:23:ASP:OD1   | 20:1U:24:LYS:N     | 2.47                     | 0.47              |
| 24:1Y:92:GLY:HA2   | 24:1Y:95:ALA:HB3   | 1.95                     | 0.47              |
| 38:1m:21:GLU:HA    | 38:1m:24:ILE:HD11  | 1.95                     | 0.47              |
| 1:1A:1:FME:HA      | 1:1A:1:FME:HE3     | 1.96                     | 0.47              |
| 2:1B:91:THR:HA     | 2:1B:119:CYS:HB3   | 1.97                     | 0.47              |
| 2:1B:114:VAL:HG22  | 2:1B:144:ILE:HB    | 1.94                     | 0.47              |
| 3:1C:39:GLN:NE2    | 43:1r:67:ILE:HG23  | 2.29                     | 0.47              |
| 4:1D:154:VAL:HG11  | 4:1D:225:LEU:HD11  | 1.96                     | 0.47              |
| 4:1D:169:TRP:HB2   | 4:1D:170:MET:HE2   | 1.96                     | 0.47              |
| 4:1D:269:LEU:HB2   | 4:1D:368:GLU:HB2   | 1.95                     | 0.47              |
| 5:1E:27:ASN:O      | 5:1E:31:ILE:HG12   | 2.14                     | 0.47              |
| 6:1F:51:LYS:HG2    | 6:1F:55:TRP:CD1    | 2.49                     | 0.47              |
| 6:1F:308:PRO:HD3   | 6:1F:421:HIS:ND1   | 2.30                     | 0.47              |
| 7:1G:125:SER:OG    | 7:1G:126:ASP:N     | 2.48                     | 0.47              |
| 7:1G:255:HIS:CD2   | 7:1G:258:ILE:HB    | 2.49                     | 0.47              |
| 7:1G:359:ARG:HA    | 7:1G:359:ARG:NH1   | 2.29                     | 0.47              |
| 13:1M:181:TYR:CE1  | 41:1p:88:GLU:HG3   | 2.49                     | 0.47              |
| 13:1M:205:VAL:HG22 | 13:1M:212:LEU:HD13 | 1.96                     | 0.47              |
| 16:1P:172:PHE:HD2  | 16:1P:204:PRO:HB2  | 1.79                     | 0.47              |
| 20:1T:45:LEU:O     | 20:1T:45:LEU:HD12  | 2.14                     | 0.47              |
| 20:1U:33:ASN:OD1   | 20:1U:33:ASN:N     | 2.47                     | 0.47              |
| 20:1U:37:MET:SD    | 20:1U:71:MET:HE1   | 2.54                     | 0.47              |
| 32:1g:37:LEU:HD22  | 32:1g:46:GLY:HA2   | 1.95                     | 0.47              |
| 41:1p:166:ARG:HD2  | 41:1p:170:LYS:HE3  | 1.96                     | 0.47              |
| 44:1s:34:ASP:HB2   | 44:1s:39:ARG:HH22  | 1.80                     | 0.47              |
| 3:1C:90:PHE:CE1    | 3:1C:113:GLU:HG3   | 2.49                     | 0.47              |
| 4:1D:161:ILE:HG13  | 4:1D:238:ARG:CZ    | 2.45                     | 0.47              |
| 4:1D:394:PRO:HD2   | 4:1D:427:GLU:OE2   | 2.13                     | 0.47              |
| 6:1F:383:ASP:HA    | 6:1F:433:PHE:CE2   | 2.50                     | 0.47              |
| 12:1L:583:LEU:HD12 | 12:1L:586:LEU:HD11 | 1.95                     | 0.47              |
| 13:1M:11:LEU:HD22  | 13:1M:100:ILE:HD12 | 1.96                     | 0.47              |
| 13:1M:89:THR:O     | 13:1M:93:LYS:HG2   | 2.14                     | 0.47              |
| 14:1N:265:MET:HG3  | 14:1N:343:LEU:HD11 | 1.95                     | 0.47              |
| 15:1O:57:HIS:HD2   | 15:1O:68:PRO:HB3   | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:1R:30:ASP:C     | 18:1R:31:ARG:HD3   | 2.39                     | 0.47              |
| 23:1X:81:PHE:HD2   | 23:1X:85:TRP:HD1   | 1.63                     | 0.47              |
| 34:1i:32:PRO:HB3   | 39:1n:114:TYR:CE1  | 2.49                     | 0.47              |
| 4:1D:180:PHE:O     | 4:1D:184:VAL:HG22  | 2.14                     | 0.47              |
| 5:1E:76:PRO:HB3    | 7:1G:170:ASP:HB3   | 1.96                     | 0.47              |
| 7:1G:372:GLU:HA    | 7:1G:398:SER:HB3   | 1.95                     | 0.47              |
| 7:1G:403:ASP:OD1   | 17:1Q:127:ARG:NH2  | 2.48                     | 0.47              |
| 7:1G:627:SER:OG    | 7:1G:629:ASN:OD1   | 2.32                     | 0.47              |
| 12:1L:53:MET:O     | 12:1L:57:THR:OG1   | 2.30                     | 0.47              |
| 12:1L:233:LEU:HB3  | 12:1L:234:PRO:HD3  | 1.96                     | 0.47              |
| 13:1M:263:MET:HE1  | 38:1m:104:PHE:CD2  | 2.49                     | 0.47              |
| 13:1M:437:MET:O    | 13:1M:441:ILE:HG22 | 2.14                     | 0.47              |
| 16:1P:13:ARG:NH1   | 16:1P:63:GLY:O     | 2.47                     | 0.47              |
| 20:1U:88:GLU:OE2   | 34:1i:19:ARG:NH1   | 2.47                     | 0.47              |
| 22:1W:42:GLU:O     | 22:1W:46:THR:HG23  | 2.13                     | 0.47              |
| 37:1l:14:PRO:HA    | 37:1l:19:GLU:OE1   | 2.15                     | 0.47              |
| 3:1C:24:ALA:HB1    | 43:1r:94:VAL:HG11  | 1.95                     | 0.47              |
| 6:1F:144:ASN:HB3   | 44:1s:43:HIS:HB2   | 1.96                     | 0.47              |
| 7:1G:99:ALA:HB1    | 7:1G:130:PHE:CE2   | 2.49                     | 0.47              |
| 14:1N:96:THR:O     | 14:1N:100:MET:HE2  | 2.14                     | 0.47              |
| 14:1N:122:ILE:HD11 | 14:1N:127:GLY:HA2  | 1.96                     | 0.47              |
| 18:1R:32:GLN:NE2   | 18:1R:34:GLU:OE1   | 2.48                     | 0.47              |
| 21:1V:24:LYS:O     | 21:1V:28:THR:HG23  | 2.14                     | 0.47              |
| 6:1F:206:LYS:HB3   | 6:1F:207:PRO:HD3   | 1.95                     | 0.47              |
| 7:1G:277:GLN:NE2   | 42:1q:137:TRP:HD1  | 2.12                     | 0.47              |
| 7:1G:325:ALA:O     | 7:1G:329:VAL:HG23  | 2.14                     | 0.47              |
| 7:1G:467:LEU:HA    | 7:1G:470:VAL:HG12  | 1.94                     | 0.47              |
| 8:1H:114:TYR:OH    | 10:1J:61:LEU:O     | 2.20                     | 0.47              |
| 12:1L:6:SER:O      | 12:1L:10:THR:HG23  | 2.15                     | 0.47              |
| 12:1L:575:ILE:O    | 12:1L:579:ASN:ND2  | 2.46                     | 0.47              |
| 14:1N:170:LEU:HD23 | 14:1N:292:PHE:HD2  | 1.79                     | 0.47              |
| 20:1U:42:LEU:HD21  | 20:1U:46:ASP:HB3   | 1.95                     | 0.47              |
| 23:1X:79:GLU:O     | 23:1X:82:THR:OG1   | 2.23                     | 0.47              |
| 30:1e:16:TRP:CE3   | 30:1e:17:MET:HB3   | 2.50                     | 0.47              |
| 2:1B:82:GLN:OE1    | 2:1B:82:GLN:N      | 2.47                     | 0.47              |
| 6:1F:282:LYS:HG3   | 6:1F:283:HIS:CD2   | 2.50                     | 0.47              |
| 6:1F:306:LEU:HD23  | 6:1F:418:LEU:HD21  | 1.95                     | 0.47              |
| 7:1G:321:GLY:HA2   | 7:1G:496:ILE:HG23  | 1.97                     | 0.47              |
| 8:1H:285:LEU:HD12  | 8:1H:285:LEU:O     | 2.15                     | 0.47              |
| 10:1J:106:TYR:CD2  | 10:1J:113:VAL:HG12 | 2.49                     | 0.47              |
| 11:1K:37:MET:HA    | 11:1K:40:LEU:HB2   | 1.97                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:271:LYS:O    | 12:1L:274:GLN:HG2  | 2.14                     | 0.47              |
| 45:1L:703:3PE:H32  | 45:1L:703:3PE:H322 | 1.52                     | 0.47              |
| 13:1M:30:HIS:HA    | 13:1M:33:LEU:HB2   | 1.95                     | 0.47              |
| 15:1O:33:SER:HA    | 15:1O:182:ARG:HH22 | 1.80                     | 0.47              |
| 15:1O:70:ASP:HB3   | 15:1O:73:LEU:HB2   | 1.96                     | 0.47              |
| 15:1O:301:GLY:O    | 15:1O:309:ASN:ND2  | 2.48                     | 0.47              |
| 16:1P:133:SER:HB3  | 16:1P:165:ILE:HD11 | 1.94                     | 0.47              |
| 17:1Q:116:LYS:HD3  | 17:1Q:116:LYS:HA   | 1.60                     | 0.47              |
| 19:1S:62:PRO:C     | 19:1S:78:LEU:HB3   | 2.40                     | 0.47              |
| 21:1V:15:VAL:HG22  | 21:1V:77:GLU:HG2   | 1.97                     | 0.47              |
| 21:1V:71:LEU:HD13  | 21:1V:79:VAL:HG11  | 1.96                     | 0.47              |
| 21:1V:100:GLU:OE1  | 21:1V:100:GLU:N    | 2.44                     | 0.47              |
| 22:1W:99:GLN:OE1   | 22:1W:99:GLN:HA    | 2.14                     | 0.47              |
| 23:1X:101:LYS:O    | 23:1X:105:LYS:HG2  | 2.15                     | 0.47              |
| 32:1g:92:GLU:OE1   | 41:1p:64:HIS:NE2   | 2.35                     | 0.47              |
| 32:1g:108:MET:HE1  | 41:1p:141:ARG:HD2  | 1.96                     | 0.47              |
| 38:1m:40:SER:OG    | 39:1n:148:PRO:O    | 2.31                     | 0.47              |
| 38:1m:44:ARG:NH1   | 38:1m:44:ARG:O     | 2.47                     | 0.47              |
| 39:1n:106:TRP:CE3  | 39:1n:110:GLU:HB3  | 2.49                     | 0.47              |
| 39:1n:120:LYS:HA   | 39:1n:123:GLN:HG2  | 1.97                     | 0.47              |
| 40:1o:30:PHE:HZ    | 40:1o:103:ARG:HD2  | 1.79                     | 0.47              |
| 4:1D:152:MET:O     | 4:1D:156:THR:OG1   | 2.22                     | 0.47              |
| 4:1D:347:HIS:NE2   | 7:1G:125:SER:O     | 2.39                     | 0.47              |
| 7:1G:400:LEU:O     | 17:1Q:127:ARG:HB2  | 2.15                     | 0.47              |
| 9:1I:50:TYR:CD1    | 9:1I:51:PRO:HA     | 2.50                     | 0.47              |
| 10:1J:171:ILE:HD13 | 11:1K:77:LEU:HD23  | 1.97                     | 0.47              |
| 16:1P:249:ALA:HB2  | 16:1P:318:LEU:HD21 | 1.95                     | 0.47              |
| 20:1T:7:THR:O      | 20:1T:11:ILE:HG12  | 2.15                     | 0.47              |
| 20:1T:56:ASP:OD1   | 20:1T:57:GLU:N     | 2.48                     | 0.47              |
| 20:1U:35:HIS:HE1   | 20:1U:37:MET:HG2   | 1.80                     | 0.47              |
| 32:1g:54:ASP:OD1   | 32:1g:55:LEU:N     | 2.48                     | 0.47              |
| 37:1l:77:ILE:HB    | 38:1m:67:TRP:HB2   | 1.96                     | 0.47              |
| 37:1l:129:GLY:H    | 40:1o:97:ARG:HB3   | 1.80                     | 0.47              |
| 5:1E:111:ARG:HE    | 5:1E:151:ALA:HA    | 1.80                     | 0.47              |
| 6:1F:31:TRP:HD1    | 6:1F:113:HIS:HA    | 1.80                     | 0.47              |
| 6:1F:256:PHE:HD2   | 6:1F:270:GLU:HB3   | 1.79                     | 0.47              |
| 7:1G:365:ASN:HD22  | 7:1G:488:LYS:HD2   | 1.79                     | 0.47              |
| 7:1G:385:ARG:HG3   | 7:1G:415:LEU:HA    | 1.97                     | 0.47              |
| 7:1G:673:MET:HG2   | 7:1G:688:VAL:HG11  | 1.97                     | 0.47              |
| 8:1H:179:TRP:CG    | 8:1H:180:PRO:HD3   | 2.49                     | 0.47              |
| 8:1H:186:PHE:CD2   | 50:1H:401:PC1:H2E1 | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:383:MET:HG3  | 12:1L:386:LEU:HB2  | 1.97                     | 0.47              |
| 15:1O:110:ASP:OD1  | 15:1O:266:LYS:NZ   | 2.38                     | 0.47              |
| 16:1P:194:ILE:O    | 16:1P:288:HIS:NE2  | 2.48                     | 0.47              |
| 16:1P:341:ASN:OD1  | 16:1P:341:ASN:N    | 2.46                     | 0.47              |
| 17:1Q:95:PHE:HA    | 17:1Q:98:LYS:HD3   | 1.97                     | 0.47              |
| 20:1U:61:GLU:OE1   | 39:1n:81:PHE:HB2   | 2.14                     | 0.47              |
| 1:1A:65:PHE:HA     | 1:1A:68:GLU:OE2    | 2.15                     | 0.47              |
| 3:1C:204:GLU:HA    | 17:1Q:50:ASN:HD21  | 1.77                     | 0.47              |
| 8:1H:29:GLY:HA2    | 8:1H:34:ARG:HE     | 1.80                     | 0.47              |
| 9:1I:68:ARG:HH12   | 9:1I:76:ARG:HD2    | 1.79                     | 0.47              |
| 10:1J:78:MET:HE3   | 10:1J:78:MET:C     | 2.40                     | 0.47              |
| 13:1M:215:TRP:CD1  | 13:1M:215:TRP:H    | 2.32                     | 0.47              |
| 15:1O:78:SER:HB3   | 15:1O:81:LYS:HB2   | 1.97                     | 0.47              |
| 17:1Q:67:ASN:HD22  | 17:1Q:72:TRP:HD1   | 1.62                     | 0.47              |
| 18:1R:19:ASP:N     | 18:1R:22:ASP:OD2   | 2.48                     | 0.47              |
| 18:1R:28:PHE:CE2   | 18:1R:33:LYS:HG3   | 2.50                     | 0.47              |
| 20:1T:22:TYR:CD2   | 20:1T:23:ASP:N     | 2.83                     | 0.47              |
| 30:1e:85:LEU:HA    | 30:1e:88:GLU:OE2   | 2.15                     | 0.47              |
| 34:1i:82:HIS:O     | 34:1i:86:LYS:HB2   | 2.15                     | 0.47              |
| 37:1l:11:GLY:O     | 38:1m:78:ASN:ND2   | 2.48                     | 0.47              |
| 39:1n:149:ARG:HD2  | 39:1n:149:ARG:HA   | 1.71                     | 0.47              |
| 4:1D:270:ARG:NH1   | 4:1D:368:GLU:HG2   | 2.30                     | 0.46              |
| 5:1E:100:ILE:HD12  | 5:1E:156:ILE:HG22  | 1.97                     | 0.46              |
| 6:1F:103:GLY:HA3   | 6:1F:335:ILE:HD11  | 1.97                     | 0.46              |
| 6:1F:276:LEU:O     | 6:1F:280:ILE:HD12  | 2.15                     | 0.46              |
| 7:1G:323:VAL:HG11  | 7:1G:525:LEU:HD22  | 1.98                     | 0.46              |
| 7:1G:626:VAL:HA    | 19:1S:19:ARG:NH2   | 2.30                     | 0.46              |
| 8:1H:112:ALA:O     | 8:1H:116:ILE:HG12  | 2.15                     | 0.46              |
| 10:1J:68:PHE:CD2   | 11:1K:75:LEU:HD21  | 2.50                     | 0.46              |
| 11:1K:55:LEU:H     | 30:1e:24:GLN:HE22  | 1.63                     | 0.46              |
| 11:1K:89:TYR:HB3   | 11:1K:91:GLN:OE1   | 2.15                     | 0.46              |
| 12:1L:444:ASN:HD21 | 35:1j:7:ILE:HD13   | 1.80                     | 0.46              |
| 14:1N:109:SER:HB3  | 14:1N:157:MET:HG3  | 1.96                     | 0.46              |
| 16:1P:182:PHE:HA   | 16:1P:185:MET:HG2  | 1.97                     | 0.46              |
| 16:1P:204:PRO:HG2  | 16:1P:310:LEU:HD12 | 1.97                     | 0.46              |
| 21:1V:63:ASP:H     | 21:1V:66:LYS:HZ1   | 1.63                     | 0.46              |
| 23:1X:46:ARG:NH1   | 25:1Z:76:GLN:OE1   | 2.48                     | 0.46              |
| 33:1h:91:MET:HE1   | 41:1p:82:LEU:HA    | 1.96                     | 0.46              |
| 5:1E:124:LEU:HD23  | 5:1E:173:ILE:HD12  | 1.97                     | 0.46              |
| 6:1F:102:PRO:HG2   | 6:1F:302:SER:HB3   | 1.97                     | 0.46              |
| 7:1G:646:ASN:O     | 7:1G:650:LYS:HG2   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:215:TYR:C     | 8:1H:220:PHE:HB2   | 2.40                     | 0.46              |
| 9:1I:68:ARG:NH1    | 9:1I:76:ARG:HD2    | 2.30                     | 0.46              |
| 11:1K:40:LEU:HD21  | 14:1N:72:MET:HB2   | 1.97                     | 0.46              |
| 12:1L:279:CYS:HA   | 37:1I:116:PHE:CZ   | 2.50                     | 0.46              |
| 13:1M:1:FME:HG3    | 13:1M:52:PHE:CD2   | 2.50                     | 0.46              |
| 14:1N:210:THR:OG1  | 14:1N:211:MET:SD   | 2.72                     | 0.46              |
| 15:1O:57:HIS:CD2   | 15:1O:68:PRO:HB3   | 2.51                     | 0.46              |
| 16:1P:46:ILE:O     | 16:1P:46:ILE:HG22  | 2.15                     | 0.46              |
| 16:1P:54:TYR:O     | 16:1P:57:MET:HB2   | 2.14                     | 0.46              |
| 19:1S:12:LYS:HB2   | 19:1S:98:ALA:C     | 2.40                     | 0.46              |
| 24:1Y:139:LYS:HG3  | 33:1h:112:ARG:HG3  | 1.95                     | 0.46              |
| 30:1e:50:ARG:NH2   | 30:1e:54:GLU:OE2   | 2.49                     | 0.46              |
| 32:1g:36:ASN:HB3   | 32:1g:39:GLU:OE2   | 2.14                     | 0.46              |
| 3:1C:39:GLN:HE21   | 43:1r:67:ILE:HG23  | 1.80                     | 0.46              |
| 4:1D:393:ALA:HB3   | 4:1D:396:PHE:HB2   | 1.98                     | 0.46              |
| 6:1F:16:LYS:HA     | 6:1F:16:LYS:HD3    | 1.81                     | 0.46              |
| 7:1G:276:ARG:CZ    | 7:1G:682:GLN:HE21  | 2.29                     | 0.46              |
| 8:1H:52:ALA:O      | 8:1H:56:VAL:HG23   | 2.15                     | 0.46              |
| 12:1L:268:GLU:N    | 12:1L:268:GLU:OE1  | 2.48                     | 0.46              |
| 14:1N:155:LEU:HD22 | 14:1N:278:MET:HE2  | 1.97                     | 0.46              |
| 16:1P:241:LEU:O    | 16:1P:245:ILE:HG22 | 2.16                     | 0.46              |
| 30:1e:93:PRO:HB2   | 30:1e:98:LEU:HD21  | 1.97                     | 0.46              |
| 33:1h:87:TYR:OH    | 41:1p:86:GLU:OE1   | 2.26                     | 0.46              |
| 39:1n:94:GLU:HA    | 39:1n:97:LYS:HG3   | 1.98                     | 0.46              |
| 42:1q:13:GLN:HB3   | 42:1q:23:TYR:HE1   | 1.80                     | 0.46              |
| 42:1q:29:ARG:NH2   | 42:1q:65:THR:O     | 2.48                     | 0.46              |
| 43:1r:105:LEU:HD21 | 43:1r:111:TYR:CE1  | 2.51                     | 0.46              |
| 1:1A:22:PHE:HZ     | 8:1H:62:ARG:HH11   | 1.63                     | 0.46              |
| 3:1C:181:LYS:HG2   | 16:1P:174:ARG:NH2  | 2.30                     | 0.46              |
| 4:1D:176:LYS:HG2   | 43:1r:26:ARG:NH1   | 2.30                     | 0.46              |
| 6:1F:347:ILE:HG12  | 6:1F:418:LEU:HD12  | 1.98                     | 0.46              |
| 7:1G:175:THR:N     | 7:1G:182:GLN:O     | 2.49                     | 0.46              |
| 12:1L:478:PRO:HG3  | 40:1o:86:TRP:CH2   | 2.50                     | 0.46              |
| 18:1R:68:HIS:CG    | 18:1R:86:TYR:HB3   | 2.51                     | 0.46              |
| 19:1S:23:CYS:HA    | 19:1S:57:CYS:O     | 2.14                     | 0.46              |
| 37:1I:82:ASP:HB2   | 37:1I:88:ARG:HH12  | 1.81                     | 0.46              |
| 39:1n:41:CYS:HA    | 39:1n:44:ARG:HB3   | 1.96                     | 0.46              |
| 41:1p:54:GLN:HE22  | 41:1p:55:HIS:HD2   | 1.63                     | 0.46              |
| 41:1p:139:GLN:O    | 41:1p:157:LYS:NZ   | 2.47                     | 0.46              |
| 43:1r:51:ASN:HB3   | 43:1r:56:ARG:HH22  | 1.81                     | 0.46              |
| 4:1D:372:GLY:HA3   | 4:1D:394:PRO:HB3   | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:195:LEU:HD11  | 7:1G:393:ALA:HB2   | 1.98                     | 0.46              |
| 7:1G:362:TYR:HH    | 7:1G:504:ASP:CG    | 2.22                     | 0.46              |
| 8:1H:200:LEU:O     | 8:1H:200:LEU:HD23  | 2.15                     | 0.46              |
| 8:1H:201:THR:HG22  | 8:1H:211:PHE:HD1   | 1.80                     | 0.46              |
| 10:1J:35:VAL:O     | 10:1J:39:VAL:HG12  | 2.16                     | 0.46              |
| 12:1L:33:PRO:HB3   | 12:1L:118:PHE:CE1  | 2.50                     | 0.46              |
| 12:1L:293:ILE:HD11 | 45:1L:704:3PE:H242 | 1.97                     | 0.46              |
| 13:1M:306:PRO:HA   | 13:1M:458:LEU:HD13 | 1.96                     | 0.46              |
| 14:1N:112:HIS:CE1  | 14:1N:164:ILE:HG21 | 2.50                     | 0.46              |
| 16:1P:8:HIS:ND1    | 17:1Q:65:TRP:HB2   | 2.30                     | 0.46              |
| 16:1P:236:TYR:HB2  | 16:1P:241:LEU:CD2  | 2.45                     | 0.46              |
| 16:1P:245:ILE:O    | 16:1P:249:ALA:N    | 2.40                     | 0.46              |
| 16:1P:256:TYR:HE2  | 16:1P:258:LEU:HD23 | 1.81                     | 0.46              |
| 23:1X:73:ILE:HD12  | 26:1a:66:LEU:HD21  | 1.97                     | 0.46              |
| 30:1e:60:ASP:HA    | 30:1e:63:VAL:HG12  | 1.98                     | 0.46              |
| 31:1f:43:LEU:HD23  | 33:1h:87:TYR:CE2   | 2.50                     | 0.46              |
| 42:1q:76:ASP:OD1   | 42:1q:76:ASP:O     | 2.34                     | 0.46              |
| 4:1D:326:ASP:OD2   | 43:1r:46:HIS:ND1   | 2.48                     | 0.46              |
| 4:1D:399:LEU:HD23  | 4:1D:428:VAL:HG11  | 1.98                     | 0.46              |
| 8:1H:108:MET:HA    | 8:1H:108:MET:HE3   | 1.98                     | 0.46              |
| 12:1L:478:PRO:HG2  | 40:1o:90:GLU:HG3   | 1.98                     | 0.46              |
| 12:1L:594:THR:OG1  | 24:1Y:38:TYR:OH    | 2.29                     | 0.46              |
| 14:1N:324:LYS:HA   | 14:1N:324:LYS:HD2  | 1.62                     | 0.46              |
| 15:1O:51:PHE:HD2   | 15:1O:107:GLN:HE21 | 1.64                     | 0.46              |
| 15:1O:168:VAL:HG13 | 15:1O:221:LEU:HD13 | 1.96                     | 0.46              |
| 18:1R:32:GLN:NE2   | 42:1q:122:GLN:O    | 2.44                     | 0.46              |
| 18:1R:75:LEU:HD21  | 18:1R:91:PHE:O     | 2.16                     | 0.46              |
| 20:1T:84:LYS:NZ    | 20:1T:86:VAL:O     | 2.47                     | 0.46              |
| 22:1W:17:VAL:HB    | 22:1W:77:ARG:CZ    | 2.45                     | 0.46              |
| 23:1X:48:GLU:OE1   | 27:1b:57:ARG:NH1   | 2.48                     | 0.46              |
| 29:1d:94:VAL:HG23  | 29:1d:101:PHE:CD2  | 2.51                     | 0.46              |
| 39:1n:57:VAL:O     | 39:1n:61:GLN:HG2   | 2.16                     | 0.46              |
| 40:1o:61:TYR:HB3   | 40:1o:86:TRP:HA    | 1.96                     | 0.46              |
| 1:1A:85:LYS:HE2    | 1:1A:85:LYS:HB3    | 1.64                     | 0.46              |
| 5:1E:14:GLU:O      | 5:1E:19:THR:OG1    | 2.27                     | 0.46              |
| 5:1E:48:LEU:O      | 5:1E:90:TYR:OH     | 2.27                     | 0.46              |
| 6:1F:50:LEU:O      | 6:1F:127:ARG:NH2   | 2.49                     | 0.46              |
| 6:1F:215:VAL:HG22  | 6:1F:220:THR:HG1   | 1.80                     | 0.46              |
| 6:1F:435:LEU:HD23  | 6:1F:435:LEU:HA    | 1.79                     | 0.46              |
| 45:1L:702:3PE:C24  | 37:1l:88:ARG:HD3   | 2.43                     | 0.46              |
| 15:1O:80:GLU:HB3   | 15:1O:190:HIS:CE1  | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:1P:31:GLY:O     | 16:1P:35:VAL:HG22  | 2.15                     | 0.46              |
| 17:1Q:52:THR:O     | 17:1Q:53:LYS:HD3   | 2.15                     | 0.46              |
| 20:1U:19:LEU:HD12  | 20:1U:19:LEU:H     | 1.79                     | 0.46              |
| 20:1U:35:HIS:CE1   | 20:1U:37:MET:HG2   | 2.51                     | 0.46              |
| 29:1d:91:PHE:HA    | 29:1d:94:VAL:HG12  | 1.98                     | 0.46              |
| 36:1k:48:GLU:HB3   | 36:1k:51:ARG:HD2   | 1.98                     | 0.46              |
| 37:1l:122:TYR:HB3  | 40:1o:8:TYR:CE2    | 2.51                     | 0.46              |
| 4:1D:387:TYR:CE2   | 21:1V:113:TRP:HH2  | 2.33                     | 0.46              |
| 5:1E:39:PRO:HB3    | 44:1s:66:PRO:HD2   | 1.98                     | 0.46              |
| 6:1F:349:ARG:HD2   | 6:1F:349:ARG:HA    | 1.68                     | 0.46              |
| 7:1G:206:GLY:N     | 46:1G:801:SF4:S1   | 2.86                     | 0.46              |
| 7:1G:514:ILE:HD12  | 7:1G:519:PRO:HG3   | 1.98                     | 0.46              |
| 9:1I:53:GLU:HG2    | 42:1q:61:TRP:HB3   | 1.98                     | 0.46              |
| 10:1J:25:SER:HB2   | 10:1J:81:GLU:HB3   | 1.97                     | 0.46              |
| 10:1J:129:ASP:OD2  | 10:1J:129:ASP:C    | 2.59                     | 0.46              |
| 11:1K:61:ILE:O     | 11:1K:65:VAL:HG23  | 2.16                     | 0.46              |
| 14:1N:108:LEU:HD22 | 14:1N:191:THR:HG21 | 1.98                     | 0.46              |
| 15:1O:75:GLY:C     | 15:1O:77:CYS:H     | 2.24                     | 0.46              |
| 20:1U:75:GLU:N     | 20:1U:75:GLU:OE1   | 2.48                     | 0.46              |
| 22:1W:57:LYS:HE3   | 22:1W:57:LYS:HB3   | 1.72                     | 0.46              |
| 22:1W:111:GLU:HG2  | 22:1W:114:ARG:NH2  | 2.31                     | 0.46              |
| 25:1Z:68:ARG:HB2   | 26:1a:43:TYR:CE2   | 2.50                     | 0.46              |
| 30:1e:90:LYS:HD3   | 30:1e:90:LYS:HA    | 1.67                     | 0.46              |
| 34:1i:48:LYS:HG2   | 34:1i:49:PHE:CD2   | 2.51                     | 0.46              |
| 2:1B:101:ARG:HD2   | 2:1B:101:ARG:HA    | 1.64                     | 0.46              |
| 7:1G:53:ARG:HH21   | 7:1G:56:LEU:HD21   | 1.81                     | 0.46              |
| 7:1G:74:MET:HB3    | 7:1G:77:TRP:CE3    | 2.51                     | 0.46              |
| 7:1G:252:PRO:HG2   | 17:1Q:44:ASN:ND2   | 2.29                     | 0.46              |
| 7:1G:628:PRO:HG2   | 19:1S:57:CYS:HB3   | 1.97                     | 0.46              |
| 8:1H:179:TRP:HE1   | 25:1Z:43:LEU:HG    | 1.81                     | 0.46              |
| 11:1K:91:GLN:O     | 11:1K:94:ASN:ND2   | 2.49                     | 0.46              |
| 12:1L:386:LEU:HD13 | 35:1j:36:ILE:HD11  | 1.98                     | 0.46              |
| 12:1L:500:LEU:HD11 | 45:1L:704:3PE:H362 | 1.97                     | 0.46              |
| 13:1M:10:MET:HG3   | 31:1f:15:LEU:HD21  | 1.98                     | 0.46              |
| 14:1N:44:LEU:HD23  | 14:1N:56:ALA:HA    | 1.97                     | 0.46              |
| 16:1P:171:ILE:HG12 | 16:1P:210:VAL:HG21 | 1.98                     | 0.46              |
| 17:1Q:39:VAL:HG11  | 17:1Q:108:ARG:HE   | 1.81                     | 0.46              |
| 19:1S:20:ILE:HD13  | 19:1S:22:LEU:HD22  | 1.96                     | 0.46              |
| 19:1S:24:GLN:CB    | 19:1S:25:ARG:HH12  | 2.27                     | 0.46              |
| 20:1T:11:ILE:HD12  | 20:1T:80:ILE:HG22  | 1.98                     | 0.46              |
| 20:1T:36:PHE:O     | 20:1T:41:GLY:N     | 2.48                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:1X:76:HIS:O     | 23:1X:78:ALA:N     | 2.48                     | 0.46              |
| 27:1b:31:LEU:O     | 27:1b:35:SER:N     | 2.49                     | 0.46              |
| 27:1b:77:LEU:HA    | 27:1b:79:TRP:NE1   | 2.30                     | 0.46              |
| 41:1p:145:LEU:HB3  | 41:1p:149:TYR:HB3  | 1.97                     | 0.46              |
| 1:1A:73:LEU:HD13   | 8:1H:103:LEU:HD11  | 1.98                     | 0.46              |
| 4:1D:228:MET:HE2   | 4:1D:228:MET:HB2   | 1.77                     | 0.46              |
| 5:1E:149:VAL:HG21  | 6:1F:267:THR:HG22  | 1.98                     | 0.46              |
| 5:1E:169:ILE:HD12  | 5:1E:172:ILE:HB    | 1.97                     | 0.46              |
| 7:1G:104:ASP:O     | 7:1G:108:CYS:N     | 2.48                     | 0.46              |
| 7:1G:284:ILE:HD11  | 7:1G:299:ALA:HA    | 1.98                     | 0.46              |
| 7:1G:306:MET:HG2   | 7:1G:542:PHE:CG    | 2.51                     | 0.46              |
| 7:1G:367:THR:HG22  | 7:1G:370:GLY:H     | 1.80                     | 0.46              |
| 7:1G:427:LYS:O     | 7:1G:430:GLN:HG3   | 2.16                     | 0.46              |
| 7:1G:622:ARG:HA    | 7:1G:625:GLU:HG2   | 1.98                     | 0.46              |
| 10:1J:132:ASP:C    | 10:1J:132:ASP:OD1  | 2.59                     | 0.46              |
| 14:1N:261:MET:HB2  | 14:1N:337:LEU:HD12 | 1.97                     | 0.46              |
| 14:1N:314:LYS:NZ   | 15:1O:270:LEU:O    | 2.50                     | 0.46              |
| 15:1O:154:GLU:HA   | 15:1O:157:LYS:NZ   | 2.31                     | 0.46              |
| 23:1X:81:PHE:CD2   | 23:1X:85:TRP:HD1   | 2.34                     | 0.46              |
| 24:1Y:93:GLY:O     | 24:1Y:97:GLY:N     | 2.39                     | 0.46              |
| 25:1Z:74:LEU:O     | 25:1Z:78:GLU:HG2   | 2.16                     | 0.46              |
| 2:1B:81:ARG:HH12   | 8:1H:63:PRO:HD3    | 1.81                     | 0.45              |
| 3:1C:101:PHE:CE1   | 43:1r:99:PRO:HB3   | 2.50                     | 0.45              |
| 4:1D:14:PHE:N      | 4:1D:14:PHE:CD1    | 2.83                     | 0.45              |
| 5:1E:51:LEU:HD21   | 5:1E:84:ALA:HB2    | 1.98                     | 0.45              |
| 6:1F:378:ARG:NH1   | 7:1G:131:LEU:HG    | 2.31                     | 0.45              |
| 7:1G:387:GLU:OE2   | 7:1G:665:GLN:HG2   | 2.16                     | 0.45              |
| 8:1H:170:GLU:HG2   | 8:1H:171:HIS:ND1   | 2.32                     | 0.45              |
| 12:1L:530:PRO:O    | 12:1L:534:HIS:HB2  | 2.16                     | 0.45              |
| 14:1N:276:ILE:C    | 14:1N:279:PRO:HD2  | 2.41                     | 0.45              |
| 15:1O:318:TRP:CD1  | 15:1O:318:TRP:H    | 2.33                     | 0.45              |
| 16:1P:262:ALA:HA   | 16:1P:265:TRP:CD1  | 2.40                     | 0.45              |
| 17:1Q:130:VAL:HG12 | 17:1Q:132:THR:H    | 1.79                     | 0.45              |
| 26:1a:27:HIS:NE2   | 26:1a:36:LYS:HE3   | 2.31                     | 0.45              |
| 33:1h:7:ARG:HH22   | 34:1i:26:GLU:HA    | 1.81                     | 0.45              |
| 36:1k:70:PHE:HD2   | 36:1k:74:PHE:HE1   | 1.63                     | 0.45              |
| 41:1p:22:GLN:H     | 41:1p:22:GLN:HG3   | 1.62                     | 0.45              |
| 1:1A:109:LYS:CG    | 1:1A:110:GLY:H     | 2.29                     | 0.45              |
| 3:1C:161:PRO:HA    | 3:1C:166:PHE:CG    | 2.51                     | 0.45              |
| 4:1D:95:THR:HA     | 4:1D:385:ARG:HG2   | 1.97                     | 0.45              |
| 5:1E:82:GLU:HA     | 5:1E:85:THR:HG22   | 1.98                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:189:LYS:HD3   | 7:1G:190:MET:H     | 1.81                     | 0.45              |
| 7:1G:252:PRO:O     | 17:1Q:44:ASN:ND2   | 2.49                     | 0.45              |
| 10:1J:103:MET:C    | 10:1J:103:MET:HE2  | 2.40                     | 0.45              |
| 11:1K:33:LEU:O     | 11:1K:36:MET:HG2   | 2.16                     | 0.45              |
| 13:1M:2:LEU:HD13   | 31:1f:26:LEU:HB3   | 1.97                     | 0.45              |
| 15:1O:14:THR:HB    | 15:1O:256:PHE:HD2  | 1.81                     | 0.45              |
| 16:1P:146:LEU:HD11 | 16:1P:289:MET:HG2  | 1.98                     | 0.45              |
| 16:1P:196:LEU:HG   | 16:1P:257:PRO:HB3  | 1.98                     | 0.45              |
| 37:1l:118:VAL:HA   | 37:1l:121:ILE:HG12 | 1.98                     | 0.45              |
| 39:1n:12:GLN:H     | 39:1n:12:GLN:CD    | 2.23                     | 0.45              |
| 39:1n:121:ARG:O    | 39:1n:125:LYS:HG2  | 2.17                     | 0.45              |
| 42:1q:94:THR:HG23  | 43:1r:34:THR:HG22  | 1.98                     | 0.45              |
| 2:1B:145:TYR:HB2   | 9:1I:141:THR:HG23  | 1.98                     | 0.45              |
| 3:1C:113:GLU:H     | 3:1C:113:GLU:CD    | 2.20                     | 0.45              |
| 5:1E:193:CYS:H     | 6:1F:26:TYR:HE1    | 1.63                     | 0.45              |
| 7:1G:454:GLY:HA2   | 7:1G:493:LEU:HB2   | 1.99                     | 0.45              |
| 13:1M:120:ILE:HG23 | 14:1N:255:PRO:HB3  | 1.96                     | 0.45              |
| 13:1M:305:THR:HB   | 13:1M:308:SER:HB2  | 1.97                     | 0.45              |
| 16:1P:26:ALA:HA    | 16:1P:31:GLY:HA3   | 1.98                     | 0.45              |
| 34:1i:105:PRO:HG3  | 40:1o:44:GLU:HG2   | 1.97                     | 0.45              |
| 37:1l:134:PRO:CB   | 40:1o:38:MET:HE2   | 2.35                     | 0.45              |
| 39:1n:103:LEU:HA   | 39:1n:103:LEU:HD23 | 1.72                     | 0.45              |
| 41:1p:161:ARG:HG2  | 41:1p:161:ARG:HH11 | 1.81                     | 0.45              |
| 3:1C:95:ASN:ND2    | 3:1C:106:ARG:HG3   | 2.31                     | 0.45              |
| 7:1G:134:LYS:H     | 18:1R:72:TYR:HE2   | 1.64                     | 0.45              |
| 7:1G:145:LEU:HD23  | 7:1G:145:LEU:H     | 1.80                     | 0.45              |
| 7:1G:290:LEU:HD13  | 7:1G:291:LEU:O     | 2.17                     | 0.45              |
| 7:1G:377:ILE:HG13  | 7:1G:450:MET:HB3   | 1.97                     | 0.45              |
| 10:1J:71:THR:O     | 10:1J:74:MET:HG3   | 2.16                     | 0.45              |
| 13:1M:447:LEU:HD21 | 13:1M:454:ILE:HG21 | 1.98                     | 0.45              |
| 16:1P:35:VAL:HG21  | 16:1P:59:LEU:HD12  | 1.98                     | 0.45              |
| 21:1V:26:LEU:O     | 21:1V:30:ILE:HG23  | 2.16                     | 0.45              |
| 28:1c:28:TRP:O     | 28:1c:32:ILE:HG23  | 2.16                     | 0.45              |
| 2:1B:70:ASP:HA     | 2:1B:74:VAL:O      | 2.17                     | 0.45              |
| 5:1E:204:GLU:CD    | 6:1F:17:ASP:HB2    | 2.42                     | 0.45              |
| 8:1H:96:ILE:HG23   | 25:1Z:144:THR:OG1  | 2.15                     | 0.45              |
| 9:1I:163:ALA:HB1   | 42:1q:103:PRO:HB3  | 1.97                     | 0.45              |
| 10:1J:95:SER:O     | 10:1J:98:MET:N     | 2.47                     | 0.45              |
| 10:1J:109:LYS:O    | 10:1J:111:GLU:HG2  | 2.17                     | 0.45              |
| 10:1J:163:ILE:HG13 | 14:1N:12:THR:HG21  | 1.98                     | 0.45              |
| 12:1L:264:TYR:N    | 12:1L:265:PRO:HD2  | 2.32                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:400:ASN:HD21 | 51:1L:701:MYR:H62  | 1.82                     | 0.45              |
| 13:1M:388:TRP:C    | 38:1m:111:LYS:HZ1  | 2.24                     | 0.45              |
| 13:1M:396:MET:HE3  | 13:1M:396:MET:HB2  | 1.86                     | 0.45              |
| 14:1N:11:MET:C     | 14:1N:11:MET:HE3   | 2.42                     | 0.45              |
| 14:1N:262:PRO:O    | 14:1N:266:ILE:HG12 | 2.15                     | 0.45              |
| 15:1O:211:LEU:HD12 | 15:1O:220:VAL:HG13 | 1.98                     | 0.45              |
| 15:1O:237:ASP:OD2  | 15:1O:237:ASP:N    | 2.36                     | 0.45              |
| 16:1P:57:MET:HA    | 16:1P:57:MET:HE3   | 1.97                     | 0.45              |
| 16:1P:77:ASP:OD2   | 16:1P:80:SER:N     | 2.49                     | 0.45              |
| 16:1P:91:VAL:HG12  | 16:1P:126:VAL:HG21 | 1.97                     | 0.45              |
| 20:1U:63:PRO:HD2   | 20:1U:79:TYR:OH    | 2.17                     | 0.45              |
| 28:1c:28:TRP:NE1   | 29:1d:66:THR:HG22  | 2.32                     | 0.45              |
| 34:1i:1:SAC:O      | 34:1i:2:GLY:N      | 2.50                     | 0.45              |
| 35:1j:60:THR:N     | 35:1j:63:GLU:OE2   | 2.50                     | 0.45              |
| 35:1j:63:GLU:HG2   | 35:1j:64:LEU:HD22  | 1.99                     | 0.45              |
| 39:1n:107:HIS:O    | 39:1n:111:LYS:HG3  | 2.16                     | 0.45              |
| 1:1A:78:ALA:HA     | 10:1J:144:ALA:HB1  | 1.98                     | 0.45              |
| 2:1B:81:ARG:HD3    | 8:1H:214:GLU:CG    | 2.46                     | 0.45              |
| 5:1E:98:TYR:HA     | 5:1E:157:ASN:CG    | 2.42                     | 0.45              |
| 5:1E:194:GLU:HB3   | 6:1F:26:TYR:CE1    | 2.52                     | 0.45              |
| 6:1F:107:ASP:HA    | 6:1F:110:ILE:HG22  | 1.99                     | 0.45              |
| 7:1G:38:PRO:HB2    | 7:1G:54:MET:HG3    | 1.99                     | 0.45              |
| 7:1G:249:ARG:NH1   | 7:1G:251:LEU:HD21  | 2.32                     | 0.45              |
| 7:1G:673:MET:HE1   | 7:1G:679:ARG:HA    | 1.99                     | 0.45              |
| 8:1H:189:THR:O     | 8:1H:193:THR:HG23  | 2.16                     | 0.45              |
| 12:1L:140:LEU:HB3  | 12:1L:182:PHE:HZ   | 1.81                     | 0.45              |
| 12:1L:331:MET:HE1  | 12:1L:468:ILE:HD12 | 1.98                     | 0.45              |
| 12:1L:387:THR:OG1  | 12:1L:461:SER:O    | 2.24                     | 0.45              |
| 12:1L:562:LEU:HB2  | 12:1L:563:PRO:HD3  | 1.97                     | 0.45              |
| 15:1O:92:ASN:O     | 15:1O:96:LEU:HB2   | 2.17                     | 0.45              |
| 15:1O:226:ARG:H    | 15:1O:226:ARG:NE   | 2.14                     | 0.45              |
| 20:1U:9:GLU:OE1    | 20:1U:9:GLU:N      | 2.38                     | 0.45              |
| 21:1V:102:LEU:H    | 21:1V:102:LEU:HD22 | 1.81                     | 0.45              |
| 33:1h:8:LEU:HB2    | 34:1i:25:GLN:O     | 2.17                     | 0.45              |
| 43:1r:34:THR:O     | 43:1r:35:GLN:NE2   | 2.49                     | 0.45              |
| 2:1B:147:PRO:HG3   | 9:1I:147:LEU:HD21  | 1.97                     | 0.45              |
| 3:1C:65:ARG:NH1    | 3:1C:123:VAL:O     | 2.50                     | 0.45              |
| 4:1D:270:ARG:HH11  | 4:1D:270:ARG:HG3   | 1.81                     | 0.45              |
| 4:1D:357:GLN:OE1   | 7:1G:122:MET:HE1   | 2.17                     | 0.45              |
| 7:1G:465:ALA:O     | 7:1G:469:ALA:N     | 2.44                     | 0.45              |
| 7:1G:692:THR:OG1   | 7:1G:693:GLU:OE2   | 2.29                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:9:GLU:H       | 9:1I:9:GLU:CD      | 2.22                     | 0.45              |
| 10:1J:118:LYS:HD2  | 10:1J:119:PHE:N    | 2.32                     | 0.45              |
| 12:1L:371:THR:O    | 12:1L:375:ILE:HG12 | 2.17                     | 0.45              |
| 13:1M:147:LEU:HD23 | 14:1N:294:MET:HE3  | 1.99                     | 0.45              |
| 13:1M:181:TYR:HE1  | 41:1p:88:GLU:HG3   | 1.82                     | 0.45              |
| 14:1N:154:MET:HA   | 14:1N:154:MET:HE3  | 1.98                     | 0.45              |
| 16:1P:113:ILE:HG13 | 16:1P:114:PRO:HD3  | 1.98                     | 0.45              |
| 17:1Q:40:PRO:HG2   | 17:1Q:51:ASN:O     | 2.17                     | 0.45              |
| 18:1R:18:TYR:HE1   | 18:1R:24:ARG:HE    | 1.65                     | 0.45              |
| 23:1X:122:GLY:HA3  | 27:1b:77:LEU:HD22  | 1.99                     | 0.45              |
| 30:1e:75:LEU:O     | 30:1e:78:ILE:HG22  | 2.17                     | 0.45              |
| 32:1g:99:TYR:O     | 32:1g:103:ASN:ND2  | 2.47                     | 0.45              |
| 34:1i:110:LEU:HD23 | 34:1i:111:GLU:OE1  | 2.17                     | 0.45              |
| 39:1n:113:MET:HE3  | 39:1n:113:MET:HB2  | 1.83                     | 0.45              |
| 41:1p:100:GLU:HA   | 41:1p:103:ASN:HD22 | 1.82                     | 0.45              |
| 2:1B:34:ASP:O      | 2:1B:38:ASN:ND2    | 2.50                     | 0.45              |
| 3:1C:40:VAL:HG22   | 43:1r:69:MET:HB3   | 1.98                     | 0.45              |
| 3:1C:89:ARG:HG3    | 3:1C:90:PHE:CD1    | 2.51                     | 0.45              |
| 3:1C:203:TRP:CZ3   | 7:1G:38:PRO:HA     | 2.51                     | 0.45              |
| 4:1D:104:ASP:OD1   | 4:1D:111:MET:HB3   | 2.17                     | 0.45              |
| 4:1D:258:VAL:HG23  | 4:1D:261:ARG:HH21  | 1.82                     | 0.45              |
| 6:1F:393:TRP:CE3   | 6:1F:419:ILE:HG21  | 2.52                     | 0.45              |
| 7:1G:100:ASN:HB3   | 7:1G:135:ARG:HG2   | 1.99                     | 0.45              |
| 7:1G:238:ILE:HG22  | 7:1G:252:PRO:HA    | 1.98                     | 0.45              |
| 7:1G:601:ARG:NH2   | 7:1G:614:ASP:OD2   | 2.50                     | 0.45              |
| 7:1G:661:LEU:H     | 7:1G:661:LEU:HD12  | 1.82                     | 0.45              |
| 8:1H:206:GLU:HG3   | 8:1H:207:LEU:HD12  | 1.99                     | 0.45              |
| 9:1I:175:TYR:CE1   | 43:1r:38:PRO:HG3   | 2.52                     | 0.45              |
| 10:1J:139:GLU:O    | 10:1J:143:ILE:HG12 | 2.17                     | 0.45              |
| 12:1L:117:PHE:HE1  | 12:1L:243:VAL:HG22 | 1.82                     | 0.45              |
| 12:1L:131:LEU:HB2  | 12:1L:143:GLY:HA3  | 1.99                     | 0.45              |
| 13:1M:19:LYS:HB2   | 13:1M:19:LYS:HE3   | 1.75                     | 0.45              |
| 13:1M:154:LEU:HA   | 13:1M:154:LEU:HD12 | 1.80                     | 0.45              |
| 13:1M:403:THR:HA   | 13:1M:406:TYR:HE2  | 1.82                     | 0.45              |
| 52:1M:501:PGT:H121 | 52:1M:501:PGT:H32  | 1.69                     | 0.45              |
| 20:1T:9:GLU:HA     | 20:1T:12:LYS:HZ2   | 1.82                     | 0.45              |
| 22:1W:92:GLU:OE2   | 22:1W:98:LYS:NZ    | 2.50                     | 0.45              |
| 23:1X:36:ASP:OD2   | 23:1X:40:LYS:HG2   | 2.16                     | 0.45              |
| 33:1h:23:LYS:HG2   | 33:1h:26:ARG:HH12  | 1.81                     | 0.45              |
| 35:1j:60:THR:OG1   | 35:1j:63:GLU:OE1   | 2.27                     | 0.45              |
| 4:1D:67:GLU:OE1    | 4:1D:74:ARG:NH2    | 2.42                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:76:CYS:SG     | 4:1D:403:ASP:HA    | 2.57                     | 0.45              |
| 4:1D:146:ARG:HE    | 4:1D:370:PRO:HB3   | 1.82                     | 0.45              |
| 4:1D:171:PHE:HA    | 4:1D:174:ARG:HD3   | 1.98                     | 0.45              |
| 6:1F:252:GLY:O     | 6:1F:272:MET:HB3   | 2.16                     | 0.45              |
| 7:1G:80:LEU:HB3    | 7:1G:83:SER:HB2    | 1.98                     | 0.45              |
| 7:1G:362:TYR:CG    | 7:1G:362:TYR:O     | 2.69                     | 0.45              |
| 7:1G:575:ASN:HD21  | 7:1G:579:ARG:HB3   | 1.81                     | 0.45              |
| 9:1I:114:THR:O     | 9:1I:114:THR:OG1   | 2.34                     | 0.45              |
| 10:1J:32:GLY:O     | 10:1J:36:SER:OG    | 2.33                     | 0.45              |
| 12:1L:37:LYS:HD3   | 12:1L:98:TRP:HE1   | 1.81                     | 0.45              |
| 12:1L:503:GLU:O    | 12:1L:507:THR:OG1  | 2.32                     | 0.45              |
| 13:1M:51:ASN:ND2   | 33:1h:90:THR:OG1   | 2.49                     | 0.45              |
| 15:1O:179:ILE:O    | 15:1O:183:ILE:HG13 | 2.17                     | 0.45              |
| 15:1O:266:LYS:O    | 15:1O:269:VAL:HG22 | 2.17                     | 0.45              |
| 16:1P:2:HIS:HB3    | 16:1P:5:LEU:HD23   | 1.98                     | 0.45              |
| 20:1U:17:TYR:OH    | 36:1k:16:PRO:O     | 2.26                     | 0.45              |
| 21:1V:19:PRO:HB2   | 21:1V:76:ILE:HG21  | 1.99                     | 0.45              |
| 21:1V:109:ASN:HA   | 21:1V:112:LYS:NZ   | 2.31                     | 0.45              |
| 24:1Y:8:TYR:O      | 24:1Y:20:LYS:NZ    | 2.47                     | 0.45              |
| 29:1d:114:GLU:OE2  | 41:1p:152:ARG:NH1  | 2.49                     | 0.45              |
| 34:1i:3:TYR:HD1    | 34:1i:7:GLU:HG2    | 1.82                     | 0.45              |
| 34:1i:68:ILE:O     | 34:1i:72:THR:HG22  | 2.16                     | 0.45              |
| 37:1l:14:PRO:HD3   | 37:1l:46:ASP:HA    | 1.98                     | 0.45              |
| 40:1o:98:MET:O     | 40:1o:102:GLU:HG2  | 2.17                     | 0.45              |
| 4:1D:233:ARG:HB3   | 9:1I:30:LEU:HD21   | 1.98                     | 0.45              |
| 5:1E:102:VAL:HG21  | 5:1E:117:LEU:HB3   | 1.99                     | 0.45              |
| 6:1F:242:PHE:CE2   | 6:1F:252:GLY:HA3   | 2.52                     | 0.45              |
| 7:1G:285:ARG:HD2   | 7:1G:291:LEU:HD13  | 1.98                     | 0.45              |
| 7:1G:298:ASP:OD2   | 7:1G:302:ARG:NH2   | 2.49                     | 0.45              |
| 7:1G:314:ASP:HA    | 7:1G:520:LYS:HD3   | 1.99                     | 0.45              |
| 8:1H:107:ALA:HB1   | 10:1J:57:PHE:HB3   | 1.99                     | 0.45              |
| 8:1H:126:LYS:O     | 8:1H:130:ILE:HG13  | 2.17                     | 0.45              |
| 8:1H:139:THR:OG1   | 8:1H:192:GLU:OE1   | 2.35                     | 0.45              |
| 9:1I:35:GLY:HA3    | 50:1I:203:PC1:H331 | 1.99                     | 0.45              |
| 12:1L:33:PRO:HB3   | 12:1L:118:PHE:CZ   | 2.52                     | 0.45              |
| 12:1L:154:LEU:HD23 | 12:1L:154:LEU:HA   | 1.77                     | 0.45              |
| 13:1M:45:LEU:HG    | 13:1M:50:LEU:HD11  | 1.99                     | 0.45              |
| 13:1M:160:LEU:O    | 13:1M:164:LEU:HD12 | 2.16                     | 0.45              |
| 15:1O:3:TYR:HB2    | 15:1O:260:ARG:HE   | 1.81                     | 0.45              |
| 15:1O:272:TYR:O    | 15:1O:275:ILE:HG12 | 2.17                     | 0.45              |
| 20:1T:11:ILE:HD12  | 20:1T:80:ILE:CG2   | 2.47                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:1U:5:PRO:HD3    | 35:1j:1:ALA:N      | 2.32                     | 0.45              |
| 22:1W:34:GLU:OE1   | 22:1W:35:LEU:N     | 2.50                     | 0.45              |
| 34:1i:24:ASP:CG    | 39:1n:124:TRP:HE1  | 2.25                     | 0.45              |
| 40:1o:25:PRO:HB2   | 40:1o:28:TYR:HB3   | 1.99                     | 0.45              |
| 3:1C:164:LYS:HB3   | 17:1Q:84:LEU:HD11  | 2.00                     | 0.44              |
| 4:1D:281:VAL:HG13  | 4:1D:283:PHE:HE1   | 1.81                     | 0.44              |
| 5:1E:33:ALA:O      | 5:1E:36:LYS:HG2    | 2.17                     | 0.44              |
| 5:1E:78:MET:O      | 5:1E:81:TYR:HB2    | 2.17                     | 0.44              |
| 5:1E:145:LEU:HD21  | 5:1E:153:MET:HG2   | 1.99                     | 0.44              |
| 6:1F:134:ALA:O     | 6:1F:176:PHE:N     | 2.31                     | 0.44              |
| 6:1F:162:ILE:HD13  | 6:1F:175:VAL:HG12  | 1.98                     | 0.44              |
| 7:1G:290:LEU:HG    | 42:1q:142:THR:C    | 2.42                     | 0.44              |
| 8:1H:26:LYS:NZ     | 8:1H:35:LYS:O      | 2.50                     | 0.44              |
| 12:1L:21:MET:HA    | 12:1L:21:MET:HE3   | 1.99                     | 0.44              |
| 12:1L:162:THR:OG1  | 37:1l:86:ARG:NH1   | 2.50                     | 0.44              |
| 12:1L:536:LEU:HB3  | 12:1L:537:PRO:HD3  | 1.98                     | 0.44              |
| 13:1M:3:LYS:HB2    | 13:1M:3:LYS:HE3    | 1.76                     | 0.44              |
| 13:1M:336:ARG:HD2  | 13:1M:426:ILE:HG23 | 1.98                     | 0.44              |
| 15:1O:27:VAL:HA    | 15:1O:170:VAL:HB   | 1.99                     | 0.44              |
| 15:1O:63:THR:HG23  | 15:1O:302:ARG:HH22 | 1.80                     | 0.44              |
| 15:1O:183:ILE:HD12 | 15:1O:184:GLN:N    | 2.32                     | 0.44              |
| 16:1P:253:PHE:CZ   | 16:1P:255:PRO:HB3  | 2.52                     | 0.44              |
| 17:1Q:14:ASP:OD1   | 17:1Q:14:ASP:N     | 2.43                     | 0.44              |
| 17:1Q:55:TRP:CZ2   | 17:1Q:108:ARG:HD2  | 2.51                     | 0.44              |
| 21:1V:29:LYS:O     | 21:1V:33:VAL:HG22  | 2.17                     | 0.44              |
| 23:1X:136:LEU:HD12 | 23:1X:137:PRO:HD2  | 1.98                     | 0.44              |
| 26:1a:65:GLY:N     | 26:1a:67:GLU:OE2   | 2.50                     | 0.44              |
| 37:1l:126:GLN:O    | 37:1l:128:VAL:N    | 2.50                     | 0.44              |
| 39:1n:125:LYS:O    | 39:1n:129:ARG:HG2  | 2.16                     | 0.44              |
| 3:1C:56:GLY:C      | 3:1C:59:PRO:HD2    | 2.43                     | 0.44              |
| 3:1C:149:ARG:HD2   | 22:1W:97:TRP:HZ3   | 1.81                     | 0.44              |
| 5:1E:200:THR:OG1   | 6:1F:283:HIS:ND1   | 2.48                     | 0.44              |
| 6:1F:205:LEU:HG    | 6:1F:404:ILE:HD12  | 1.98                     | 0.44              |
| 6:1F:309:LYS:HE3   | 6:1F:309:LYS:HB3   | 1.64                     | 0.44              |
| 6:1F:394:GLU:HB2   | 7:1G:129:ARG:HH22  | 1.82                     | 0.44              |
| 7:1G:20:VAL:HG21   | 7:1G:73:VAL:HG11   | 1.99                     | 0.44              |
| 7:1G:285:ARG:HB3   | 42:1q:144:TYR:H    | 1.81                     | 0.44              |
| 7:1G:666:LEU:HD12  | 7:1G:666:LEU:HA    | 1.84                     | 0.44              |
| 11:1K:47:ILE:HG12  | 14:1N:79:LEU:HD13  | 1.99                     | 0.44              |
| 12:1L:149:ILE:HD12 | 12:1L:172:ILE:HD11 | 1.99                     | 0.44              |
| 12:1L:236:ALA:HB1  | 12:1L:248:HIS:CE1  | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:316:THR:HB   | 12:1L:395:ILE:HD12 | 2.00                     | 0.44              |
| 12:1L:432:LEU:HD21 | 36:1k:65:ALA:HB2   | 1.98                     | 0.44              |
| 14:1N:40:MET:SD    | 14:1N:134:GLN:NE2  | 2.91                     | 0.44              |
| 14:1N:80:TYR:HA    | 30:1e:67:LEU:HD21  | 1.98                     | 0.44              |
| 15:1O:104:ARG:NH1  | 54:1O:401:GTP:N7   | 2.64                     | 0.44              |
| 16:1P:38:LEU:O     | 16:1P:43:SER:OG    | 2.30                     | 0.44              |
| 16:1P:256:TYR:CE2  | 16:1P:258:LEU:HD23 | 2.51                     | 0.44              |
| 17:1Q:112:LYS:O    | 17:1Q:114:LYS:NZ   | 2.45                     | 0.44              |
| 25:1Z:6:VAL:HG21   | 43:1r:41:PRO:HB3   | 1.99                     | 0.44              |
| 33:1h:70:PRO:HA    | 33:1h:73:ARG:HD3   | 2.00                     | 0.44              |
| 34:1i:86:LYS:HB3   | 34:1i:87:TYR:CD1   | 2.53                     | 0.44              |
| 38:1m:5:TYR:HE2    | 38:1m:14:PRO:HD3   | 1.81                     | 0.44              |
| 2:1B:59:MET:HA     | 2:1B:156:LEU:HD21  | 1.99                     | 0.44              |
| 4:1D:202:ASP:CG    | 43:1r:40:LEU:HD11  | 2.43                     | 0.44              |
| 7:1G:58:GLU:HB3    | 7:1G:65:VAL:HG22   | 1.99                     | 0.44              |
| 7:1G:259:ASN:HA    | 7:1G:390:LEU:HD22  | 1.98                     | 0.44              |
| 7:1G:383:ASN:C     | 7:1G:387:GLU:HG2   | 2.42                     | 0.44              |
| 9:1I:168:ASN:HD21  | 42:1q:93:MET:HE1   | 1.82                     | 0.44              |
| 12:1L:150:MET:HE3  | 12:1L:153:LEU:HD12 | 1.98                     | 0.44              |
| 12:1L:217:LEU:HD12 | 12:1L:277:THR:HG22 | 1.98                     | 0.44              |
| 12:1L:298:ILE:HG22 | 12:1L:354:GLN:O    | 2.17                     | 0.44              |
| 12:1L:306:THR:HG22 | 12:1L:336:LYS:HD2  | 1.99                     | 0.44              |
| 13:1M:364:LEU:HG   | 13:1M:369:LEU:HD22 | 1.99                     | 0.44              |
| 13:1M:421:HIS:HB3  | 38:1m:50:TYR:OH    | 2.17                     | 0.44              |
| 15:1O:257:HIS:O    | 15:1O:261:MET:HG2  | 2.17                     | 0.44              |
| 16:1P:237:LEU:HB3  | 16:1P:240:ASP:HB2  | 1.99                     | 0.44              |
| 21:1V:27:TYR:HD2   | 21:1V:55:LEU:HB2   | 1.83                     | 0.44              |
| 22:1W:24:ASP:CG    | 22:1W:25:MET:N     | 2.74                     | 0.44              |
| 25:1Z:144:THR:O    | 26:1a:36:LYS:NZ    | 2.50                     | 0.44              |
| 33:1h:49:GLU:OE2   | 33:1h:69:HIS:NE2   | 2.48                     | 0.44              |
| 37:1l:43:GLY:HA3   | 38:1m:75:ILE:HG13  | 1.99                     | 0.44              |
| 37:1l:139:TYR:CE1  | 37:1l:144:GLY:HA3  | 2.52                     | 0.44              |
| 41:1p:69:ARG:NH2   | 41:1p:94:ASP:OD1   | 2.50                     | 0.44              |
| 3:1C:152:LEU:HD22  | 4:1D:84:HIS:ND1    | 2.32                     | 0.44              |
| 6:1F:26:TYR:HD2    | 6:1F:28:ARG:HG2    | 1.82                     | 0.44              |
| 7:1G:159:CYS:HA    | 7:1G:199:ILE:HD11  | 2.00                     | 0.44              |
| 7:1G:396:ARG:HA    | 7:1G:399:TRP:HB3   | 2.00                     | 0.44              |
| 7:1G:539:LYS:HB3   | 7:1G:540:ASP:OD1   | 2.18                     | 0.44              |
| 8:1H:260:VAL:HG21  | 26:1a:17:PHE:HA    | 2.00                     | 0.44              |
| 8:1H:281:ARG:HG3   | 8:1H:281:ARG:HH11  | 1.82                     | 0.44              |
| 8:1H:287:HIS:NE2   | 50:1H:401:PC1:H141 | 2.32                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 13:1M:447:LEU:HD11 | 13:1M:454:ILE:HG23 | 2.00                     | 0.44              |
| 16:1P:28:GLY:HA3   | 56:1P:501:NDP:O1N  | 2.18                     | 0.44              |
| 21:1V:81:LEU:O     | 21:1V:84:GLU:HG3   | 2.17                     | 0.44              |
| 22:1W:23:ARG:HH21  | 22:1W:27:GLU:HG2   | 1.81                     | 0.44              |
| 23:1X:23:VAL:HG13  | 23:1X:81:PHE:CZ    | 2.53                     | 0.44              |
| 24:1Y:23:ALA:O     | 24:1Y:26:SER:OG    | 2.32                     | 0.44              |
| 33:1h:30:LEU:HD12  | 33:1h:34:ILE:HG23  | 1.99                     | 0.44              |
| 34:1i:118:LEU:HD23 | 34:1i:118:LEU:H    | 1.82                     | 0.44              |
| 1:1A:87:MET:HA     | 10:1J:147:TYR:HB3  | 1.99                     | 0.44              |
| 3:1C:82:ASP:HB2    | 3:1C:138:PHE:HE2   | 1.83                     | 0.44              |
| 4:1D:246:THR:OG1   | 21:1V:12:GLY:HA3   | 2.18                     | 0.44              |
| 4:1D:305:ARG:NH2   | 25:1Z:23:ARG:HG3   | 2.32                     | 0.44              |
| 4:1D:345:LEU:HD22  | 7:1G:103:LEU:HD23  | 1.99                     | 0.44              |
| 6:1F:89:ARG:HG2    | 17:1Q:124:TRP:HB2  | 1.99                     | 0.44              |
| 6:1F:136:ILE:CD1   | 6:1F:177:VAL:HA    | 2.48                     | 0.44              |
| 7:1G:296:TRP:HZ3   | 7:1G:561:LEU:HD22  | 1.83                     | 0.44              |
| 7:1G:640:ASN:CG    | 7:1G:641:TYR:N     | 2.75                     | 0.44              |
| 7:1G:688:VAL:O     | 7:1G:692:THR:OG1   | 2.36                     | 0.44              |
| 8:1H:303:TRP:NE1   | 25:1Z:47:TYR:OH    | 2.48                     | 0.44              |
| 9:1I:56:PRO:O      | 9:1I:57:LEU:HD13   | 2.17                     | 0.44              |
| 12:1L:145:GLU:OE2  | 12:1L:176:ARG:NE   | 2.50                     | 0.44              |
| 12:1L:481:THR:C    | 12:1L:482:MET:HE3  | 2.42                     | 0.44              |
| 12:1L:485:TYR:CE2  | 51:1L:701:MYR:H52  | 2.52                     | 0.44              |
| 12:1L:511:LEU:HD11 | 39:1n:38:TYR:CE1   | 2.53                     | 0.44              |
| 14:1N:92:PRO:O     | 14:1N:96:THR:HG23  | 2.18                     | 0.44              |
| 14:1N:209:ILE:HG23 | 14:1N:213:LEU:HD23 | 1.99                     | 0.44              |
| 16:1P:9:GLY:HA3    | 16:1P:15:SER:HB3   | 2.00                     | 0.44              |
| 16:1P:84:VAL:HG23  | 16:1P:85:VAL:HG13  | 2.00                     | 0.44              |
| 16:1P:112:LYS:O    | 16:1P:115:HIS:ND1  | 2.51                     | 0.44              |
| 16:1P:132:ILE:HG22 | 16:1P:166:ILE:HB   | 2.00                     | 0.44              |
| 16:1P:196:LEU:HB3  | 16:1P:239:PHE:CE2  | 2.51                     | 0.44              |
| 22:1W:21:PHE:O     | 22:1W:23:ARG:NH1   | 2.49                     | 0.44              |
| 39:1n:82:PRO:HA    | 39:1n:87:GLY:HA3   | 2.00                     | 0.44              |
| 2:1B:49:THR:HA     | 2:1B:87:ILE:HB     | 2.00                     | 0.44              |
| 2:1B:116:MET:HG3   | 2:1B:151:PRO:HG2   | 1.99                     | 0.44              |
| 2:1B:127:HIS:ND1   | 9:1I:115:LYS:HD3   | 2.32                     | 0.44              |
| 3:1C:41:GLN:NE2    | 43:1r:65:PRO:O     | 2.45                     | 0.44              |
| 3:1C:129:TRP:HZ2   | 4:1D:78:PRO:HD2    | 1.83                     | 0.44              |
| 3:1C:198:ASP:OD1   | 3:1C:198:ASP:N     | 2.50                     | 0.44              |
| 4:1D:116:GLN:NE2   | 4:1D:138:ARG:HG2   | 2.31                     | 0.44              |
| 4:1D:317:LYS:HA    | 4:1D:317:LYS:HD2   | 1.92                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:249:ARG:HD2   | 7:1G:251:LEU:HD11  | 2.00                     | 0.44              |
| 7:1G:332:LYS:HB2   | 7:1G:507:TYR:HE1   | 1.83                     | 0.44              |
| 8:1H:86:TRP:HA     | 8:1H:89:LEU:HD23   | 2.00                     | 0.44              |
| 11:1K:48:ILE:HG13  | 11:1K:48:ILE:H     | 1.60                     | 0.44              |
| 16:1P:185:MET:HA   | 16:1P:188:PHE:CD2  | 2.52                     | 0.44              |
| 17:1Q:127:ARG:HH11 | 44:1s:70:ARG:CZ    | 2.31                     | 0.44              |
| 20:1T:17:TYR:HB2   | 20:1T:20:LYS:HE3   | 2.00                     | 0.44              |
| 20:1T:43:ASP:OD1   | 20:1T:46:ASP:N     | 2.33                     | 0.44              |
| 23:1X:77:CYS:SG    | 23:1X:113:LYS:NZ   | 2.91                     | 0.44              |
| 40:1o:32:GLU:OE2   | 40:1o:32:GLU:N     | 2.51                     | 0.44              |
| 3:1C:155:TYR:HB2   | 22:1W:102:HIS:CE1  | 2.52                     | 0.44              |
| 6:1F:22:PHE:HD1    | 6:1F:117:LYS:HD2   | 1.83                     | 0.44              |
| 7:1G:326:GLU:OE1   | 7:1G:572:THR:N     | 2.50                     | 0.44              |
| 7:1G:386:PHE:HB2   | 7:1G:665:GLN:HB3   | 2.00                     | 0.44              |
| 8:1H:181:LEU:HA    | 8:1H:184:MET:HB2   | 1.98                     | 0.44              |
| 10:1J:61:LEU:HA    | 10:1J:61:LEU:HD12  | 1.70                     | 0.44              |
| 10:1J:152:TRP:CD2  | 30:1e:13:LEU:HD11  | 2.53                     | 0.44              |
| 12:1L:293:ILE:HG22 | 12:1L:422:TYR:HB3  | 2.00                     | 0.44              |
| 13:1M:47:GLU:OE1   | 13:1M:47:GLU:N     | 2.51                     | 0.44              |
| 13:1M:70:THR:HA    | 13:1M:103:GLN:NE2  | 2.32                     | 0.44              |
| 45:1N:401:3PE:O14  | 15:1O:303:LYS:NZ   | 2.44                     | 0.44              |
| 16:1P:172:PHE:HB2  | 16:1P:179:LEU:HD22 | 2.00                     | 0.44              |
| 16:1P:201:VAL:O    | 16:1P:290:SER:OG   | 2.35                     | 0.44              |
| 16:1P:202:LYS:HA   | 16:1P:291:ASP:HB3  | 2.00                     | 0.44              |
| 33:1h:41:THR:O     | 33:1h:45:VAL:HG22  | 2.18                     | 0.44              |
| 34:1i:107:ASP:H    | 40:1o:67:LYS:NZ    | 2.16                     | 0.44              |
| 35:1j:26:GLU:H     | 35:1j:26:GLU:HG2   | 1.69                     | 0.44              |
| 41:1p:119:SER:OG   | 41:1p:123:ASN:ND2  | 2.50                     | 0.44              |
| 2:1B:52:LEU:HD12   | 2:1B:89:ALA:O      | 2.17                     | 0.44              |
| 2:1B:55:CYS:SG     | 2:1B:117:GLY:HA3   | 2.57                     | 0.44              |
| 3:1C:67:HIS:HB3    | 3:1C:70:ALA:HB3    | 2.00                     | 0.44              |
| 3:1C:149:ARG:HA    | 22:1W:88:MET:CE    | 2.47                     | 0.44              |
| 6:1F:121:GLY:HA3   | 6:1F:228:VAL:O     | 2.18                     | 0.44              |
| 6:1F:279:LEU:HD22  | 6:1F:317:MET:HE1   | 1.99                     | 0.44              |
| 6:1F:364:PRO:HB2   | 6:1F:403:THR:HG22  | 1.98                     | 0.44              |
| 7:1G:378:LEU:HB3   | 7:1G:451:VAL:HG13  | 2.00                     | 0.44              |
| 7:1G:386:PHE:CZ    | 7:1G:668:ILE:HD12  | 2.53                     | 0.44              |
| 7:1G:389:PRO:CD    | 7:1G:390:LEU:N     | 2.80                     | 0.44              |
| 8:1H:15:LEU:HB3    | 26:1a:15:CYS:SG    | 2.58                     | 0.44              |
| 9:1I:33:GLY:O      | 9:1I:37:THR:HG23   | 2.18                     | 0.44              |
| 12:1L:335:PHE:CE1  | 12:1L:380:LEU:HD23 | 2.53                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:1M:501:PGT:H181 | 52:1M:501:PGT:H152 | 1.63                     | 0.44              |
| 16:1P:170:ASP:O    | 16:1P:204:PRO:HA   | 2.18                     | 0.44              |
| 19:1S:17:GLU:CD    | 19:1S:53:LEU:HG    | 2.42                     | 0.44              |
| 19:1S:35:PHE:CD1   | 19:1S:35:PHE:C     | 2.96                     | 0.44              |
| 20:1T:58:PHE:HB3   | 20:1T:60:PHE:CE2   | 2.53                     | 0.44              |
| 20:1T:60:PHE:CD1   | 20:1T:60:PHE:C     | 2.96                     | 0.44              |
| 21:1V:39:LYS:HD3   | 21:1V:44:ARG:HD3   | 2.00                     | 0.44              |
| 21:1V:79:VAL:HA    | 21:1V:82:GLN:HE22  | 1.82                     | 0.44              |
| 40:1o:51:MET:O     | 40:1o:55:ARG:HG3   | 2.17                     | 0.44              |
| 41:1p:29:VAL:O     | 41:1p:33:THR:OG1   | 2.32                     | 0.44              |
| 42:1q:5:GLN:O      | 42:1q:9:ARG:HG3    | 2.17                     | 0.44              |
| 1:1A:18:VAL:HG21   | 8:1H:76:ILE:HD11   | 2.00                     | 0.44              |
| 2:1B:41:ARG:HH11   | 2:1B:110:PRO:HG3   | 1.83                     | 0.44              |
| 4:1D:4:TRP:CE2     | 13:1M:140:THR:HG23 | 2.52                     | 0.44              |
| 4:1D:98:GLN:O      | 4:1D:101:PRO:HD2   | 2.18                     | 0.44              |
| 5:1E:97:LYS:HD2    | 5:1E:97:LYS:HA     | 1.70                     | 0.44              |
| 6:1F:371:TRP:HZ2   | 7:1G:130:PHE:HA    | 1.82                     | 0.44              |
| 10:1J:57:PHE:CE2   | 10:1J:61:LEU:HD23  | 2.53                     | 0.44              |
| 10:1J:151:THR:OG1  | 50:1J:201:PC1:H32  | 2.17                     | 0.44              |
| 12:1L:3:PRO:HB3    | 41:1p:36:PHE:CE2   | 2.53                     | 0.44              |
| 12:1L:496:MET:O    | 12:1L:500:LEU:HG   | 2.17                     | 0.44              |
| 13:1M:278:ARG:NH1  | 37:1l:83:MET:HE3   | 2.33                     | 0.44              |
| 14:1N:194:LEU:HD23 | 14:1N:201:THR:HG21 | 2.00                     | 0.44              |
| 16:1P:234:ASN:C    | 16:1P:234:ASN:OD1  | 2.61                     | 0.44              |
| 56:1P:501:NDP:H51A | 56:1P:501:NDP:C8A  | 2.44                     | 0.44              |
| 19:1S:20:ILE:HD11  | 19:1S:54:ILE:HG23  | 2.00                     | 0.44              |
| 20:1T:22:TYR:HD2   | 20:1T:23:ASP:N     | 2.16                     | 0.44              |
| 22:1W:53:ASP:N     | 22:1W:53:ASP:OD1   | 2.51                     | 0.44              |
| 24:1Y:31:THR:O     | 24:1Y:35:VAL:HG12  | 2.17                     | 0.44              |
| 29:1d:96:SER:OG    | 29:1d:97:HIS:ND1   | 2.49                     | 0.44              |
| 35:1j:44:SER:O     | 35:1j:48:LEU:HD23  | 2.18                     | 0.44              |
| 40:1o:72:SER:HA    | 41:1p:23:THR:OG1   | 2.18                     | 0.44              |
| 42:1q:6:VAL:HG22   | 42:1q:9:ARG:HH21   | 1.83                     | 0.44              |
| 6:1F:261:HIS:N     | 6:1F:336:VAL:O     | 2.46                     | 0.43              |
| 6:1F:262:VAL:HG13  | 6:1F:265:PRO:HG3   | 2.00                     | 0.43              |
| 7:1G:199:ILE:HD12  | 7:1G:199:ILE:HA    | 1.85                     | 0.43              |
| 7:1G:496:ILE:HB    | 7:1G:499:GLN:HB2   | 2.00                     | 0.43              |
| 7:1G:569:LYS:HZ3   | 7:1G:571:ALA:HB3   | 1.82                     | 0.43              |
| 8:1H:281:ARG:HD3   | 8:1H:281:ARG:HA    | 1.87                     | 0.43              |
| 11:1K:27:MET:O     | 11:1K:31:LEU:HD12  | 2.18                     | 0.43              |
| 13:1M:84:LEU:O     | 13:1M:86:LYS:N     | 2.51                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:1O:97:GLN:HG2   | 15:1O:135:LEU:HB2  | 1.99                     | 0.43              |
| 16:1P:195:SER:O    | 16:1P:195:SER:OG   | 2.36                     | 0.43              |
| 16:1P:238:LEU:O    | 16:1P:242:VAL:HG23 | 2.17                     | 0.43              |
| 22:1W:90:LEU:O     | 22:1W:94:ILE:HD12  | 2.18                     | 0.43              |
| 23:1X:25:LYS:HA    | 23:1X:28:ALA:HB2   | 2.00                     | 0.43              |
| 24:1Y:28:GLY:O     | 24:1Y:62:SER:OG    | 2.29                     | 0.43              |
| 40:1o:88:TYR:CZ    | 40:1o:92:LEU:HD11  | 2.53                     | 0.43              |
| 41:1p:27:ASN:HD21  | 41:1p:29:VAL:HB    | 1.82                     | 0.43              |
| 41:1p:73:ILE:HA    | 41:1p:76:CYS:HB2   | 1.98                     | 0.43              |
| 3:1C:147:ASP:OD2   | 3:1C:149:ARG:NH1   | 2.42                     | 0.43              |
| 3:1C:206:PHE:CE1   | 4:1D:360:PRO:HD3   | 2.53                     | 0.43              |
| 5:1E:149:VAL:O     | 6:1F:265:PRO:HB2   | 2.17                     | 0.43              |
| 6:1F:351:ILE:HA    | 6:1F:354:TYR:HB2   | 2.00                     | 0.43              |
| 9:1I:73:GLY:HA2    | 42:1q:108:TYR:HE1  | 1.83                     | 0.43              |
| 9:1I:141:THR:OG1   | 9:1I:146:GLU:OE2   | 2.36                     | 0.43              |
| 10:1J:87:LYS:HA    | 10:1J:87:LYS:HD3   | 1.79                     | 0.43              |
| 12:1L:141:PHE:HB2  | 12:1L:186:MET:HE1  | 1.99                     | 0.43              |
| 12:1L:331:MET:N    | 12:1L:331:MET:SD   | 2.91                     | 0.43              |
| 12:1L:386:LEU:HD12 | 12:1L:386:LEU:HA   | 1.82                     | 0.43              |
| 12:1L:495:ILE:O    | 12:1L:499:MET:HG3  | 2.18                     | 0.43              |
| 12:1L:529:TYR:HB3  | 12:1L:530:PRO:HD3  | 2.00                     | 0.43              |
| 13:1M:14:MET:HG3   | 31:1f:12:VAL:HB    | 2.00                     | 0.43              |
| 15:1O:28:ASP:C     | 15:1O:35:LYS:HD2   | 2.43                     | 0.43              |
| 16:1P:93:ASN:OD1   | 16:1P:94:LEU:N     | 2.51                     | 0.43              |
| 17:1Q:22:LEU:HB3   | 22:1W:82:LEU:HD21  | 1.99                     | 0.43              |
| 18:1R:28:PHE:N     | 18:1R:28:PHE:CD1   | 2.86                     | 0.43              |
| 20:1U:9:GLU:HA     | 20:1U:12:LYS:HE3   | 1.99                     | 0.43              |
| 20:1U:47:GLN:HA    | 20:1U:50:ILE:HG12  | 2.00                     | 0.43              |
| 30:1e:46:ILE:HG23  | 30:1e:50:ARG:NH1   | 2.33                     | 0.43              |
| 1:1A:55:PHE:HB2    | 10:1J:70:TYR:OH    | 2.18                     | 0.43              |
| 2:1B:93:THR:HG23   | 2:1B:96:MET:H      | 1.82                     | 0.43              |
| 3:1C:127:ALA:HA    | 3:1C:130:TYR:CD1   | 2.52                     | 0.43              |
| 3:1C:150:ARG:NH2   | 3:1C:157:PHE:O     | 2.52                     | 0.43              |
| 5:1E:34:ILE:HD13   | 5:1E:34:ILE:HA     | 1.88                     | 0.43              |
| 5:1E:165:THR:N     | 5:1E:168:ASP:OD2   | 2.47                     | 0.43              |
| 6:1F:31:TRP:CZ2    | 6:1F:148:ASN:HB3   | 2.53                     | 0.43              |
| 6:1F:256:PHE:CD2   | 6:1F:270:GLU:HB3   | 2.54                     | 0.43              |
| 7:1G:315:VAL:HG13  | 7:1G:340:SER:HB2   | 1.99                     | 0.43              |
| 7:1G:386:PHE:HB3   | 7:1G:671:PHE:CD1   | 2.53                     | 0.43              |
| 7:1G:652:VAL:HG22  | 7:1G:653:ASN:N     | 2.27                     | 0.43              |
| 8:1H:136:VAL:O     | 8:1H:140:ILE:HG13  | 2.18                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:190:LEU:H     | 8:1H:190:LEU:HD12  | 1.84                     | 0.43              |
| 8:1H:235:ASN:O     | 8:1H:239:ALA:N     | 2.32                     | 0.43              |
| 9:1I:146:GLU:HA    | 42:1q:124:TYR:HD2  | 1.83                     | 0.43              |
| 10:1J:129:ASP:OD1  | 11:1K:52:HIS:NE2   | 2.51                     | 0.43              |
| 12:1L:121:LEU:HD23 | 12:1L:121:LEU:HA   | 1.84                     | 0.43              |
| 12:1L:556:ILE:HD13 | 12:1L:556:ILE:HA   | 1.88                     | 0.43              |
| 13:1M:30:HIS:CD2   | 31:1f:16:VAL:HB    | 2.54                     | 0.43              |
| 13:1M:214:LEU:HD23 | 13:1M:214:LEU:HA   | 1.68                     | 0.43              |
| 14:1N:2:ASN:HB3    | 14:1N:5:ILE:CD1    | 2.48                     | 0.43              |
| 14:1N:7:THR:HA     | 53:1N:402:CDL:H112 | 2.00                     | 0.43              |
| 14:1N:190:MET:H    | 14:1N:190:MET:HG2  | 1.56                     | 0.43              |
| 14:1N:338:PRO:O    | 23:1X:169:TRP:NE1  | 2.51                     | 0.43              |
| 16:1P:97:ARG:HA    | 16:1P:97:ARG:HD3   | 1.79                     | 0.43              |
| 35:1j:64:LEU:HD13  | 35:1j:64:LEU:HA    | 1.80                     | 0.43              |
| 36:1k:39:GLY:O     | 36:1k:40:LEU:HD23  | 2.18                     | 0.43              |
| 38:1m:38:ILE:HG22  | 38:1m:41:ARG:NH2   | 2.33                     | 0.43              |
| 40:1o:41:THR:OG1   | 40:1o:42:GLN:N     | 2.51                     | 0.43              |
| 3:1C:126:ALA:HB2   | 4:1D:252:ASN:O     | 2.18                     | 0.43              |
| 4:1D:46:ASN:HA     | 4:1D:68:LEU:O      | 2.18                     | 0.43              |
| 5:1E:9:HIS:NE2     | 5:1E:63:ILE:HG13   | 2.34                     | 0.43              |
| 10:1J:78:MET:C     | 10:1J:80:PRO:HD3   | 2.43                     | 0.43              |
| 11:1K:43:MET:O     | 11:1K:47:ILE:HD12  | 2.18                     | 0.43              |
| 12:1L:287:PHE:CZ   | 12:1L:527:GLY:HA3  | 2.53                     | 0.43              |
| 12:1L:578:SER:HB2  | 14:1N:172:GLN:NE2  | 2.29                     | 0.43              |
| 13:1M:75:LEU:HD23  | 13:1M:78:MET:HE3   | 1.99                     | 0.43              |
| 13:1M:420:THR:HB   | 13:1M:423:ILE:HD12 | 1.99                     | 0.43              |
| 14:1N:331:VAL:HG21 | 29:1d:41:SER:HA    | 1.99                     | 0.43              |
| 15:1O:136:GLU:O    | 15:1O:140:ARG:HG2  | 2.19                     | 0.43              |
| 19:1S:35:PHE:C     | 19:1S:35:PHE:HD1   | 2.27                     | 0.43              |
| 20:1T:11:ILE:HG22  | 20:1T:77:VAL:HG13  | 1.99                     | 0.43              |
| 25:1Z:113:THR:HG22 | 25:1Z:115:ARG:H    | 1.84                     | 0.43              |
| 34:1i:87:TYR:CZ    | 41:1p:48:ARG:HG2   | 2.53                     | 0.43              |
| 37:1l:10:PRO:HD2   | 38:1m:69:TYR:HD2   | 1.82                     | 0.43              |
| 37:1l:138:LEU:HD12 | 37:1l:142:ARG:NH1  | 2.32                     | 0.43              |
| 39:1n:137:LYS:HB3  | 39:1n:137:LYS:HE3  | 1.55                     | 0.43              |
| 40:1o:50:LEU:O     | 40:1o:55:ARG:NE    | 2.34                     | 0.43              |
| 41:1p:54:GLN:NE2   | 41:1p:55:HIS:HD2   | 2.17                     | 0.43              |
| 43:1r:54:CYS:HA    | 43:1r:57:ASP:HB2   | 2.01                     | 0.43              |
| 43:1r:92:LYS:HE2   | 43:1r:92:LYS:H     | 1.83                     | 0.43              |
| 2:1B:32:LYS:HA     | 2:1B:32:LYS:HD2    | 1.91                     | 0.43              |
| 2:1B:48:MET:O      | 2:1B:87:ILE:N      | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:1D:209:ASP:OD1   | 25:1Z:16:TYR:OH    | 2.36                     | 0.43              |
| 4:1D:270:ARG:HB3   | 4:1D:283:PHE:CZ    | 2.53                     | 0.43              |
| 6:1F:129:MET:HG3   | 6:1F:131:ALA:H     | 1.84                     | 0.43              |
| 7:1G:100:ASN:OD1   | 7:1G:135:ARG:NH1   | 2.52                     | 0.43              |
| 10:1J:6:ALA:HA     | 10:1J:9:LEU:HB2    | 1.99                     | 0.43              |
| 11:1K:90:VAL:HA    | 11:1K:93:LEU:HB2   | 2.01                     | 0.43              |
| 13:1M:455:LEU:HA   | 13:1M:455:LEU:HD23 | 1.72                     | 0.43              |
| 14:1N:219:LEU:O    | 14:1N:223:SER:N    | 2.51                     | 0.43              |
| 15:1O:97:GLN:NE2   | 54:1O:401:GTP:HN1  | 2.16                     | 0.43              |
| 15:1O:186:LYS:HB2  | 15:1O:191:GLU:OE2  | 2.18                     | 0.43              |
| 19:1S:36:ILE:HA    | 19:1S:40:TYR:HB2   | 2.00                     | 0.43              |
| 21:1V:31:LEU:HD23  | 21:1V:31:LEU:HA    | 1.88                     | 0.43              |
| 34:1i:123:PRO:HB2  | 34:1i:125:GLN:OE1  | 2.18                     | 0.43              |
| 37:1l:93:PRO:HB3   | 38:1m:14:PRO:HG3   | 2.00                     | 0.43              |
| 37:1l:112:MET:O    | 37:1l:116:PHE:HB2  | 2.19                     | 0.43              |
| 43:1r:12:ASN:O     | 43:1r:16:GLY:N     | 2.49                     | 0.43              |
| 43:1r:105:LEU:HD12 | 43:1r:105:LEU:HA   | 1.84                     | 0.43              |
| 7:1G:106:PRO:O     | 9:1I:104:ARG:NH2   | 2.51                     | 0.43              |
| 7:1G:395:ILE:O     | 7:1G:399:TRP:N     | 2.39                     | 0.43              |
| 8:1H:132:ALA:O     | 8:1H:136:VAL:HG13  | 2.17                     | 0.43              |
| 11:1K:67:ALA:HA    | 11:1K:70:GLU:OE1   | 2.18                     | 0.43              |
| 12:1L:119:LYS:HB3  | 12:1L:119:LYS:HE2  | 1.77                     | 0.43              |
| 30:1e:29:PRO:HB3   | 33:1h:138:LYS:HG3  | 2.00                     | 0.43              |
| 32:1g:66:PHE:HB2   | 33:1h:28:TYR:HE2   | 1.81                     | 0.43              |
| 36:1k:50:TRP:CE2   | 36:1k:51:ARG:HG2   | 2.53                     | 0.43              |
| 37:1l:60:PRO:HG3   | 37:1l:70:ARG:NH2   | 2.33                     | 0.43              |
| 40:1o:30:PHE:CZ    | 40:1o:103:ARG:HD2  | 2.54                     | 0.43              |
| 3:1C:76:ALA:HB3    | 3:1C:95:ASN:HB3    | 2.00                     | 0.43              |
| 4:1D:103:PHE:HA    | 4:1D:106:LEU:HB2   | 1.99                     | 0.43              |
| 7:1G:232:ASP:OD2   | 7:1G:388:ALA:HA    | 2.19                     | 0.43              |
| 8:1H:59:GLU:HA     | 8:1H:60:PRO:HD3    | 1.80                     | 0.43              |
| 9:1I:8:ARG:NH1     | 9:1I:8:ARG:HA      | 2.34                     | 0.43              |
| 12:1L:3:PRO:O      | 12:1L:7:LEU:HD23   | 2.18                     | 0.43              |
| 12:1L:88:MET:HE2   | 12:1L:88:MET:HA    | 2.00                     | 0.43              |
| 12:1L:250:SER:CB   | 12:1L:333:ALA:HA   | 2.47                     | 0.43              |
| 14:1N:25:HIS:HB2   | 30:1e:14:ASP:HB2   | 2.01                     | 0.43              |
| 14:1N:321:LYS:HD3  | 14:1N:323:MET:HB3  | 2.00                     | 0.43              |
| 16:1P:175:GLU:OE2  | 16:1P:175:GLU:N    | 2.52                     | 0.43              |
| 16:1P:234:ASN:HB2  | 16:1P:341:ASN:HB3  | 2.01                     | 0.43              |
| 16:1P:280:THR:H    | 16:1P:283:LYS:HE2  | 1.83                     | 0.43              |
| 17:1Q:112:LYS:HB3  | 17:1Q:114:LYS:NZ   | 2.34                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:1S:83:ALA:O     | 19:1S:87:THR:OG1   | 2.37                     | 0.43              |
| 21:1V:81:LEU:O     | 21:1V:85:ASN:ND2   | 2.52                     | 0.43              |
| 23:1X:12:LEU:HD23  | 23:1X:12:LEU:H     | 1.84                     | 0.43              |
| 40:1o:14:LYS:HE2   | 40:1o:112:LYS:NZ   | 2.34                     | 0.43              |
| 43:1r:56:ARG:O     | 43:1r:58:GLY:N     | 2.51                     | 0.43              |
| 1:1A:1:FME:O1      | 1:1A:2:ASN:N       | 2.52                     | 0.43              |
| 1:1A:81:THR:O      | 27:1b:45:ASN:ND2   | 2.52                     | 0.43              |
| 3:1C:39:GLN:HB3    | 3:1C:51:PHE:CD2    | 2.53                     | 0.43              |
| 3:1C:66:ASP:HB2    | 21:1V:89:LEU:HD12  | 2.01                     | 0.43              |
| 3:1C:78:LEU:HA     | 3:1C:93:VAL:O      | 2.19                     | 0.43              |
| 5:1E:37:ASN:OD1    | 44:1s:62:ARG:NH2   | 2.52                     | 0.43              |
| 6:1F:422:PHE:HB3   | 6:1F:425:GLU:HB2   | 2.01                     | 0.43              |
| 7:1G:9:ILE:HG12    | 7:1G:22:PRO:HG3    | 2.00                     | 0.43              |
| 7:1G:108:CYS:SG    | 7:1G:206:GLY:HA3   | 2.58                     | 0.43              |
| 7:1G:110:GLN:HG3   | 7:1G:205:VAL:C     | 2.44                     | 0.43              |
| 7:1G:230:VAL:HG11  | 7:1G:566:TYR:CD1   | 2.54                     | 0.43              |
| 11:1K:42:ILE:O     | 11:1K:46:LEU:HD23  | 2.19                     | 0.43              |
| 12:1L:203:MET:HE2  | 41:1p:113:GLN:HG2  | 2.01                     | 0.43              |
| 12:1L:572:LYS:O    | 12:1L:575:ILE:HB   | 2.18                     | 0.43              |
| 13:1M:225:ILE:HD13 | 13:1M:331:ASN:HB2  | 1.99                     | 0.43              |
| 15:1O:58:TYR:OH    | 15:1O:110:ASP:OD2  | 2.33                     | 0.43              |
| 15:1O:144:ILE:HD12 | 15:1O:148:CYS:HB2  | 2.00                     | 0.43              |
| 20:1U:7:THR:O      | 20:1U:11:ILE:HD12  | 2.19                     | 0.43              |
| 20:1U:17:TYR:O     | 20:1U:21:LEU:HB2   | 2.19                     | 0.43              |
| 22:1W:90:LEU:HD23  | 22:1W:91:GLU:OE1   | 2.19                     | 0.43              |
| 25:1Z:143:TYR:HE2  | 26:1a:48:MET:SD    | 2.42                     | 0.43              |
| 31:1f:37:PHE:O     | 33:1h:88:GLU:HB3   | 2.19                     | 0.43              |
| 34:1i:112:THR:OG1  | 34:1i:114:GLU:HG3  | 2.18                     | 0.43              |
| 40:1o:90:GLU:O     | 40:1o:94:TYR:HB2   | 2.19                     | 0.43              |
| 3:1C:15:ASN:OD1    | 3:1C:15:ASN:C      | 2.61                     | 0.43              |
| 7:1G:37:ILE:HD12   | 7:1G:37:ILE:N      | 2.34                     | 0.43              |
| 7:1G:149:ILE:O     | 7:1G:149:ILE:HG22  | 2.18                     | 0.43              |
| 7:1G:194:GLU:CD    | 7:1G:385:ARG:HH21  | 2.24                     | 0.43              |
| 7:1G:467:LEU:HA    | 7:1G:467:LEU:HD12  | 1.89                     | 0.43              |
| 12:1L:47:SER:C     | 12:1L:50:PRO:HD2   | 2.43                     | 0.43              |
| 13:1M:243:MET:HB2  | 13:1M:301:ILE:HD12 | 2.01                     | 0.43              |
| 14:1N:3:PRO:HA     | 14:1N:6:TYR:HB3    | 2.01                     | 0.43              |
| 16:1P:219:LYS:HE3  | 16:1P:219:LYS:HB3  | 1.77                     | 0.43              |
| 29:1d:16:ASN:HA    | 29:1d:19:ARG:HH21  | 1.84                     | 0.43              |
| 35:1j:29:SER:O     | 35:1j:32:MET:HG3   | 2.19                     | 0.43              |
| 38:1m:5:TYR:CE2    | 38:1m:14:PRO:HD3   | 2.54                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 41:1p:59:ARG:HD3  | 41:1p:59:ARG:HA    | 1.69                     | 0.43              |
| 1:1A:68:GLU:HA    | 1:1A:71:LEU:HD23   | 2.00                     | 0.43              |
| 2:1B:50:PHE:N     | 2:1B:87:ILE:O      | 2.33                     | 0.43              |
| 2:1B:92:LEU:HD21  | 2:1B:100:LEU:HD23  | 2.01                     | 0.43              |
| 2:1B:118:SER:N    | 46:1B:201:SF4:S1   | 2.91                     | 0.43              |
| 3:1C:27:GLN:HA    | 3:1C:30:ALA:HB3    | 2.01                     | 0.43              |
| 4:1D:101:PRO:HB3  | 4:1D:105:ARG:NH2   | 2.34                     | 0.43              |
| 5:1E:131:THR:OG1  | 5:1E:138:THR:HG22  | 2.19                     | 0.43              |
| 5:1E:195:PRO:HB3  | 6:1F:264:HIS:HB3   | 2.00                     | 0.43              |
| 7:1G:105:CYS:HB2  | 7:1G:106:PRO:HD3   | 2.00                     | 0.43              |
| 7:1G:147:LYS:HA   | 7:1G:147:LYS:HD3   | 1.78                     | 0.43              |
| 7:1G:194:GLU:OE1  | 7:1G:385:ARG:NH2   | 2.39                     | 0.43              |
| 7:1G:584:LYS:HA   | 7:1G:584:LYS:HD2   | 1.57                     | 0.43              |
| 10:1J:68:PHE:CE1  | 11:1K:31:LEU:HG    | 2.54                     | 0.43              |
| 12:1L:49:VAL:HA   | 12:1L:52:LEU:HD23  | 2.01                     | 0.43              |
| 12:1L:141:PHE:HE2 | 13:1M:375:LEU:HD21 | 1.84                     | 0.43              |
| 12:1L:294:THR:O   | 12:1L:524:ASN:ND2  | 2.51                     | 0.43              |
| 12:1L:395:ILE:O   | 12:1L:399:VAL:HG13 | 2.19                     | 0.43              |
| 12:1L:496:MET:HE3 | 12:1L:500:LEU:HD23 | 2.01                     | 0.43              |
| 13:1M:86:LYS:H    | 13:1M:86:LYS:HG3   | 1.59                     | 0.43              |
| 13:1M:354:LEU:HB2 | 33:1h:18:ASP:OD2   | 2.19                     | 0.43              |
| 14:1N:170:LEU:O   | 14:1N:295:ARG:NH1  | 2.50                     | 0.43              |
| 15:1O:95:ARG:HG3  | 15:1O:282:ILE:HG22 | 2.01                     | 0.43              |
| 15:1O:223:TYR:OH  | 15:1O:237:ASP:OD1  | 2.28                     | 0.43              |
| 16:1P:73:TRP:HZ2  | 56:1P:501:NDP:H2A  | 1.84                     | 0.43              |
| 16:1P:149:LYS:O   | 16:1P:153:GLU:N    | 2.48                     | 0.43              |
| 16:1P:226:LYS:HG3 | 16:1P:227:THR:H    | 1.84                     | 0.43              |
| 21:1V:43:TYR:O    | 21:1V:47:THR:HG23  | 2.18                     | 0.43              |
| 22:1W:90:LEU:C    | 22:1W:94:ILE:HD12  | 2.44                     | 0.43              |
| 37:1l:30:ARG:HH22 | 38:1m:35:ARG:N     | 2.17                     | 0.43              |
| 40:1o:7:ARG:HG2   | 40:1o:8:TYR:CD1    | 2.54                     | 0.43              |
| 40:1o:57:TYR:HB2  | 40:1o:93:ASP:OD2   | 2.19                     | 0.43              |
| 41:1p:159:LYS:O   | 41:1p:163:LEU:HD23 | 2.18                     | 0.43              |
| 42:1q:86:TRP:CD1  | 42:1q:98:PRO:HG2   | 2.54                     | 0.43              |
| 43:1r:32:LYS:HA   | 43:1r:32:LYS:HD3   | 1.88                     | 0.43              |
| 3:1C:66:ASP:N     | 3:1C:66:ASP:OD1    | 2.52                     | 0.42              |
| 3:1C:94:TYR:HB2   | 3:1C:107:VAL:CG2   | 2.47                     | 0.42              |
| 3:1C:116:PRO:HB3  | 3:1C:141:PHE:CD2   | 2.54                     | 0.42              |
| 4:1D:6:PRO:HB3    | 4:1D:10:TRP:CD1    | 2.53                     | 0.42              |
| 4:1D:165:THR:OG1  | 8:1H:276:SER:HA    | 2.19                     | 0.42              |
| 4:1D:373:GLU:C    | 4:1D:394:PRO:HG3   | 2.44                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:25:THR:HG22   | 7:1G:28:GLN:HB2    | 2.01                     | 0.42              |
| 7:1G:47:SER:OG     | 7:1G:48:VAL:N      | 2.52                     | 0.42              |
| 7:1G:302:ARG:HG3   | 7:1G:542:PHE:HE2   | 1.84                     | 0.42              |
| 7:1G:426:PRO:HB3   | 7:1G:466:ILE:HD11  | 2.00                     | 0.42              |
| 7:1G:432:ILE:HG13  | 7:1G:440:SER:OG    | 2.19                     | 0.42              |
| 10:1J:20:PHE:CE1   | 10:1J:33:LEU:HD23  | 2.54                     | 0.42              |
| 12:1L:60:GLU:CD    | 12:1L:83:ASP:HA    | 2.44                     | 0.42              |
| 45:1L:702:3PE:H231 | 37:1l:88:ARG:HA    | 2.00                     | 0.42              |
| 13:1M:45:LEU:HD12  | 33:1h:86:ASN:HD22  | 1.84                     | 0.42              |
| 13:1M:75:LEU:HD13  | 13:1M:440:HIS:NE2  | 2.33                     | 0.42              |
| 15:1O:51:PHE:HB3   | 15:1O:107:GLN:HE21 | 1.84                     | 0.42              |
| 16:1P:299:GLY:N    | 16:1P:302:ASP:OD1  | 2.50                     | 0.42              |
| 21:1V:22:ARG:HA    | 21:1V:22:ARG:HD2   | 1.86                     | 0.42              |
| 24:1Y:114:CYS:O    | 24:1Y:116:TYR:N    | 2.52                     | 0.42              |
| 34:1i:121:GLU:OE1  | 34:1i:121:GLU:N    | 2.52                     | 0.42              |
| 38:1m:91:LEU:O     | 38:1m:96:PRO:HD3   | 2.19                     | 0.42              |
| 41:1p:77:GLU:HG3   | 41:1p:80:ASP:HB2   | 2.00                     | 0.42              |
| 42:1q:14:VAL:HA    | 42:1q:23:TYR:HD1   | 1.84                     | 0.42              |
| 2:1B:116:MET:SD    | 2:1B:156:LEU:HD22  | 2.59                     | 0.42              |
| 2:1B:125:TYR:HB2   | 9:1I:117:ILE:HG23  | 2.02                     | 0.42              |
| 3:1C:96:LEU:HB2    | 3:1C:105:ILE:HD12  | 2.00                     | 0.42              |
| 6:1F:22:PHE:CE2    | 6:1F:255:LEU:HD11  | 2.54                     | 0.42              |
| 7:1G:61:LYS:HD2    | 7:1G:61:LYS:O      | 2.18                     | 0.42              |
| 7:1G:159:CYS:CB    | 7:1G:199:ILE:HD11  | 2.49                     | 0.42              |
| 7:1G:278:ARG:HD3   | 7:1G:549:HIS:CE1   | 2.54                     | 0.42              |
| 7:1G:283:MET:HE3   | 7:1G:291:LEU:C     | 2.44                     | 0.42              |
| 7:1G:408:LEU:O     | 7:1G:421:HIS:HA    | 2.19                     | 0.42              |
| 7:1G:524:LEU:O     | 7:1G:545:TYR:HA    | 2.18                     | 0.42              |
| 7:1G:675:ASP:OD2   | 7:1G:676:SER:N     | 2.52                     | 0.42              |
| 8:1H:151:LEU:O     | 8:1H:155:LEU:HB2   | 2.19                     | 0.42              |
| 8:1H:299:ALA:HB1   | 27:1b:24:ILE:HB    | 2.01                     | 0.42              |
| 9:1I:8:ARG:NH2     | 43:1r:112:LEU:O    | 2.53                     | 0.42              |
| 11:1K:48:ILE:HG23  | 11:1K:53:PHE:HB3   | 2.01                     | 0.42              |
| 12:1L:5:ALA:HB2    | 12:1L:61:MET:SD    | 2.59                     | 0.42              |
| 12:1L:71:LEU:HD22  | 13:1M:307:TRP:CH2  | 2.54                     | 0.42              |
| 13:1M:14:MET:HB2   | 31:1f:15:LEU:HD13  | 2.02                     | 0.42              |
| 14:1N:25:HIS:O     | 14:1N:29:ILE:HG12  | 2.19                     | 0.42              |
| 16:1P:93:ASN:HB3   | 16:1P:131:HIS:HA   | 2.01                     | 0.42              |
| 20:1U:22:TYR:HE1   | 36:1k:43:PRO:HB2   | 1.84                     | 0.42              |
| 22:1W:69:LYS:HB2   | 22:1W:69:LYS:HE2   | 1.73                     | 0.42              |
| 25:1Z:68:ARG:HB2   | 26:1a:43:TYR:HE2   | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:1q:2:GLU:HA     | 42:1q:5:GLN:NE2    | 2.33                     | 0.42              |
| 4:1D:204:PRO:HA    | 9:1I:175:TYR:CE2   | 2.54                     | 0.42              |
| 6:1F:111:ILE:HD13  | 6:1F:138:ILE:HD13  | 2.02                     | 0.42              |
| 7:1G:211:LYS:O     | 7:1G:214:ALA:HB2   | 2.18                     | 0.42              |
| 7:1G:215:PHE:CD2   | 9:1I:104:ARG:HD3   | 2.54                     | 0.42              |
| 7:1G:230:VAL:HG23  | 7:1G:573:TYR:CE2   | 2.54                     | 0.42              |
| 8:1H:1:FME:HA      | 8:1H:4:ILE:HD11    | 1.91                     | 0.42              |
| 8:1H:196:ALA:N     | 8:1H:199:ASP:HB3   | 2.33                     | 0.42              |
| 8:1H:222:MET:O     | 8:1H:226:ALA:N     | 2.43                     | 0.42              |
| 10:1J:83:TRP:HB3   | 10:1J:90:PHE:HE1   | 1.84                     | 0.42              |
| 13:1M:181:TYR:HB3  | 41:1p:84:MET:HE3   | 2.01                     | 0.42              |
| 13:1M:203:PHE:CE1  | 13:1M:242:GLY:HA3  | 2.54                     | 0.42              |
| 13:1M:329:LEU:HD23 | 13:1M:359:TRP:CD2  | 2.54                     | 0.42              |
| 14:1N:125:GLN:HG3  | 14:1N:220:ILE:HD13 | 2.00                     | 0.42              |
| 19:1S:68:TYR:HD1   | 19:1S:72:GLN:HE22  | 1.67                     | 0.42              |
| 20:1U:28:GLU:OE2   | 20:1U:29:LYS:NZ    | 2.26                     | 0.42              |
| 21:1V:88:SER:O     | 21:1V:92:LYS:HG2   | 2.20                     | 0.42              |
| 21:1V:92:LYS:HB3   | 21:1V:96:TRP:CZ2   | 2.54                     | 0.42              |
| 23:1X:125:SER:HA   | 27:1b:53:PRO:HG3   | 2.01                     | 0.42              |
| 25:1Z:98:MET:HG3   | 25:1Z:101:VAL:HG21 | 2.00                     | 0.42              |
| 38:1m:109:ASP:O    | 38:1m:112:GLU:HG3  | 2.20                     | 0.42              |
| 4:1D:208:LEU:HA    | 4:1D:211:ILE:HD12  | 2.01                     | 0.42              |
| 5:1E:55:GLN:NE2    | 5:1E:59:GLY:O      | 2.52                     | 0.42              |
| 6:1F:150:GLN:HE21  | 6:1F:177:VAL:HG11  | 1.85                     | 0.42              |
| 8:1H:240:ILE:HD13  | 8:1H:240:ILE:HA    | 1.92                     | 0.42              |
| 12:1L:48:LEU:O     | 12:1L:51:LEU:HB2   | 2.19                     | 0.42              |
| 12:1L:79:SER:HB2   | 12:1L:135:ASN:HB3  | 2.00                     | 0.42              |
| 12:1L:202:PHE:CE1  | 12:1L:265:PRO:HG2  | 2.55                     | 0.42              |
| 12:1L:587:TYR:OH   | 14:1N:117:GLU:OE2  | 2.35                     | 0.42              |
| 13:1M:458:LEU:HD23 | 13:1M:458:LEU:HA   | 1.90                     | 0.42              |
| 20:1T:60:PHE:HE1   | 20:1T:62:ILE:HG22  | 1.84                     | 0.42              |
| 22:1W:46:THR:O     | 22:1W:50:PHE:HB2   | 2.20                     | 0.42              |
| 26:1a:2:TRP:CD1    | 26:1a:2:TRP:H      | 2.36                     | 0.42              |
| 34:1i:72:THR:HG23  | 34:1i:73:HIS:ND1   | 2.34                     | 0.42              |
| 37:1l:130:PRO:HD3  | 40:1o:21:MET:HE1   | 2.02                     | 0.42              |
| 2:1B:150:PRO:HG3   | 4:1D:189:MET:HE2   | 2.02                     | 0.42              |
| 4:1D:217:ASN:O     | 4:1D:221:ARG:HG2   | 2.19                     | 0.42              |
| 6:1F:37:GLN:HA     | 6:1F:41:ASP:O      | 2.20                     | 0.42              |
| 7:1G:231:MET:HG2   | 7:1G:266:LYS:HD2   | 2.01                     | 0.42              |
| 7:1G:260:GLU:OE2   | 7:1G:394:ARG:NH1   | 2.53                     | 0.42              |
| 7:1G:275:LYS:HA    | 42:1q:134:ILE:HA   | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:95:GLU:HG3    | 9:1I:108:ARG:HB3   | 2.01                     | 0.42              |
| 9:1I:96:ALA:HB2    | 9:1I:106:THR:HA    | 2.01                     | 0.42              |
| 12:1L:76:LEU:HD11  | 12:1L:196:TRP:HZ3  | 1.84                     | 0.42              |
| 12:1L:190:LEU:HD21 | 13:1M:307:TRP:CH2  | 2.55                     | 0.42              |
| 12:1L:288:THR:HG21 | 12:1L:307:SER:OG   | 2.18                     | 0.42              |
| 12:1L:338:MET:HE1  | 12:1L:461:SER:OG   | 2.19                     | 0.42              |
| 12:1L:350:LEU:O    | 12:1L:350:LEU:HD23 | 2.20                     | 0.42              |
| 16:1P:76:LYS:HD3   | 16:1P:76:LYS:HA    | 1.72                     | 0.42              |
| 16:1P:249:ALA:HB1  | 16:1P:251:ARG:HG2  | 2.00                     | 0.42              |
| 19:1S:87:THR:O     | 19:1S:91:GLU:HG2   | 2.20                     | 0.42              |
| 22:1W:91:GLU:HA    | 22:1W:94:ILE:HD12  | 2.02                     | 0.42              |
| 26:1a:28:LYS:HE3   | 26:1a:28:LYS:HB3   | 1.61                     | 0.42              |
| 32:1g:96:LEU:HD11  | 32:1g:100:ARG:NH2  | 2.35                     | 0.42              |
| 37:1l:46:ASP:OD1   | 37:1l:46:ASP:N     | 2.44                     | 0.42              |
| 37:1l:82:ASP:HB2   | 37:1l:88:ARG:NH1   | 2.34                     | 0.42              |
| 37:1l:139:TYR:CD2  | 37:1l:150:PRO:HG3  | 2.55                     | 0.42              |
| 38:1m:112:GLU:OE2  | 38:1m:113:LYS:NZ   | 2.43                     | 0.42              |
| 39:1n:128:ARG:HD2  | 39:1n:167:TRP:CD2  | 2.54                     | 0.42              |
| 40:1o:74:PRO:HG3   | 41:1p:28:PRO:HD3   | 2.01                     | 0.42              |
| 42:1q:1:MET:O      | 42:1q:4:VAL:HG12   | 2.20                     | 0.42              |
| 43:1r:1:ALA:HB1    | 43:1r:23:LEU:HD22  | 2.02                     | 0.42              |
| 2:1B:51:GLY:HA2    | 2:1B:89:ALA:O      | 2.19                     | 0.42              |
| 4:1D:83:LEU:HD12   | 4:1D:83:LEU:HA     | 1.90                     | 0.42              |
| 5:1E:124:LEU:H     | 5:1E:124:LEU:HG    | 1.72                     | 0.42              |
| 7:1G:187:ILE:HD11  | 7:1G:189:LYS:HB2   | 2.01                     | 0.42              |
| 7:1G:384:PRO:HD2   | 7:1G:415:LEU:HD11  | 2.00                     | 0.42              |
| 7:1G:421:HIS:ND1   | 7:1G:421:HIS:O     | 2.53                     | 0.42              |
| 7:1G:675:ASP:CG    | 7:1G:676:SER:N     | 2.78                     | 0.42              |
| 10:1J:106:TYR:HA   | 10:1J:109:LYS:HG2  | 2.00                     | 0.42              |
| 14:1N:319:HIS:CD2  | 14:1N:321:LYS:H    | 2.34                     | 0.42              |
| 16:1P:107:GLU:O    | 16:1P:111:VAL:HG22 | 2.19                     | 0.42              |
| 16:1P:143:SER:HB3  | 16:1P:146:LEU:HG   | 2.01                     | 0.42              |
| 16:1P:335:LYS:HD2  | 16:1P:335:LYS:O    | 2.18                     | 0.42              |
| 19:1S:23:CYS:HB3   | 19:1S:26:SER:HB3   | 2.01                     | 0.42              |
| 19:1S:41:VAL:HG22  | 19:1S:45:LYS:HZ1   | 1.84                     | 0.42              |
| 21:1V:6:LYS:HE2    | 21:1V:6:LYS:HB2    | 1.63                     | 0.42              |
| 22:1W:62:LYS:HE3   | 22:1W:62:LYS:HB3   | 1.90                     | 0.42              |
| 23:1X:34:GLN:HG3   | 23:1X:116:TRP:CD2  | 2.55                     | 0.42              |
| 29:1d:116:PHE:CE2  | 41:1p:157:LYS:HG3  | 2.54                     | 0.42              |
| 30:1e:37:LYS:HB3   | 30:1e:37:LYS:HE3   | 1.71                     | 0.42              |
| 34:1i:31:GLU:OE1   | 39:1n:115:PRO:HD2  | 2.19                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:1k:24:GLU:H     | 36:1k:24:GLU:CD    | 2.26                     | 0.42              |
| 39:1n:54:LYS:HA    | 39:1n:54:LYS:HD2   | 1.80                     | 0.42              |
| 4:1D:145:THR:OG1   | 4:1D:181:TYR:OH    | 2.25                     | 0.42              |
| 4:1D:162:GLY:HA3   | 8:1H:279:ARG:N     | 2.35                     | 0.42              |
| 4:1D:285:VAL:HA    | 4:1D:286:PRO:HD3   | 1.88                     | 0.42              |
| 6:1F:226:GLU:O     | 6:1F:230:VAL:HG13  | 2.20                     | 0.42              |
| 7:1G:142:ILE:C     | 7:1G:190:MET:HE1   | 2.44                     | 0.42              |
| 7:1G:161:ARG:HH11  | 7:1G:161:ARG:HG3   | 1.84                     | 0.42              |
| 10:1J:130:THR:HG21 | 25:1Z:124:LEU:HD12 | 2.01                     | 0.42              |
| 12:1L:8:THR:HG21   | 12:1L:82:MET:HG3   | 2.02                     | 0.42              |
| 12:1L:279:CYS:HA   | 37:1l:116:PHE:CE2  | 2.55                     | 0.42              |
| 12:1L:355:ASP:OD1  | 12:1L:357:ARG:NE   | 2.44                     | 0.42              |
| 13:1M:293:HIS:NE2  | 13:1M:366:ASN:OD1  | 2.52                     | 0.42              |
| 13:1M:373:ILE:HG21 | 13:1M:454:ILE:HD11 | 2.02                     | 0.42              |
| 52:1M:501:PGT:H352 | 52:1M:501:PGT:H321 | 1.77                     | 0.42              |
| 14:1N:88:LYS:HE3   | 14:1N:88:LYS:HB3   | 1.75                     | 0.42              |
| 15:1O:73:LEU:HD21  | 15:1O:295:LYS:HD3  | 2.02                     | 0.42              |
| 19:1S:82:SER:HB3   | 19:1S:85:GLN:HB3   | 2.01                     | 0.42              |
| 20:1T:78:ASP:OD1   | 20:1T:79:TYR:N     | 2.52                     | 0.42              |
| 20:1U:32:VAL:O     | 20:1U:74:GLN:N     | 2.53                     | 0.42              |
| 22:1W:65:GLU:OE1   | 22:1W:66:MET:N     | 2.53                     | 0.42              |
| 32:1g:66:PHE:O     | 32:1g:70:LEU:HB3   | 2.20                     | 0.42              |
| 34:1i:93:PRO:HG3   | 41:1p:9:TYR:CE2    | 2.55                     | 0.42              |
| 34:1i:125:GLN:HB2  | 40:1o:61:TYR:OH    | 2.20                     | 0.42              |
| 35:1j:60:THR:O     | 35:1j:64:LEU:HD23  | 2.20                     | 0.42              |
| 37:1l:97:SER:HA    | 38:1m:5:TYR:CD1    | 2.54                     | 0.42              |
| 38:1m:84:LYS:HA    | 38:1m:84:LYS:HD3   | 1.68                     | 0.42              |
| 39:1n:47:PHE:HA    | 39:1n:50:HIS:CE1   | 2.54                     | 0.42              |
| 42:1q:52:ASN:OD1   | 42:1q:52:ASN:C     | 2.62                     | 0.42              |
| 42:1q:106:ARG:HB2  | 42:1q:109:ILE:HG13 | 2.01                     | 0.42              |
| 3:1C:84:PRO:HB2    | 17:1Q:86:PHE:HE1   | 1.84                     | 0.42              |
| 4:1D:161:ILE:HG21  | 4:1D:235:TRP:CE3   | 2.55                     | 0.42              |
| 4:1D:290:ARG:H     | 4:1D:290:ARG:HG3   | 1.70                     | 0.42              |
| 5:1E:102:VAL:HA    | 5:1E:154:VAL:HG23  | 2.00                     | 0.42              |
| 6:1F:247:ARG:NH1   | 6:1F:316:LEU:HD23  | 2.35                     | 0.42              |
| 8:1H:314:ILE:HD11  | 27:1b:44:ILE:HD11  | 2.02                     | 0.42              |
| 10:1J:17:PHE:CD1   | 10:1J:20:PHE:HE2   | 2.37                     | 0.42              |
| 11:1K:27:MET:N     | 11:1K:88:ASP:OD2   | 2.52                     | 0.42              |
| 12:1L:90:ILE:HB    | 12:1L:91:PRO:HD3   | 2.02                     | 0.42              |
| 12:1L:226:GLN:OE1  | 12:1L:284:THR:HG21 | 2.20                     | 0.42              |
| 13:1M:42:LEU:HD12  | 13:1M:453:MET:HB3  | 2.01                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 15:1O:87:LYS:HZ1  | 15:1O:141:GLN:C    | 2.28                     | 0.42              |
| 16:1P:340:VAL:O   | 16:1P:340:VAL:HG22 | 2.19                     | 0.42              |
| 20:1T:58:PHE:O    | 20:1T:60:PHE:N     | 2.47                     | 0.42              |
| 22:1W:102:HIS:HA  | 22:1W:105:ARG:NH1  | 2.35                     | 0.42              |
| 29:1d:58:LEU:HD23 | 29:1d:58:LEU:HA    | 1.81                     | 0.42              |
| 31:1f:44:PHE:CD2  | 33:1h:84:GLU:HB3   | 2.55                     | 0.42              |
| 35:1j:18:THR:O    | 35:1j:22:LEU:HD12  | 2.19                     | 0.42              |
| 39:1n:34:ASP:N    | 39:1n:34:ASP:OD1   | 2.52                     | 0.42              |
| 39:1n:65:GLN:O    | 39:1n:68:GLU:HG3   | 2.19                     | 0.42              |
| 39:1n:176:ARG:HE  | 39:1n:176:ARG:HB2  | 1.61                     | 0.42              |
| 40:1o:57:TYR:CD1  | 40:1o:57:TYR:N     | 2.87                     | 0.42              |
| 2:1B:175:ILE:HD13 | 2:1B:175:ILE:HA    | 1.85                     | 0.42              |
| 3:1C:41:GLN:NE2   | 43:1r:65:PRO:HB2   | 2.35                     | 0.42              |
| 3:1C:155:TYR:O    | 22:1W:102:HIS:ND1  | 2.53                     | 0.42              |
| 7:1G:315:VAL:CG1  | 7:1G:340:SER:HB2   | 2.50                     | 0.42              |
| 7:1G:432:ILE:HD11 | 7:1G:437:HIS:CD2   | 2.53                     | 0.42              |
| 7:1G:601:ARG:NH1  | 7:1G:605:GLU:HB2   | 2.35                     | 0.42              |
| 8:1H:88:PRO:HG3   | 8:1H:104:PHE:CD2   | 2.54                     | 0.42              |
| 9:1I:148:LEU:HB3  | 17:1Q:70:MET:HE1   | 2.02                     | 0.42              |
| 12:1L:101:MET:HG3 | 12:1L:118:PHE:HE2  | 1.85                     | 0.42              |
| 12:1L:533:MET:O   | 45:1L:702:3PE:H362 | 2.20                     | 0.42              |
| 14:1N:347:ASN:HB3 | 29:1d:2:MET:HG3    | 2.01                     | 0.42              |
| 16:1P:66:GLY:HA3  | 17:1Q:69:LEU:HD22  | 2.01                     | 0.42              |
| 18:1R:87:CYS:SG   | 18:1R:89:LEU:HG    | 2.60                     | 0.42              |
| 19:1S:44:LYS:O    | 19:1S:44:LYS:HD3   | 2.20                     | 0.42              |
| 20:1T:36:PHE:HB2  | 20:1T:37:MET:CE    | 2.46                     | 0.42              |
| 22:1W:29:LYS:HD3  | 22:1W:29:LYS:HA    | 1.82                     | 0.42              |
| 23:1X:64:GLN:O    | 23:1X:67:LEU:HB3   | 2.20                     | 0.42              |
| 30:1e:78:ILE:O    | 30:1e:82:ARG:HB2   | 2.20                     | 0.42              |
| 32:1g:112:CYS:N   | 41:1p:158:GLN:OE1  | 2.49                     | 0.42              |
| 33:1h:45:VAL:O    | 33:1h:46:PHE:HD1   | 2.02                     | 0.42              |
| 39:1n:100:GLU:OE2 | 39:1n:167:TRP:NE1  | 2.51                     | 0.42              |
| 2:1B:87:ILE:HD13  | 2:1B:114:VAL:HB    | 2.01                     | 0.42              |
| 3:1C:176:TYR:OH   | 3:1C:181:LYS:HE3   | 2.20                     | 0.42              |
| 4:1D:225:LEU:O    | 4:1D:229:LEU:HB2   | 2.20                     | 0.42              |
| 5:1E:190:ARG:NH2  | 6:1F:265:PRO:O     | 2.53                     | 0.42              |
| 6:1F:188:GLU:OE1  | 6:1F:190:THR:N     | 2.53                     | 0.42              |
| 7:1G:197:GLY:H    | 7:1G:265:ASP:CG    | 2.25                     | 0.42              |
| 7:1G:568:GLU:OE2  | 7:1G:590:PRO:HD3   | 2.20                     | 0.42              |
| 11:1K:43:MET:HE3  | 14:1N:72:MET:SD    | 2.59                     | 0.42              |
| 12:1L:230:HIS:O   | 12:1L:232:TRP:N    | 2.52                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:1L:366:MET:HB3  | 12:1L:369:THR:HB   | 2.01                     | 0.42              |
| 12:1L:522:PHE:HA   | 12:1L:528:TYR:CE1  | 2.55                     | 0.42              |
| 16:1P:222:ASP:OD1  | 16:1P:222:ASP:N    | 2.53                     | 0.42              |
| 20:1T:75:GLU:HA    | 20:1T:78:ASP:OD2   | 2.20                     | 0.42              |
| 23:1X:57:GLU:HA    | 23:1X:60:LYS:HE3   | 2.02                     | 0.42              |
| 25:1Z:22:LYS:HA    | 25:1Z:22:LYS:HD3   | 1.90                     | 0.42              |
| 25:1Z:77:ALA:HB1   | 25:1Z:81:ARG:NH2   | 2.35                     | 0.42              |
| 26:1a:48:MET:HE3   | 26:1a:60:TYR:CG    | 2.55                     | 0.42              |
| 33:1h:48:GLY:HA2   | 41:1p:55:HIS:NE2   | 2.34                     | 0.42              |
| 40:1o:46:ASN:ND2   | 40:1o:55:ARG:HH12  | 2.18                     | 0.42              |
| 4:1D:76:CYS:SG     | 4:1D:406:SER:HB3   | 2.60                     | 0.41              |
| 5:1E:36:LYS:HE3    | 44:1s:59:SER:HA    | 2.01                     | 0.41              |
| 5:1E:165:THR:H     | 5:1E:168:ASP:CG    | 2.26                     | 0.41              |
| 6:1F:261:HIS:HE1   | 6:1F:341:THR:HB    | 1.83                     | 0.41              |
| 6:1F:305:PRO:HG2   | 6:1F:327:THR:HA    | 2.02                     | 0.41              |
| 6:1F:389:ILE:HG23  | 6:1F:419:ILE:HG12  | 2.01                     | 0.41              |
| 7:1G:143:GLY:N     | 7:1G:190:MET:HE1   | 2.35                     | 0.41              |
| 8:1H:203:GLY:O     | 8:1H:207:LEU:N     | 2.52                     | 0.41              |
| 8:1H:314:ILE:HD12  | 25:1Z:58:ARG:HD3   | 2.02                     | 0.41              |
| 12:1L:315:VAL:HG11 | 12:1L:412:THR:HG21 | 2.00                     | 0.41              |
| 12:1L:486:MET:C    | 12:1L:489:THR:HG1  | 2.24                     | 0.41              |
| 15:1O:96:LEU:O     | 15:1O:100:LEU:HB2  | 2.20                     | 0.41              |
| 16:1P:2:HIS:HE1    | 18:1R:22:ASP:OD1   | 2.03                     | 0.41              |
| 18:1R:28:PHE:N     | 18:1R:28:PHE:HD1   | 2.18                     | 0.41              |
| 19:1S:82:SER:OG    | 19:1S:84:ASP:OD1   | 2.35                     | 0.41              |
| 22:1W:112:ALA:O    | 22:1W:114:ARG:NH2  | 2.53                     | 0.41              |
| 25:1Z:103:ASP:OD1  | 25:1Z:103:ASP:N    | 2.52                     | 0.41              |
| 31:1f:46:ARG:HD2   | 31:1f:47:GLU:O     | 2.20                     | 0.41              |
| 32:1g:40:LYS:HA    | 32:1g:40:LYS:HD2   | 1.61                     | 0.41              |
| 34:1i:65:ARG:HG2   | 34:1i:65:ARG:NH1   | 2.33                     | 0.41              |
| 42:1q:9:ARG:O      | 42:1q:13:GLN:HG2   | 2.19                     | 0.41              |
| 1:1A:7:LEU:HD23    | 1:1A:7:LEU:HA      | 1.89                     | 0.41              |
| 2:1B:40:ALA:HB1    | 8:1H:54:LYS:HB2    | 2.03                     | 0.41              |
| 4:1D:68:LEU:HD12   | 4:1D:70:GLY:H      | 1.84                     | 0.41              |
| 4:1D:347:HIS:CD2   | 7:1G:126:ASP:HA    | 2.54                     | 0.41              |
| 5:1E:52:ASP:O      | 5:1E:56:ARG:N      | 2.53                     | 0.41              |
| 7:1G:147:LYS:HD2   | 7:1G:702:SER:O     | 2.20                     | 0.41              |
| 7:1G:426:PRO:HD3   | 7:1G:661:LEU:HD11  | 2.01                     | 0.41              |
| 7:1G:430:GLN:O     | 7:1G:434:SER:OG    | 2.38                     | 0.41              |
| 7:1G:594:ARG:NH2   | 22:1W:125:GLY:HA2  | 2.35                     | 0.41              |
| 7:1G:594:ARG:CD    | 22:1W:126:HIS:HB3  | 2.48                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:1G:667:THR:HB    | 7:1G:669:LYS:HG2   | 2.02                     | 0.41              |
| 9:1I:42:PHE:HB3    | 43:1r:7:ILE:HD11   | 2.03                     | 0.41              |
| 10:1J:152:TRP:HZ3  | 50:1J:201:PC1:H272 | 1.85                     | 0.41              |
| 12:1L:542:LEU:HD23 | 12:1L:542:LEU:HA   | 1.82                     | 0.41              |
| 13:1M:60:SER:OG    | 32:1g:83:TYR:OH    | 2.33                     | 0.41              |
| 13:1M:76:MET:HE2   | 13:1M:230:VAL:HG22 | 2.00                     | 0.41              |
| 13:1M:347:GLY:N    | 13:1M:414:THR:O    | 2.53                     | 0.41              |
| 13:1M:450:ASN:HB2  | 50:1M:502:PC1:H221 | 2.02                     | 0.41              |
| 14:1N:2:ASN:OD1    | 14:1N:4:ILE:HG22   | 2.19                     | 0.41              |
| 14:1N:86:ILE:HG23  | 14:1N:86:ILE:O     | 2.21                     | 0.41              |
| 15:1O:25:ILE:HD12  | 15:1O:238:ILE:HD11 | 2.02                     | 0.41              |
| 15:1O:304:TYR:CE2  | 29:1d:52:PRO:HG3   | 2.54                     | 0.41              |
| 16:1P:198:LYS:C    | 16:1P:237:LEU:HD11 | 2.45                     | 0.41              |
| 17:1Q:30:ILE:HD12  | 17:1Q:101:TRP:NE1  | 2.35                     | 0.41              |
| 20:1T:19:LEU:HD12  | 20:1T:19:LEU:HA    | 1.83                     | 0.41              |
| 20:1T:58:PHE:HD2   | 20:1T:58:PHE:HA    | 1.73                     | 0.41              |
| 22:1W:63:VAL:O     | 22:1W:67:PHE:HD2   | 2.03                     | 0.41              |
| 24:1Y:99:THR:O     | 24:1Y:103:ARG:HG2  | 2.20                     | 0.41              |
| 38:1m:50:TYR:O     | 39:1n:168:HIS:HE1  | 2.03                     | 0.41              |
| 39:1n:9:LEU:HD23   | 39:1n:9:LEU:HA     | 1.74                     | 0.41              |
| 1:1A:106:TRP:CD2   | 45:1A:201:3PE:H231 | 2.56                     | 0.41              |
| 2:1B:48:MET:HE3    | 2:1B:80:PRO:CA     | 2.50                     | 0.41              |
| 3:1C:12:ARG:NH2    | 4:1D:124:LYS:HG3   | 2.35                     | 0.41              |
| 3:1C:151:ILE:C     | 3:1C:151:ILE:HD12  | 2.45                     | 0.41              |
| 4:1D:120:LEU:HD23  | 4:1D:120:LEU:HA    | 1.87                     | 0.41              |
| 4:1D:149:ASN:ND2   | 4:1D:371:LYS:HG2   | 2.35                     | 0.41              |
| 4:1D:217:ASN:ND2   | 43:1r:23:LEU:O     | 2.51                     | 0.41              |
| 4:1D:233:ARG:HH12  | 50:1H:401:PC1:H31  | 1.85                     | 0.41              |
| 6:1F:82:MET:SD     | 6:1F:129:MET:SD    | 3.19                     | 0.41              |
| 6:1F:277:LYS:HD2   | 6:1F:277:LYS:HA    | 1.89                     | 0.41              |
| 6:1F:406:ALA:HB3   | 48:1F:501:FMN:HM82 | 2.03                     | 0.41              |
| 7:1G:566:TYR:HA    | 7:1G:569:LYS:HZ2   | 1.84                     | 0.41              |
| 7:1G:646:ASN:HB3   | 7:1G:650:LYS:HE2   | 2.02                     | 0.41              |
| 8:1H:253:GLU:O     | 8:1H:256:THR:OG1   | 2.29                     | 0.41              |
| 12:1L:103:PHE:CE2  | 12:1L:242:PRO:HG3  | 2.55                     | 0.41              |
| 12:1L:183:VAL:HG12 | 13:1M:382:ILE:HG21 | 2.02                     | 0.41              |
| 12:1L:407:TRP:CE2  | 37:1l:115:MET:HE2  | 2.55                     | 0.41              |
| 12:1L:504:LEU:HD23 | 45:1L:704:3PE:O22  | 2.19                     | 0.41              |
| 13:1M:78:MET:HE1   | 13:1M:439:LEU:HD23 | 2.02                     | 0.41              |
| 13:1M:399:ASN:O    | 13:1M:403:THR:OG1  | 2.33                     | 0.41              |
| 15:1O:28:ASP:OD2   | 15:1O:126:ARG:HA   | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:1P:10:LYS:HA    | 16:1P:10:LYS:HD3   | 1.83                     | 0.41              |
| 16:1P:283:LYS:O    | 16:1P:287:VAL:HG13 | 2.21                     | 0.41              |
| 23:1X:46:ARG:HB3   | 33:1h:141:PRO:HB3  | 2.01                     | 0.41              |
| 27:1b:77:LEU:HD12  | 27:1b:80:LEU:HD23  | 2.02                     | 0.41              |
| 38:1m:34:GLU:H     | 38:1m:34:GLU:HG2   | 1.68                     | 0.41              |
| 39:1n:25:HIS:CE1   | 39:1n:78:PRO:HB3   | 2.55                     | 0.41              |
| 1:1A:75:LEU:HA     | 1:1A:78:ALA:HB3    | 2.01                     | 0.41              |
| 2:1B:81:ARG:NH1    | 8:1H:61:LEU:O      | 2.54                     | 0.41              |
| 2:1B:94:ASN:OD1    | 2:1B:131:SER:HA    | 2.20                     | 0.41              |
| 3:1C:101:PHE:HE1   | 43:1r:99:PRO:HB3   | 1.86                     | 0.41              |
| 3:1C:151:ILE:HD12  | 3:1C:152:LEU:HG    | 2.02                     | 0.41              |
| 5:1E:106:THR:HA    | 5:1E:109:MET:HG3   | 2.02                     | 0.41              |
| 7:1G:107:ILE:HA    | 9:1I:104:ARG:NH2   | 2.31                     | 0.41              |
| 7:1G:613:TYR:CB    | 7:1G:618:GLN:HB3   | 2.51                     | 0.41              |
| 8:1H:141:SER:C     | 8:1H:289:LEU:HD21  | 2.45                     | 0.41              |
| 8:1H:252:PRO:O     | 8:1H:256:THR:HG23  | 2.20                     | 0.41              |
| 12:1L:384:PRO:O    | 35:1j:36:ILE:HD12  | 2.20                     | 0.41              |
| 12:1L:475:MET:O    | 40:1o:51:MET:HE1   | 2.21                     | 0.41              |
| 12:1L:535:ARG:NH1  | 37:1l:92:SER:O     | 2.43                     | 0.41              |
| 14:1N:41:ILE:N     | 14:1N:42:PRO:HD2   | 2.35                     | 0.41              |
| 17:1Q:125:ASN:OD1  | 17:1Q:125:ASN:N    | 2.50                     | 0.41              |
| 17:1Q:126:LYS:HD3  | 17:1Q:126:LYS:HA   | 1.67                     | 0.41              |
| 18:1R:34:GLU:OE1   | 42:1q:124:TYR:HA   | 2.20                     | 0.41              |
| 20:1U:54:MET:HE3   | 20:1U:76:ILE:HG21  | 2.03                     | 0.41              |
| 29:1d:11:LEU:HD11  | 30:1e:3:PHE:HB3    | 2.02                     | 0.41              |
| 30:1e:70:LYS:NZ    | 30:1e:74:ARG:HB2   | 2.35                     | 0.41              |
| 32:1g:66:PHE:CD1   | 33:1h:28:TYR:HE2   | 2.38                     | 0.41              |
| 37:1l:158:ILE:HD11 | 40:1o:99:LYS:C     | 2.45                     | 0.41              |
| 40:1o:60:HIS:HD1   | 40:1o:60:HIS:H     | 1.67                     | 0.41              |
| 42:1q:44:TYR:HE2   | 42:1q:83:PRO:HB3   | 1.85                     | 0.41              |
| 43:1r:8:GLN:O      | 43:1r:12:ASN:ND2   | 2.54                     | 0.41              |
| 4:1D:100:LEU:HD12  | 4:1D:118:TYR:CD2   | 2.55                     | 0.41              |
| 4:1D:112:MET:SD    | 4:1D:194:ILE:HG12  | 2.61                     | 0.41              |
| 4:1D:234:ILE:HA    | 4:1D:237:ASN:ND2   | 2.35                     | 0.41              |
| 7:1G:198:ASN:CG    | 7:1G:262:TRP:HB3   | 2.46                     | 0.41              |
| 7:1G:200:ILE:HD13  | 7:1G:210:SER:HB3   | 2.01                     | 0.41              |
| 7:1G:285:ARG:CG    | 7:1G:291:LEU:HA    | 2.50                     | 0.41              |
| 7:1G:344:CYS:HB2   | 7:1G:510:GLY:O     | 2.21                     | 0.41              |
| 7:1G:577:GLU:OE2   | 7:1G:577:GLU:HA    | 2.21                     | 0.41              |
| 7:1G:592:LEU:HD22  | 16:1P:6:ILE:HG23   | 2.02                     | 0.41              |
| 8:1H:74:ALA:HB3    | 8:1H:75:PRO:HD3    | 2.03                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:1I:31:VAL:O      | 9:1I:35:GLY:N      | 2.53                     | 0.41              |
| 9:1I:69:ARG:NH1    | 9:1I:155:LEU:HD12  | 2.36                     | 0.41              |
| 11:1K:55:LEU:HD12  | 11:1K:55:LEU:HA    | 1.77                     | 0.41              |
| 12:1L:487:LYS:NZ   | 35:1j:49:GLY:HA2   | 2.35                     | 0.41              |
| 13:1M:73:LEU:HA    | 13:1M:76:MET:SD    | 2.60                     | 0.41              |
| 14:1N:275:SER:HB2  | 24:1Y:136:ALA:HB3  | 2.03                     | 0.41              |
| 15:1O:14:THR:HG21  | 15:1O:116:LEU:HG   | 2.01                     | 0.41              |
| 16:1P:83:LYS:HE2   | 16:1P:83:LYS:HB3   | 1.82                     | 0.41              |
| 16:1P:133:SER:O    | 16:1P:167:LYS:HA   | 2.19                     | 0.41              |
| 16:1P:144:ARG:O    | 16:1P:148:SER:OG   | 2.38                     | 0.41              |
| 16:1P:157:ARG:NH2  | 16:1P:225:GLY:O    | 2.45                     | 0.41              |
| 17:1Q:23:THR:HG23  | 17:1Q:25:VAL:H     | 1.85                     | 0.41              |
| 19:1S:19:ARG:O     | 19:1S:65:TRP:N     | 2.39                     | 0.41              |
| 20:1T:8:LEU:O      | 20:1T:11:ILE:HB    | 2.20                     | 0.41              |
| 20:1U:78:ASP:HB3   | 34:1i:15:ARG:CZ    | 2.50                     | 0.41              |
| 21:1V:72:GLN:NE2   | 43:1r:99:PRO:HB2   | 2.36                     | 0.41              |
| 25:1Z:5:LYS:HE2    | 25:1Z:5:LYS:HA     | 2.01                     | 0.41              |
| 53:1a:101:CDL:H552 | 53:1a:101:CDL:H741 | 2.03                     | 0.41              |
| 37:1l:5:THR:HG23   | 37:1l:7:ASP:OD1    | 2.20                     | 0.41              |
| 37:1l:128:VAL:HG11 | 40:1o:94:TYR:OH    | 2.19                     | 0.41              |
| 2:1B:69:MET:HE1    | 2:1B:76:PHE:N      | 2.35                     | 0.41              |
| 4:1D:144:ILE:HD13  | 4:1D:144:ILE:HA    | 1.88                     | 0.41              |
| 5:1E:99:HIS:H      | 5:1E:157:ASN:HA    | 1.85                     | 0.41              |
| 5:1E:105:THR:OG1   | 5:1E:106:THR:N     | 2.54                     | 0.41              |
| 6:1F:298:ILE:HG13  | 6:1F:306:LEU:HD13  | 2.02                     | 0.41              |
| 6:1F:317:MET:HA    | 6:1F:322:LEU:HD21  | 2.02                     | 0.41              |
| 7:1G:478:ARG:HE    | 7:1G:483:VAL:HB    | 1.86                     | 0.41              |
| 7:1G:503:LEU:CD1   | 7:1G:509:PRO:HB3   | 2.48                     | 0.41              |
| 8:1H:149:ILE:HG23  | 8:1H:181:LEU:HD22  | 2.03                     | 0.41              |
| 8:1H:216:ALA:O     | 8:1H:220:PHE:HB3   | 2.21                     | 0.41              |
| 11:1K:57:ASN:O     | 11:1K:60:PRO:HD2   | 2.20                     | 0.41              |
| 12:1L:129:MET:O    | 12:1L:133:THR:OG1  | 2.35                     | 0.41              |
| 12:1L:548:SER:HA   | 12:1L:552:LEU:HB3  | 2.03                     | 0.41              |
| 45:1L:703:3PE:H2   | 45:1L:703:3PE:H221 | 1.50                     | 0.41              |
| 13:1M:204:MET:HE3  | 13:1M:204:MET:HB3  | 1.78                     | 0.41              |
| 14:1N:173:THR:O    | 14:1N:227:THR:OG1  | 2.38                     | 0.41              |
| 17:1Q:69:LEU:HD12  | 17:1Q:69:LEU:HA    | 1.71                     | 0.41              |
| 20:1T:52:MET:HE3   | 22:1W:40:TYR:HD2   | 1.85                     | 0.41              |
| 22:1W:75:ASP:O     | 22:1W:79:VAL:HG12  | 2.21                     | 0.41              |
| 25:1Z:98:MET:HG2   | 25:1Z:104:TRP:CE2  | 2.55                     | 0.41              |
| 29:1d:115:GLU:HG2  | 29:1d:115:GLU:O    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:1f:55:THR:O     | 31:1f:56:TRP:C     | 2.64                     | 0.41              |
| 33:1h:114:MET:HE1  | 33:1h:121:PRO:HD2  | 2.02                     | 0.41              |
| 35:1j:60:THR:HG1   | 35:1j:63:GLU:CD    | 2.27                     | 0.41              |
| 39:1n:40:ALA:O     | 39:1n:44:ARG:N     | 2.44                     | 0.41              |
| 40:1o:71:ASP:HB3   | 41:1p:22:GLN:HG3   | 2.03                     | 0.41              |
| 6:1F:32:ARG:HG3    | 6:1F:34:LYS:HG2    | 2.03                     | 0.41              |
| 6:1F:215:VAL:O     | 6:1F:218:CYS:HB2   | 2.21                     | 0.41              |
| 6:1F:247:ARG:N     | 6:1F:250:ASN:O     | 2.54                     | 0.41              |
| 7:1G:644:GLN:OE1   | 7:1G:644:GLN:N     | 2.52                     | 0.41              |
| 8:1H:142:TYR:CZ    | 8:1H:289:LEU:HB2   | 2.56                     | 0.41              |
| 8:1H:293:PHE:O     | 8:1H:297:THR:OG1   | 2.32                     | 0.41              |
| 9:1I:79:ALA:HB2    | 9:1I:106:THR:HG22  | 2.02                     | 0.41              |
| 12:1L:95:PHE:CE1   | 12:1L:456:ARG:HG2  | 2.56                     | 0.41              |
| 13:1M:1:FME:O      | 13:1M:5:ILE:HD12   | 2.20                     | 0.41              |
| 13:1M:16:TRP:CH2   | 45:1N:401:3PE:H241 | 2.55                     | 0.41              |
| 13:1M:442:LEU:HD11 | 32:1g:70:LEU:HD21  | 2.03                     | 0.41              |
| 14:1N:304:MET:HB2  | 14:1N:304:MET:HE2  | 1.82                     | 0.41              |
| 15:1O:58:TYR:O     | 15:1O:62:THR:HG23  | 2.21                     | 0.41              |
| 15:1O:169:VAL:HG11 | 15:1O:214:MET:HE1  | 2.02                     | 0.41              |
| 16:1P:30:LEU:HD21  | 16:1P:94:LEU:HB2   | 2.02                     | 0.41              |
| 16:1P:165:ILE:HG23 | 16:1P:227:THR:HG23 | 2.02                     | 0.41              |
| 17:1Q:35:VAL:HG21  | 17:1Q:101:TRP:HB3  | 2.02                     | 0.41              |
| 20:1T:83:LYS:NZ    | 20:1T:84:LYS:HB3   | 2.33                     | 0.41              |
| 20:1U:35:HIS:NE2   | 20:1U:38:LYS:HD3   | 2.35                     | 0.41              |
| 21:1V:80:ILE:H     | 21:1V:80:ILE:HG12  | 1.70                     | 0.41              |
| 23:1X:100:ARG:HA   | 23:1X:100:ARG:HD3  | 1.90                     | 0.41              |
| 23:1X:166:LEU:HG   | 23:1X:167:PHE:HD2  | 1.85                     | 0.41              |
| 25:1Z:87:LEU:HD23  | 25:1Z:87:LEU:HA    | 1.78                     | 0.41              |
| 27:1b:62:MET:N     | 27:1b:62:MET:SD    | 2.94                     | 0.41              |
| 28:1c:1:LYS:HD3    | 28:1c:3:TYR:HD2    | 1.86                     | 0.41              |
| 31:1f:48:LEU:HD21  | 31:1f:53:GLU:C     | 2.45                     | 0.41              |
| 50:1f:101:PC1:H3I1 | 33:1h:39:GLY:HA3   | 2.02                     | 0.41              |
| 33:1h:24:LEU:O     | 33:1h:28:TYR:HB3   | 2.21                     | 0.41              |
| 38:1m:119:LYS:HA   | 38:1m:119:LYS:HD2  | 1.89                     | 0.41              |
| 39:1n:107:HIS:CD2  | 39:1n:108:PRO:HD2  | 2.56                     | 0.41              |
| 41:1p:48:ARG:O     | 41:1p:52:GLU:HG2   | 2.21                     | 0.41              |
| 42:1q:72:ASP:OD2   | 42:1q:72:ASP:C     | 2.64                     | 0.41              |
| 2:1B:47:PRO:HA     | 2:1B:85:VAL:O      | 2.21                     | 0.41              |
| 2:1B:59:MET:HG3    | 2:1B:116:MET:HE1   | 2.03                     | 0.41              |
| 2:1B:113:VAL:HG11  | 2:1B:140:VAL:HG12  | 2.02                     | 0.41              |
| 3:1C:46:ASN:OD1    | 3:1C:46:ASN:N      | 2.54                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:86:PHE:HB2    | 6:1F:200:GLN:NE2   | 2.36                     | 0.41              |
| 6:1F:199:LYS:HD2   | 6:1F:200:GLN:H     | 1.85                     | 0.41              |
| 7:1G:14:ASP:OD1    | 7:1G:81:THR:N      | 2.48                     | 0.41              |
| 8:1H:127:TYR:OH    | 8:1H:208:VAL:HG23  | 2.21                     | 0.41              |
| 8:1H:197:PRO:HG2   | 8:1H:198:PHE:CD1   | 2.56                     | 0.41              |
| 12:1L:188:TRP:CD2  | 12:1L:212:PRO:HG3  | 2.55                     | 0.41              |
| 12:1L:500:LEU:HD12 | 12:1L:501:ALA:H    | 1.86                     | 0.41              |
| 45:1L:704:3PE:H222 | 45:1L:704:3PE:O31  | 2.21                     | 0.41              |
| 13:1M:210:TYR:HB2  | 13:1M:268:GLY:HA3  | 2.02                     | 0.41              |
| 13:1M:411:LEU:HA   | 13:1M:411:LEU:HD12 | 1.82                     | 0.41              |
| 16:1P:173:GLY:N    | 16:1P:176:ASP:HB3  | 2.36                     | 0.41              |
| 20:1T:14:ARG:O     | 20:1T:18:VAL:HG13  | 2.20                     | 0.41              |
| 20:1T:85:ASP:OD1   | 20:1T:85:ASP:N     | 2.54                     | 0.41              |
| 20:1U:51:ILE:HD13  | 20:1U:62:ILE:HD11  | 2.02                     | 0.41              |
| 21:1V:25:ILE:O     | 21:1V:29:LYS:HD2   | 2.20                     | 0.41              |
| 21:1V:76:ILE:N     | 21:1V:76:ILE:HD13  | 2.36                     | 0.41              |
| 24:1Y:119:LEU:O    | 24:1Y:123:LEU:N    | 2.46                     | 0.41              |
| 36:1k:35:LEU:HD11  | 36:1k:42:ASP:N     | 2.35                     | 0.41              |
| 39:1n:52:ASN:N     | 39:1n:52:ASN:OD1   | 2.54                     | 0.41              |
| 42:1q:32:ASP:OD2   | 42:1q:34:ARG:NH2   | 2.54                     | 0.41              |
| 1:1A:72:LEU:HD11   | 8:1H:148:ILE:HD12  | 2.03                     | 0.41              |
| 2:1B:54:CYS:O      | 4:1D:189:MET:HE1   | 2.21                     | 0.41              |
| 3:1C:51:PHE:HB3    | 21:1V:111:TRP:CZ2  | 2.56                     | 0.41              |
| 3:1C:84:PRO:HB3    | 17:1Q:95:PHE:CE1   | 2.56                     | 0.41              |
| 3:1C:127:ALA:O     | 3:1C:128:ASN:C     | 2.64                     | 0.41              |
| 3:1C:136:ASP:OD1   | 3:1C:150:ARG:HA    | 2.21                     | 0.41              |
| 3:1C:149:ARG:HA    | 22:1W:88:MET:HE1   | 2.03                     | 0.41              |
| 4:1D:162:GLY:HA3   | 8:1H:279:ARG:HB3   | 2.02                     | 0.41              |
| 4:1D:389:CYS:O     | 4:1D:389:CYS:SG    | 2.79                     | 0.41              |
| 5:1E:205:PRO:HA    | 5:1E:206:PRO:HD3   | 1.96                     | 0.41              |
| 6:1F:89:ARG:HB3    | 6:1F:218:CYS:SG    | 2.61                     | 0.41              |
| 6:1F:93:LEU:HB3    | 6:1F:134:ALA:HA    | 2.03                     | 0.41              |
| 6:1F:145:GLU:OE1   | 6:1F:145:GLU:N     | 2.48                     | 0.41              |
| 6:1F:224:ASN:O     | 6:1F:228:VAL:HG23  | 2.21                     | 0.41              |
| 7:1G:203:CYS:HB3   | 49:1G:804:K:K      | 2.14                     | 0.41              |
| 7:1G:227:SER:O     | 7:1G:228:ILE:HD13  | 2.21                     | 0.41              |
| 7:1G:285:ARG:HB3   | 42:1q:144:TYR:N    | 2.36                     | 0.41              |
| 7:1G:328:LEU:HD13  | 7:1G:502:ALA:HA    | 2.02                     | 0.41              |
| 7:1G:433:ALA:HB1   | 7:1G:472:ASN:ND2   | 2.35                     | 0.41              |
| 7:1G:460:ARG:HG2   | 7:1G:461:SER:H     | 1.86                     | 0.41              |
| 8:1H:179:TRP:CD1   | 8:1H:180:PRO:HD3   | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:1H:312:ALA:HA    | 27:1b:41:ALA:HB2   | 2.02                     | 0.41              |
| 50:1H:401:PC1:H331 | 9:1I:27:TRP:CZ2    | 2.56                     | 0.41              |
| 9:1I:99:ARG:HB2    | 9:1I:103:SER:O     | 2.21                     | 0.41              |
| 10:1J:59:ILE:CD1   | 11:1K:64:LEU:HD22  | 2.51                     | 0.41              |
| 10:1J:119:PHE:CD1  | 11:1K:1:FME:HB2    | 2.55                     | 0.41              |
| 12:1L:28:LYS:HD2   | 12:1L:30:ASN:H     | 1.85                     | 0.41              |
| 12:1L:367:PRO:O    | 12:1L:371:THR:OG1  | 2.30                     | 0.41              |
| 12:1L:373:LEU:HD12 | 12:1L:373:LEU:HA   | 1.87                     | 0.41              |
| 12:1L:528:TYR:CG   | 37:1I:101:MET:HE1  | 2.56                     | 0.41              |
| 12:1L:543:SER:OG   | 12:1L:547:LYS:NZ   | 2.52                     | 0.41              |
| 12:1L:544:MET:O    | 12:1L:548:SER:OG   | 2.23                     | 0.41              |
| 12:1L:558:LEU:HD23 | 12:1L:558:LEU:HA   | 1.96                     | 0.41              |
| 45:1L:703:3PE:H371 | 45:1L:703:3PE:C23  | 2.50                     | 0.41              |
| 13:1M:116:ILE:HD13 | 13:1M:164:LEU:HD22 | 2.03                     | 0.41              |
| 13:1M:116:ILE:O    | 13:1M:120:ILE:HD12 | 2.21                     | 0.41              |
| 13:1M:250:LEU:HD23 | 13:1M:250:LEU:HA   | 1.84                     | 0.41              |
| 13:1M:277:LEU:O    | 37:1I:88:ARG:NH2   | 2.54                     | 0.41              |
| 13:1M:286:ILE:O    | 13:1M:289:SER:OG   | 2.24                     | 0.41              |
| 13:1M:360:LEU:HD23 | 13:1M:411:LEU:HD21 | 2.03                     | 0.41              |
| 14:1N:221:HIS:CD2  | 14:1N:323:MET:HE3  | 2.55                     | 0.41              |
| 16:1P:178:PHE:CD1  | 16:1P:178:PHE:N    | 2.87                     | 0.41              |
| 16:1P:294:LEU:HD11 | 16:1P:297:LEU:HD12 | 2.02                     | 0.41              |
| 16:1P:297:LEU:HD23 | 16:1P:297:LEU:HA   | 1.88                     | 0.41              |
| 20:1T:70:LEU:HD11  | 20:1T:79:TYR:HD2   | 1.85                     | 0.41              |
| 21:1V:63:ASP:OD1   | 21:1V:65:LYS:HE3   | 2.20                     | 0.41              |
| 22:1W:52:LEU:HD23  | 22:1W:52:LEU:HA    | 1.76                     | 0.41              |
| 24:1Y:120:THR:HA   | 24:1Y:123:LEU:HB2  | 2.02                     | 0.41              |
| 26:1a:2:TRP:HH2    | 53:1a:101:CDL:H751 | 1.86                     | 0.41              |
| 27:1b:59:ASP:OD1   | 27:1b:59:ASP:N     | 2.52                     | 0.41              |
| 29:1d:31:LEU:HD21  | 29:1d:69:VAL:HG13  | 2.03                     | 0.41              |
| 33:1h:7:ARG:NH2    | 34:1i:27:LEU:H     | 2.19                     | 0.41              |
| 40:1o:38:MET:HE3   | 40:1o:57:TYR:HA    | 2.02                     | 0.41              |
| 40:1o:105:ARG:O    | 40:1o:109:GLN:OE1  | 2.38                     | 0.41              |
| 41:1p:126:LYS:HE3  | 41:1p:126:LYS:HB3  | 1.81                     | 0.41              |
| 42:1q:95:ASP:H     | 43:1r:34:THR:HG23  | 1.86                     | 0.41              |
| 43:1r:104:GLU:N    | 43:1r:104:GLU:CD   | 2.78                     | 0.41              |
| 2:1B:126:TYR:N     | 2:1B:126:TYR:CD2   | 2.89                     | 0.41              |
| 4:1D:30:PRO:HA     | 4:1D:31:PRO:HD3    | 1.99                     | 0.41              |
| 4:1D:124:LYS:HB2   | 4:1D:124:LYS:HE3   | 1.65                     | 0.41              |
| 4:1D:161:ILE:HA    | 4:1D:238:ARG:NH2   | 2.36                     | 0.41              |
| 4:1D:184:VAL:HG23  | 4:1D:185:SER:H     | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:1F:92:TYR:CE2    | 6:1F:133:ALA:HB3   | 2.56                     | 0.41              |
| 6:1F:123:LEU:HD12  | 6:1F:124:VAL:HG13  | 2.01                     | 0.41              |
| 7:1G:58:GLU:HG3    | 7:1G:86:SER:OG     | 2.21                     | 0.41              |
| 7:1G:88:LYS:HE2    | 7:1G:88:LYS:HB2    | 1.62                     | 0.41              |
| 7:1G:373:GLU:H     | 7:1G:373:GLU:CD    | 2.24                     | 0.41              |
| 11:1K:73:LEU:HD22  | 14:1N:38:LEU:HD12  | 2.03                     | 0.41              |
| 45:1L:704:3PE:H231 | 45:1L:704:3PE:H321 | 2.01                     | 0.41              |
| 13:1M:12:LEU:HB3   | 13:1M:13:PRO:HD3   | 2.01                     | 0.41              |
| 15:1O:105:LEU:HA   | 15:1O:128:ILE:HG21 | 2.03                     | 0.41              |
| 18:1R:10:LYS:HB3   | 18:1R:10:LYS:HE3   | 1.69                     | 0.41              |
| 19:1S:24:GLN:CB    | 19:1S:25:ARG:NH1   | 2.84                     | 0.41              |
| 23:1X:139:ASN:OD1  | 23:1X:139:ASN:N    | 2.54                     | 0.41              |
| 26:1a:61:HIS:ND1   | 26:1a:61:HIS:O     | 2.53                     | 0.41              |
| 53:1a:101:CDL:H312 | 53:1a:101:CDL:OB9  | 2.21                     | 0.41              |
| 29:1d:5:ARG:O      | 29:1d:8:ARG:HB2    | 2.21                     | 0.41              |
| 41:1p:167:LYS:HD2  | 41:1p:171:GLU:OE1  | 2.21                     | 0.41              |
| 42:1q:31:ASN:HD22  | 42:1q:31:ASN:HA    | 1.68                     | 0.41              |
| 4:1D:99:ALA:HA     | 4:1D:102:TYR:CD2   | 2.54                     | 0.40              |
| 4:1D:124:LYS:HD2   | 4:1D:363:THR:HG21  | 2.03                     | 0.40              |
| 4:1D:171:PHE:HA    | 4:1D:174:ARG:HG3   | 2.03                     | 0.40              |
| 5:1E:110:LEU:HD22  | 6:1F:261:HIS:CE1   | 2.56                     | 0.40              |
| 5:1E:186:PRO:C     | 5:1E:187:ARG:HD2   | 2.46                     | 0.40              |
| 7:1G:278:ARG:HA    | 7:1G:278:ARG:HD2   | 1.85                     | 0.40              |
| 7:1G:374:ALA:HA    | 7:1G:448:LYS:HB3   | 2.03                     | 0.40              |
| 8:1H:234:MET:O     | 8:1H:238:THR:OG1   | 2.28                     | 0.40              |
| 9:1I:107:THR:O     | 42:1q:129:THR:HG23 | 2.20                     | 0.40              |
| 12:1L:534:HIS:HB3  | 45:1L:702:3PE:H31  | 2.02                     | 0.40              |
| 12:1L:550:SER:O    | 12:1L:554:ASP:HB3  | 2.21                     | 0.40              |
| 13:1M:116:ILE:HD13 | 13:1M:116:ILE:HA   | 1.81                     | 0.40              |
| 13:1M:254:THR:O    | 13:1M:258:ALA:N    | 2.54                     | 0.40              |
| 14:1N:186:HIS:O    | 14:1N:190:MET:HG2  | 2.21                     | 0.40              |
| 16:1P:46:ILE:HG23  | 18:1R:26:VAL:HG21  | 2.02                     | 0.40              |
| 16:1P:140:LYS:H    | 16:1P:140:LYS:HG3  | 1.57                     | 0.40              |
| 19:1S:86:VAL:O     | 19:1S:90:LEU:HG    | 2.21                     | 0.40              |
| 21:1V:17:GLU:O     | 21:1V:19:PRO:HD3   | 2.21                     | 0.40              |
| 23:1X:78:ALA:O     | 23:1X:82:THR:HG23  | 2.21                     | 0.40              |
| 45:1Y:201:3PE:H252 | 45:1Y:201:3PE:H221 | 1.95                     | 0.40              |
| 37:1l:101:MET:HA   | 37:1l:101:MET:HE3  | 2.03                     | 0.40              |
| 39:1n:97:LYS:HZ3   | 39:1n:173:PRO:HB2  | 1.87                     | 0.40              |
| 41:1p:145:LEU:HD11 | 41:1p:154:CYS:HA   | 2.02                     | 0.40              |
| 4:1D:170:MET:N     | 4:1D:170:MET:SD    | 2.94                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:1E:148:CYS:SG    | 6:1F:103:GLY:N     | 2.84                     | 0.40              |
| 6:1F:150:GLN:O     | 6:1F:153:ILE:HG22  | 2.21                     | 0.40              |
| 6:1F:232:PRO:HB2   | 6:1F:236:ARG:NH2   | 2.36                     | 0.40              |
| 6:1F:348:ALA:HB2   | 6:1F:376:MET:SD    | 2.62                     | 0.40              |
| 48:1F:501:FMN:H1'2 | 48:1F:501:FMN:H4'  | 1.85                     | 0.40              |
| 7:1G:285:ARG:NH2   | 42:1q:144:TYR:HD1  | 2.18                     | 0.40              |
| 8:1H:142:TYR:CD1   | 8:1H:289:LEU:HD13  | 2.56                     | 0.40              |
| 8:1H:261:LEU:HD23  | 8:1H:261:LEU:HA    | 1.89                     | 0.40              |
| 10:1J:153:LEU:HD23 | 10:1J:153:LEU:HA   | 1.89                     | 0.40              |
| 13:1M:371:PRO:HG2  | 13:1M:448:THR:HG21 | 2.03                     | 0.40              |
| 14:1N:48:PHE:CD1   | 14:1N:48:PHE:O     | 2.74                     | 0.40              |
| 14:1N:95:MET:HE3   | 14:1N:148:SER:O    | 2.22                     | 0.40              |
| 14:1N:151:PRO:HG2  | 24:1Y:137:GLU:OE1  | 2.21                     | 0.40              |
| 14:1N:191:THR:HA   | 14:1N:194:LEU:HB2  | 2.02                     | 0.40              |
| 15:1O:59:ALA:O     | 15:1O:62:THR:OG1   | 2.30                     | 0.40              |
| 16:1P:48:PRO:HB3   | 16:1P:73:TRP:CG    | 2.57                     | 0.40              |
| 16:1P:136:ASN:HD21 | 16:1P:291:ASP:HA   | 1.85                     | 0.40              |
| 16:1P:318:LEU:HD23 | 16:1P:318:LEU:O    | 2.21                     | 0.40              |
| 17:1Q:57:MET:HE1   | 17:1Q:101:TRP:HZ3  | 1.86                     | 0.40              |
| 20:1U:15:VAL:O     | 20:1U:19:LEU:HD12  | 2.21                     | 0.40              |
| 22:1W:62:LYS:HD3   | 22:1W:107:PHE:CD2  | 2.56                     | 0.40              |
| 25:1Z:51:MET:SD    | 25:1Z:55:ARG:NE    | 2.94                     | 0.40              |
| 25:1Z:86:MET:HE2   | 25:1Z:86:MET:HB2   | 1.92                     | 0.40              |
| 37:1l:47:TYR:OH    | 37:1l:77:ILE:O     | 2.22                     | 0.40              |
| 40:1o:30:PHE:CD2   | 40:1o:33:ARG:HD2   | 2.57                     | 0.40              |
| 40:1o:46:ASN:ND2   | 41:1p:122:GLN:HE21 | 2.19                     | 0.40              |
| 1:1A:87:MET:C      | 1:1A:87:MET:SD     | 3.04                     | 0.40              |
| 45:1A:201:3PE:H2D1 | 8:1H:302:MET:HE1   | 2.03                     | 0.40              |
| 3:1C:70:ALA:HB1    | 3:1C:72:PHE:HD1    | 1.86                     | 0.40              |
| 3:1C:72:PHE:CE2    | 3:1C:105:ILE:HG13  | 2.56                     | 0.40              |
| 3:1C:155:TYR:HD2   | 22:1W:98:LYS:HA    | 1.86                     | 0.40              |
| 5:1E:101:GLN:OE1   | 5:1E:101:GLN:HA    | 2.21                     | 0.40              |
| 6:1F:52:GLY:O      | 6:1F:56:ILE:HD12   | 2.21                     | 0.40              |
| 7:1G:287:GLU:CD    | 7:1G:287:GLU:H     | 2.29                     | 0.40              |
| 7:1G:424:ASP:O     | 7:1G:660:PRO:HA    | 2.22                     | 0.40              |
| 8:1H:4:ILE:H       | 8:1H:4:ILE:HG13    | 1.37                     | 0.40              |
| 8:1H:141:SER:OG    | 8:1H:290:TRP:NE1   | 2.53                     | 0.40              |
| 8:1H:219:PRO:HA    | 8:1H:222:MET:HG2   | 2.02                     | 0.40              |
| 8:1H:307:LEU:HB3   | 8:1H:308:PRO:HD3   | 2.03                     | 0.40              |
| 8:1H:315:PRO:HB3   | 25:1Z:54:ASN:HD21  | 1.86                     | 0.40              |
| 10:1J:123:GLY:O    | 10:1J:126:VAL:HG22 | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:1K:34:GLU:O     | 11:1K:37:MET:HG3   | 2.21                     | 0.40              |
| 13:1M:119:TYR:CD1  | 13:1M:160:LEU:HD23 | 2.57                     | 0.40              |
| 15:1O:132:PHE:CD1  | 15:1O:132:PHE:C    | 2.99                     | 0.40              |
| 16:1P:6:ILE:HA     | 16:1P:7:PRO:HD3    | 1.91                     | 0.40              |
| 21:1V:22:ARG:O     | 21:1V:22:ARG:NH1   | 2.54                     | 0.40              |
| 22:1W:63:VAL:HA    | 22:1W:66:MET:HE3   | 2.04                     | 0.40              |
| 23:1X:67:LEU:O     | 23:1X:71:ARG:N     | 2.53                     | 0.40              |
| 25:1Z:30:LEU:HB3   | 25:1Z:34:SER:OG    | 2.22                     | 0.40              |
| 25:1Z:72:MET:N     | 25:1Z:73:PRO:HD2   | 2.36                     | 0.40              |
| 37:1l:98:TRP:HA    | 37:1l:101:MET:HB2  | 2.02                     | 0.40              |
| 38:1m:42:LEU:HD23  | 38:1m:42:LEU:HA    | 1.89                     | 0.40              |
| 42:1q:137:TRP:CD1  | 42:1q:138:VAL:H    | 2.39                     | 0.40              |
| 1:1A:98:LEU:HD12   | 1:1A:98:LEU:HA     | 1.84                     | 0.40              |
| 4:1D:139:VAL:HG23  | 4:1D:278:TYR:HE1   | 1.86                     | 0.40              |
| 5:1E:21:PHE:CD2    | 5:1E:65:ALA:HA     | 2.57                     | 0.40              |
| 6:1F:22:PHE:HB2    | 6:1F:25:LEU:HB2    | 2.02                     | 0.40              |
| 6:1F:42:TRP:CE3    | 6:1F:161:LEU:HD13  | 2.57                     | 0.40              |
| 6:1F:108:ARG:HE    | 6:1F:108:ARG:HB3   | 1.71                     | 0.40              |
| 7:1G:354:ALA:HB2   | 7:1G:648:LEU:HB3   | 2.04                     | 0.40              |
| 7:1G:378:LEU:HD12  | 7:1G:409:ILE:HD11  | 2.03                     | 0.40              |
| 9:1I:160:LYS:HD2   | 9:1I:161:TRP:CD1   | 2.56                     | 0.40              |
| 12:1L:48:LEU:HA    | 12:1L:48:LEU:HD12  | 1.78                     | 0.40              |
| 13:1M:1:FME:HE3    | 13:1M:111:THR:HG21 | 2.03                     | 0.40              |
| 14:1N:144:GLN:HE21 | 30:1e:2:PHE:N      | 2.20                     | 0.40              |
| 14:1N:230:LEU:HD12 | 14:1N:230:LEU:HA   | 1.76                     | 0.40              |
| 14:1N:248:LEU:HD11 | 14:1N:296:LEU:HB3  | 2.02                     | 0.40              |
| 16:1P:238:LEU:HD12 | 16:1P:238:LEU:HA   | 1.90                     | 0.40              |
| 22:1W:39:TRP:O     | 22:1W:43:VAL:HG23  | 2.22                     | 0.40              |
| 23:1X:54:ARG:HA    | 23:1X:54:ARG:HD3   | 1.81                     | 0.40              |
| 23:1X:77:CYS:HB3   | 23:1X:80:PRO:HG2   | 2.02                     | 0.40              |
| 26:1a:18:ILE:N     | 26:1a:19:PRO:HD2   | 2.36                     | 0.40              |
| 30:1e:87:LYS:HE2   | 30:1e:87:LYS:HB2   | 1.80                     | 0.40              |
| 32:1g:55:LEU:O     | 32:1g:59:ARG:HG3   | 2.21                     | 0.40              |
| 32:1g:113:PHE:N    | 41:1p:158:GLN:OE1  | 2.53                     | 0.40              |
| 38:1m:48:LEU:HD23  | 38:1m:48:LEU:HA    | 1.90                     | 0.40              |
| 39:1n:82:PRO:HB3   | 39:1n:89:SER:H     | 1.86                     | 0.40              |
| 1:1A:97:LEU:HD13   | 1:1A:97:LEU:HA     | 1.94                     | 0.40              |
| 4:1D:260:LEU:HB3   | 4:1D:265:ILE:HB    | 2.03                     | 0.40              |
| 4:1D:284:ASP:O     | 4:1D:306:GLN:HG3   | 2.22                     | 0.40              |
| 4:1D:322:GLU:CD    | 43:1r:44:PRO:HD3   | 2.46                     | 0.40              |
| 6:1F:115:PRO:O     | 6:1F:119:VAL:HG23  | 2.22                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:1F:136:ILE:HD11 | 6:1F:177:VAL:HG22  | 2.03                     | 0.40              |
| 6:1F:248:GLU:C    | 6:1F:250:ASN:H     | 2.30                     | 0.40              |
| 6:1F:300:GLY:HA2  | 6:1F:333:ALA:N     | 2.36                     | 0.40              |
| 7:1G:460:ARG:NH2  | 7:1G:657:LEU:HB3   | 2.36                     | 0.40              |
| 7:1G:474:ALA:O    | 7:1G:478:ARG:HB2   | 2.22                     | 0.40              |
| 8:1H:55:LEU:HD23  | 8:1H:55:LEU:HA     | 1.89                     | 0.40              |
| 8:1H:272:TRP:CZ2  | 9:1I:38:LEU:HG     | 2.57                     | 0.40              |
| 12:1L:293:ILE:CD1 | 12:1L:294:THR:HG23 | 2.50                     | 0.40              |
| 13:1M:121:LEU:H   | 13:1M:121:LEU:HG   | 1.75                     | 0.40              |
| 13:1M:135:ARG:HE  | 45:1N:401:3PE:H362 | 1.87                     | 0.40              |
| 13:1M:438:ALA:O   | 13:1M:442:LEU:HG   | 2.21                     | 0.40              |
| 14:1N:183:SER:HB2 | 14:1N:208:TYR:OH   | 2.21                     | 0.40              |
| 14:1N:278:MET:HB2 | 14:1N:279:PRO:HD3  | 2.03                     | 0.40              |
| 16:1P:27:THR:O    | 16:1P:27:THR:OG1   | 2.37                     | 0.40              |
| 16:1P:319:ARG:HA  | 16:1P:322:ARG:HD3  | 2.04                     | 0.40              |
| 19:1S:13:LEU:H    | 19:1S:13:LEU:HG    | 1.75                     | 0.40              |
| 23:1X:82:THR:O    | 23:1X:86:THR:OG1   | 2.26                     | 0.40              |
| 30:1e:13:LEU:HD12 | 30:1e:13:LEU:HA    | 1.85                     | 0.40              |
| 30:1e:49:ILE:H    | 30:1e:49:ILE:HG12  | 1.73                     | 0.40              |
| 37:1l:116:PHE:O   | 37:1l:116:PHE:HD1  | 2.04                     | 0.40              |
| 39:1n:113:MET:HG2 | 39:1n:114:TYR:CE2  | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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    | 83/115 (72%)  | 78 (94%)  | 3 (4%)  | 2 (2%)   | 4           | 29  |
| 2   | 1B    | 153/258 (59%) | 140 (92%) | 13 (8%) | 0        | 100         | 100 |
| 3   | 1C    | 207/264 (78%) | 192 (93%) | 15 (7%) | 0        | 100         | 100 |
| 4   | 1D    | 414/476 (87%) | 380 (92%) | 34 (8%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 5   | 1E    | 212/249 (85%)  | 193 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 6   | 1F    | 430/464 (93%)  | 397 (92%) | 33 (8%)  | 0        | 100         | 100 |
| 7   | 1G    | 697/727 (96%)  | 620 (89%) | 71 (10%) | 6 (1%)   | 14          | 45  |
| 8   | 1H    | 316/318 (99%)  | 290 (92%) | 24 (8%)  | 2 (1%)   | 21          | 52  |
| 9   | 1I    | 174/239 (73%)  | 164 (94%) | 10 (6%)  | 0        | 100         | 100 |
| 10  | 1J    | 173/175 (99%)  | 160 (92%) | 12 (7%)  | 1 (1%)   | 21          | 52  |
| 11  | 1K    | 96/98 (98%)    | 90 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 12  | 1L    | 604/606 (100%) | 557 (92%) | 44 (7%)  | 3 (0%)   | 24          | 56  |
| 13  | 1M    | 457/459 (100%) | 436 (95%) | 20 (4%)  | 1 (0%)   | 43          | 72  |
| 14  | 1N    | 345/347 (99%)  | 326 (94%) | 19 (6%)  | 0        | 100         | 100 |
| 15  | 1O    | 318/357 (89%)  | 288 (91%) | 30 (9%)  | 0        | 100         | 100 |
| 16  | 1P    | 340/377 (90%)  | 304 (89%) | 35 (10%) | 1 (0%)   | 36          | 65  |
| 17  | 1Q    | 127/175 (73%)  | 115 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 18  | 1R    | 94/123 (76%)   | 83 (88%)  | 10 (11%) | 1 (1%)   | 11          | 42  |
| 19  | 1S    | 85/99 (86%)    | 77 (91%)  | 8 (9%)   | 0        | 100         | 100 |
| 20  | 1T    | 83/156 (53%)   | 76 (92%)  | 7 (8%)   | 0        | 100         | 100 |
| 20  | 1U    | 84/156 (54%)   | 79 (94%)  | 5 (6%)   | 0        | 100         | 100 |
| 21  | 1V    | 113/116 (97%)  | 99 (88%)  | 14 (12%) | 0        | 100         | 100 |
| 22  | 1W    | 113/128 (88%)  | 106 (94%) | 6 (5%)   | 1 (1%)   | 14          | 45  |
| 23  | 1X    | 169/172 (98%)  | 160 (95%) | 9 (5%)   | 0        | 100         | 100 |
| 24  | 1Y    | 137/141 (97%)  | 129 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 25  | 1Z    | 139/144 (96%)  | 126 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 26  | 1a    | 68/70 (97%)    | 63 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 27  | 1b    | 81/84 (96%)    | 77 (95%)  | 4 (5%)   | 0        | 100         | 100 |
| 28  | 1c    | 47/76 (62%)    | 45 (96%)  | 2 (4%)   | 0        | 100         | 100 |
| 29  | 1d    | 117/123 (95%)  | 109 (93%) | 8 (7%)   | 0        | 100         | 100 |
| 30  | 1e    | 97/106 (92%)   | 94 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 31  | 1f    | 55/135 (41%)   | 47 (86%)  | 8 (14%)  | 0        | 100         | 100 |
| 32  | 1g    | 98/154 (64%)   | 89 (91%)  | 8 (8%)   | 1 (1%)   | 12          | 43  |
| 33  | 1h    | 136/189 (72%)  | 132 (97%) | 4 (3%)   | 0        | 100         | 100 |
| 34  | 1i    | 124/128 (97%)  | 113 (91%) | 11 (9%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 35  | 1j    | 69/105 (66%)    | 63 (91%)   | 5 (7%)   | 1 (1%)   | 9           | 37  |
| 36  | 1k    | 79/98 (81%)     | 73 (92%)   | 6 (8%)   | 0        | 100         | 100 |
| 37  | 1l    | 154/186 (83%)   | 141 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 38  | 1m    | 126/129 (98%)   | 116 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 39  | 1n    | 170/179 (95%)   | 163 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 40  | 1o    | 120/137 (88%)   | 117 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 41  | 1p    | 171/176 (97%)   | 168 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 42  | 1q    | 143/145 (99%)   | 131 (92%)  | 11 (8%)  | 1 (1%)   | 18          | 50  |
| 43  | 1r    | 90/114 (79%)    | 82 (91%)   | 8 (9%)   | 0        | 100         | 100 |
| 44  | 1s    | 43/471 (9%)     | 37 (86%)   | 6 (14%)  | 0        | 100         | 100 |
| All | All   | 8151/9744 (84%) | 7525 (92%) | 605 (7%) | 21 (0%)  | 37          | 65  |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 109 | LYS  |
| 7   | 1G    | 652 | VAL  |
| 7   | 1G    | 671 | PHE  |
| 8   | 1H    | 92  | PRO  |
| 12  | 1L    | 464 | ALA  |
| 13  | 1M    | 85  | SER  |
| 16  | 1P    | 222 | ASP  |
| 18  | 1R    | 79  | THR  |
| 32  | 1g    | 24  | ILE  |
| 1   | 1A    | 75  | LEU  |
| 8   | 1H    | 213 | VAL  |
| 10  | 1J    | 116 | ILE  |
| 12  | 1L    | 549 | ALA  |
| 7   | 1G    | 166 | ILE  |
| 7   | 1G    | 256 | GLU  |
| 7   | 1G    | 72  | PRO  |
| 12  | 1L    | 159 | HIS  |
| 42  | 1q    | 134 | ILE  |
| 7   | 1G    | 367 | THR  |
| 35  | 1j    | 50  | HIS  |
| 22  | 1W    | 96  | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 1A    | 75/99 (76%)    | 73 (97%)   | 2 (3%)   | 39          | 59  |
| 2   | 1B    | 131/212 (62%)  | 129 (98%)  | 2 (2%)   | 57          | 68  |
| 3   | 1C    | 190/227 (84%)  | 187 (98%)  | 3 (2%)   | 55          | 68  |
| 4   | 1D    | 364/405 (90%)  | 362 (100%) | 2 (0%)   | 81          | 80  |
| 5   | 1E    | 183/207 (88%)  | 183 (100%) | 0        | 100         | 100 |
| 6   | 1F    | 346/368 (94%)  | 344 (99%)  | 2 (1%)   | 78          | 79  |
| 7   | 1G    | 588/610 (96%)  | 584 (99%)  | 4 (1%)   | 76          | 77  |
| 8   | 1H    | 274/274 (100%) | 267 (97%)  | 7 (3%)   | 40          | 60  |
| 9   | 1I    | 151/201 (75%)  | 149 (99%)  | 2 (1%)   | 61          | 71  |
| 10  | 1J    | 140/140 (100%) | 139 (99%)  | 1 (1%)   | 76          | 77  |
| 11  | 1K    | 84/84 (100%)   | 84 (100%)  | 0        | 100         | 100 |
| 12  | 1L    | 539/539 (100%) | 535 (99%)  | 4 (1%)   | 76          | 77  |
| 13  | 1M    | 408/408 (100%) | 405 (99%)  | 3 (1%)   | 76          | 77  |
| 14  | 1N    | 310/310 (100%) | 309 (100%) | 1 (0%)   | 86          | 83  |
| 15  | 1O    | 283/307 (92%)  | 281 (99%)  | 2 (1%)   | 76          | 77  |
| 16  | 1P    | 296/323 (92%)  | 294 (99%)  | 2 (1%)   | 76          | 77  |
| 17  | 1Q    | 117/152 (77%)  | 117 (100%) | 0        | 100         | 100 |
| 18  | 1R    | 79/97 (81%)    | 78 (99%)   | 1 (1%)   | 61          | 71  |
| 19  | 1S    | 77/82 (94%)    | 76 (99%)   | 1 (1%)   | 61          | 71  |
| 20  | 1T    | 79/133 (59%)   | 76 (96%)   | 3 (4%)   | 29          | 53  |
| 20  | 1U    | 79/133 (59%)   | 79 (100%)  | 0        | 100         | 100 |
| 21  | 1V    | 100/101 (99%)  | 99 (99%)   | 1 (1%)   | 68          | 74  |
| 22  | 1W    | 107/112 (96%)  | 106 (99%)  | 1 (1%)   | 70          | 75  |
| 23  | 1X    | 153/154 (99%)  | 150 (98%)  | 3 (2%)   | 48          | 64  |
| 24  | 1Y    | 101/102 (99%)  | 101 (100%) | 0        | 100         | 100 |
| 25  | 1Z    | 123/124 (99%)  | 123 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 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    | 107/109 (98%)   | 107 (100%) | 0        | 100         | 100 |
| 30  | 1e    | 87/94 (93%)     | 86 (99%)   | 1 (1%)   | 65          | 73  |
| 31  | 1f    | 54/113 (48%)    | 54 (100%)  | 0        | 100         | 100 |
| 32  | 1g    | 92/129 (71%)    | 92 (100%)  | 0        | 100         | 100 |
| 33  | 1h    | 121/158 (77%)   | 121 (100%) | 0        | 100         | 100 |
| 34  | 1i    | 119/120 (99%)   | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 35  | 1j    | 62/84 (74%)     | 62 (100%)  | 0        | 100         | 100 |
| 36  | 1k    | 63/76 (83%)     | 61 (97%)   | 2 (3%)   | 34          | 56  |
| 37  | 1l    | 141/161 (88%)   | 141 (100%) | 0        | 100         | 100 |
| 38  | 1m    | 113/114 (99%)   | 112 (99%)  | 1 (1%)   | 70          | 75  |
| 39  | 1n    | 156/160 (98%)   | 156 (100%) | 0        | 100         | 100 |
| 40  | 1o    | 110/120 (92%)   | 110 (100%) | 0        | 100         | 100 |
| 41  | 1p    | 154/156 (99%)   | 153 (99%)  | 1 (1%)   | 78          | 79  |
| 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 |
| All | All   | 7188/8272 (87%) | 7135 (99%) | 53 (1%)  | 73          | 77  |

All (53) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1A    | 65  | PHE  |
| 1   | 1A    | 97  | LEU  |
| 2   | 1B    | 68  | ASP  |
| 2   | 1B    | 156 | LEU  |
| 3   | 1C    | 11  | ILE  |
| 3   | 1C    | 20  | LYS  |
| 3   | 1C    | 183 | VAL  |
| 4   | 1D    | 4   | TRP  |
| 4   | 1D    | 376 | VAL  |
| 6   | 1F    | 31  | TRP  |
| 6   | 1F    | 149 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | 1G    | 77  | TRP  |
| 7   | 1G    | 283 | MET  |
| 7   | 1G    | 525 | LEU  |
| 7   | 1G    | 636 | VAL  |
| 8   | 1H    | 32  | GLN  |
| 8   | 1H    | 33  | LEU  |
| 8   | 1H    | 143 | GLU  |
| 8   | 1H    | 145 | THR  |
| 8   | 1H    | 213 | VAL  |
| 8   | 1H    | 284 | GLN  |
| 8   | 1H    | 300 | LEU  |
| 9   | 1I    | 92  | ILE  |
| 9   | 1I    | 141 | THR  |
| 10  | 1J    | 17  | PHE  |
| 12  | 1L    | 66  | TRP  |
| 12  | 1L    | 163 | ASP  |
| 12  | 1L    | 459 | ILE  |
| 12  | 1L    | 471 | ASN  |
| 13  | 1M    | 86  | LYS  |
| 13  | 1M    | 439 | LEU  |
| 13  | 1M    | 455 | LEU  |
| 14  | 1N    | 164 | ILE  |
| 15  | 1O    | 96  | LEU  |
| 15  | 1O    | 270 | LEU  |
| 16  | 1P    | 140 | LYS  |
| 16  | 1P    | 258 | LEU  |
| 18  | 1R    | 43  | LEU  |
| 19  | 1S    | 87  | THR  |
| 20  | 1T    | 15  | VAL  |
| 20  | 1T    | 58  | PHE  |
| 20  | 1T    | 66  | ASP  |
| 21  | 1V    | 94  | LEU  |
| 22  | 1W    | 126 | HIS  |
| 23  | 1X    | 93  | LEU  |
| 23  | 1X    | 107 | ASP  |
| 23  | 1X    | 144 | ARG  |
| 30  | 1e    | 6   | GLN  |
| 34  | 1i    | 47  | ASN  |
| 36  | 1k    | 28  | LEU  |
| 36  | 1k    | 29  | GLU  |
| 38  | 1m    | 126 | ILE  |
| 41  | 1p    | 62  | TYR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1B    | 162 | GLN  |
| 3   | 1C    | 38  | GLN  |
| 3   | 1C    | 67  | HIS  |
| 3   | 1C    | 69  | ASN  |
| 3   | 1C    | 95  | ASN  |
| 3   | 1C    | 211 | GLN  |
| 4   | 1D    | 27  | HIS  |
| 4   | 1D    | 34  | ASN  |
| 4   | 1D    | 150 | HIS  |
| 5   | 1E    | 55  | GLN  |
| 5   | 1E    | 91  | ASN  |
| 6   | 1F    | 37  | GLN  |
| 6   | 1F    | 116 | HIS  |
| 7   | 1G    | 182 | GLN  |
| 7   | 1G    | 237 | ASN  |
| 7   | 1G    | 255 | HIS  |
| 7   | 1G    | 499 | GLN  |
| 7   | 1G    | 517 | ASN  |
| 7   | 1G    | 682 | GLN  |
| 8   | 1H    | 138 | GLN  |
| 8   | 1H    | 284 | GLN  |
| 9   | 1I    | 150 | ASN  |
| 9   | 1I    | 156 | ASN  |
| 11  | 1K    | 94  | ASN  |
| 12  | 1L    | 23  | ASN  |
| 12  | 1L    | 248 | HIS  |
| 12  | 1L    | 296 | ASN  |
| 12  | 1L    | 321 | GLN  |
| 12  | 1L    | 471 | ASN  |
| 12  | 1L    | 506 | ASN  |
| 12  | 1L    | 579 | ASN  |
| 13  | 1M    | 44  | GLN  |
| 13  | 1M    | 103 | GLN  |
| 14  | 1N    | 36  | ASN  |
| 14  | 1N    | 134 | GLN  |
| 14  | 1N    | 152 | ASN  |
| 14  | 1N    | 174 | GLN  |
| 14  | 1N    | 235 | ASN  |
| 15  | 1O    | 50  | HIS  |
| 15  | 1O    | 204 | ASN  |
| 15  | 1O    | 265 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | 1P    | 2   | HIS  |
| 16  | 1P    | 3   | HIS  |
| 16  | 1P    | 180 | ASN  |
| 16  | 1P    | 203 | GLN  |
| 16  | 1P    | 216 | ASN  |
| 17  | 1Q    | 6   | GLN  |
| 17  | 1Q    | 46  | GLN  |
| 17  | 1Q    | 50  | ASN  |
| 17  | 1Q    | 81  | ASN  |
| 18  | 1R    | 16  | GLN  |
| 18  | 1R    | 36  | ASN  |
| 19  | 1S    | 24  | GLN  |
| 19  | 1S    | 80  | ASN  |
| 21  | 1V    | 70  | GLN  |
| 21  | 1V    | 85  | ASN  |
| 22  | 1W    | 26  | ASN  |
| 22  | 1W    | 51  | GLN  |
| 22  | 1W    | 102 | HIS  |
| 23  | 1X    | 150 | ASN  |
| 24  | 1Y    | 133 | GLN  |
| 27  | 1b    | 45  | ASN  |
| 29  | 1d    | 61  | GLN  |
| 29  | 1d    | 117 | HIS  |
| 30  | 1e    | 97  | HIS  |
| 34  | 1i    | 44  | GLN  |
| 37  | 1l    | 28  | ASN  |
| 37  | 1l    | 55  | GLN  |
| 38  | 1m    | 78  | ASN  |
| 39  | 1n    | 65  | GLN  |
| 40  | 1o    | 46  | ASN  |
| 40  | 1o    | 75  | ASN  |
| 41  | 1p    | 55  | HIS  |
| 41  | 1p    | 58  | ASN  |
| 41  | 1p    | 103 | ASN  |
| 41  | 1p    | 122 | GLN  |
| 41  | 1p    | 123 | ASN  |
| 43  | 1r    | 12  | ASN  |
| 43  | 1r    | 24  | GLN  |
| 44  | 1s    | 40  | ASN  |
| 44  | 1s    | 75  | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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$ |
| 10  | FME  | 1J    | 1   | 10   | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.92 | 1 (12%)     |
| 12  | FME  | 1L    | 1   | 12   | 8,9,10       | 0.55 | 0           | 8,9,11      | 1.01 | 1 (12%)     |
| 13  | FME  | 1M    | 1   | 13   | 8,9,10       | 0.55 | 0           | 8,9,11      | 0.98 | 1 (12%)     |
| 8   | FME  | 1H    | 1   | 8    | 8,9,10       | 0.65 | 0           | 8,9,11      | 1.02 | 1 (12%)     |
| 1   | FME  | 1A    | 1   | 1    | 8,9,10       | 0.54 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 11  | FME  | 1K    | 1   | 11   | 8,9,10       | 0.56 | 0           | 8,9,11      | 0.96 | 1 (12%)     |
| 14  | FME  | 1N    | 1   | 14   | 8,9,10       | 0.54 | 0           | 8,9,11      | 0.91 | 1 (12%)     |
| 34  | SAC  | 1i    | 1   | -    | 7,8,9        | 0.56 | 0           | 7,9,11      | 1.17 | 1 (14%)     |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 10  | FME  | 1J    | 1   | 10   | -       | 2/7/9/11 | -     |
| 12  | FME  | 1L    | 1   | 12   | -       | 0/7/9/11 | -     |
| 13  | FME  | 1M    | 1   | 13   | -       | 1/7/9/11 | -     |
| 8   | FME  | 1H    | 1   | 8    | -       | 1/7/9/11 | -     |
| 1   | FME  | 1A    | 1   | 1    | -       | 0/7/9/11 | -     |
| 11  | FME  | 1K    | 1   | 11   | -       | 1/7/9/11 | -     |
| 14  | FME  | 1N    | 1   | 14   | -       | 0/7/9/11 | -     |
| 34  | SAC  | 1i    | 1   | -    | -       | 2/7/8/10 | -     |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 34  | 1i    | 1   | SAC  | O-C-CA | -3.03 | 116.97      | 124.77   |
| 11  | 1K    | 1   | FME  | O-C-CA | -2.67 | 117.92      | 124.77   |
| 8   | 1H    | 1   | FME  | O-C-CA | -2.65 | 117.95      | 124.77   |
| 12  | 1L    | 1   | FME  | O-C-CA | -2.63 | 118.02      | 124.77   |
| 10  | 1J    | 1   | FME  | O-C-CA | -2.58 | 118.13      | 124.77   |
| 13  | 1M    | 1   | FME  | O-C-CA | -2.51 | 118.32      | 124.77   |
| 14  | 1N    | 1   | FME  | O-C-CA | -2.48 | 118.39      | 124.77   |
| 1   | 1A    | 1   | FME  | O-C-CA | -2.47 | 118.43      | 124.77   |

There are no chirality outliers.

All (7) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | 1H    | 1   | FME  | O1-CN-N-CA  |
| 10  | 1J    | 1   | FME  | N-CA-CB-CG  |
| 11  | 1K    | 1   | FME  | N-CA-CB-CG  |
| 10  | 1J    | 1   | FME  | C-CA-CB-CG  |
| 34  | 1i    | 1   | SAC  | CB-CA-N-C1A |
| 34  | 1i    | 1   | SAC  | C-CA-N-C1A  |
| 13  | 1M    | 1   | FME  | C-CA-CB-CG  |

There are no ring outliers.

7 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | 1L    | 1   | FME  | 2       | 0            |
| 13  | 1M    | 1   | FME  | 3       | 0            |
| 8   | 1H    | 1   | FME  | 1       | 0            |
| 1   | 1A    | 1   | FME  | 2       | 0            |
| 11  | 1K    | 1   | FME  | 1       | 0            |
| 14  | 1N    | 1   | FME  | 1       | 0            |
| 34  | 1i    | 1   | SAC  | 2       | 0            |

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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 |
| 54  | GTP  | 1O    | 401 | 55   | 33,34,34     | 0.60 | 0        | 50,54,54    | 0.61 | 0        |
| 45  | 3PE  | 1L    | 703 | -    | 30,30,50     | 0.37 | 0        | 33,35,55    | 0.59 | 0        |
| 45  | 3PE  | 1L    | 702 | -    | 45,45,50     | 0.30 | 0        | 48,50,55    | 0.32 | 0        |
| 45  | 3PE  | 1N    | 401 | -    | 50,50,50     | 0.28 | 0        | 53,55,55    | 0.40 | 0        |
| 46  | SF4  | 1B    | 201 | 2    | 0,12,12      | -    | -        | -           |      |          |
| 46  | SF4  | 1G    | 801 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 48  | FMN  | 1F    | 501 | -    | 33,33,33     | 0.59 | 0        | 48,50,50    | 0.64 | 1 (2%)   |
| 50  | PC1  | 1f    | 101 | -    | 45,45,53     | 0.28 | 0        | 51,53,61    | 0.34 | 0        |
| 53  | CDL  | 1N    | 402 | -    | 76,76,99     | 0.30 | 0        | 82,88,111   | 0.37 | 0        |
| 47  | FES  | 1E    | 301 | 5    | 0,4,4        | -    | -        | -           |      |          |
| 45  | 3PE  | 1Y    | 201 | -    | 50,50,50     | 0.27 | 0        | 53,55,55    | 0.43 | 0        |
| 45  | 3PE  | 1A    | 201 | -    | 46,46,50     | 0.28 | 0        | 49,51,55    | 0.39 | 0        |
| 46  | SF4  | 1G    | 802 | 7    | 0,12,12      | -    | -        | -           |      |          |
| 50  | PC1  | 1H    | 401 | -    | 53,53,53     | 0.27 | 0        | 59,61,61    | 0.32 | 0        |
| 47  | FES  | 1G    | 803 | 7    | 0,4,4        | -    | -        | -           |      |          |
| 56  | NDP  | 1P    | 501 | -    | 51,52,52     | 0.51 | 0        | 71,80,80    | 0.78 | 1 (1%)   |
| 45  | 3PE  | 1L    | 704 | -    | 41,41,50     | 0.31 | 0        | 44,46,55    | 1.30 | 5 (11%)  |
| 50  | PC1  | 1M    | 502 | -    | 43,43,53     | 0.29 | 0        | 49,51,61    | 0.44 | 0        |
| 58  | EHZ  | 1n    | 201 | -    | 31,36,37     | 0.18 | 0        | 36,44,47    | 1.31 | 2 (5%)   |
| 52  | PGT  | 1M    | 501 | -    | 50,50,50     | 0.49 | 0        | 53,56,56    | 0.48 | 0        |
| 46  | SF4  | 1I    | 202 | 9    | 0,12,12      | -    | -        | -           |      |          |
| 53  | CDL  | 1a    | 101 | -    | 60,60,99     | 0.33 | 0        | 66,72,111   | 0.42 | 0        |
| 58  | EHZ  | 1W    | 201 | -    | 31,36,37     | 0.20 | 0        | 36,44,47    | 1.16 | 1 (2%)   |
| 46  | SF4  | 1I    | 201 | 9    | 0,12,12      | -    | -        | -           |      |          |
| 46  | SF4  | 1F    | 502 | 6    | 0,12,12      | -    | -        | -           |      |          |
| 50  | PC1  | 1J    | 201 | -    | 34,34,53     | 0.32 | 0        | 40,42,61    | 0.32 | 0        |
| 50  | PC1  | 1I    | 203 | -    | 43,43,53     | 0.29 | 0        | 49,51,61    | 0.39 | 0        |
| 51  | MYR  | 1L    | 701 | -    | 13,14,15     | 0.29 | 0        | 12,13,15    | 0.29 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions     | Rings   |
|-----|------|-------|-----|------|---------|--------------|---------|
| 54  | GTP  | 1O    | 401 | 55   | -       | 3/22/38/38   | 0/3/3/3 |
| 45  | 3PE  | 1L    | 703 | -    | -       | 7/34/34/54   | -       |
| 45  | 3PE  | 1L    | 702 | -    | -       | 2/49/49/54   | -       |
| 45  | 3PE  | 1N    | 401 | -    | -       | 8/54/54/54   | -       |
| 46  | SF4  | 1B    | 201 | 2    | -       | -            | 0/6/5/5 |
| 46  | SF4  | 1G    | 801 | 7    | -       | -            | 0/6/5/5 |
| 48  | FMN  | 1F    | 501 | -    | -       | 2/18/18/18   | 0/3/3/3 |
| 50  | PC1  | 1f    | 101 | -    | -       | 6/49/49/57   | -       |
| 53  | CDL  | 1N    | 402 | -    | -       | 9/87/87/110  | -       |
| 47  | FES  | 1E    | 301 | 5    | -       | -            | 0/1/1/1 |
| 45  | 3PE  | 1Y    | 201 | -    | -       | 8/54/54/54   | -       |
| 45  | 3PE  | 1A    | 201 | -    | -       | 3/50/50/54   | -       |
| 46  | SF4  | 1G    | 802 | 7    | -       | -            | 0/6/5/5 |
| 50  | PC1  | 1H    | 401 | -    | -       | 5/57/57/57   | -       |
| 47  | FES  | 1G    | 803 | 7    | -       | -            | 0/1/1/1 |
| 56  | NDP  | 1P    | 501 | -    | -       | 10/34/77/77  | 0/5/5/5 |
| 45  | 3PE  | 1L    | 704 | -    | -       | 7/45/45/54   | -       |
| 50  | PC1  | 1M    | 502 | -    | -       | 7/47/47/57   | -       |
| 58  | EHZ  | 1n    | 201 | -    | -       | 15/42/44/45  | -       |
| 52  | PGT  | 1M    | 501 | -    | -       | 22/55/55/55  | -       |
| 46  | SF4  | 1I    | 202 | 9    | -       | -            | 0/6/5/5 |
| 53  | CDL  | 1a    | 101 | -    | -       | 10/71/71/110 | -       |
| 58  | EHZ  | 1W    | 201 | -    | -       | 6/42/44/45   | -       |
| 50  | PC1  | 1J    | 201 | -    | -       | 5/38/38/57   | -       |
| 46  | SF4  | 1F    | 502 | 6    | -       | -            | 0/6/5/5 |
| 46  | SF4  | 1I    | 201 | 9    | -       | -            | 0/6/5/5 |
| 50  | PC1  | 1I    | 203 | -    | -       | 5/47/47/57   | -       |
| 51  | MYR  | 1L    | 701 | -    | -       | 2/12/12/13   | -       |

There are no bond length outliers.

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 58  | 1W    | 201 | EHZ  | C10-S1-C9   | 6.49 | 121.03      | 101.84   |
| 58  | 1n    | 201 | EHZ  | C10-S1-C9   | 6.45 | 120.90      | 101.84   |
| 45  | 1L    | 704 | 3PE  | O21-C21-C22 | 6.44 | 125.41      | 111.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 56  | 1P    | 501 | NDP  | P2B-O2B-C2B | -4.62 | 111.09      | 123.43   |
| 58  | 1n    | 201 | EHZ  | C14-C13-C12 | 3.04  | 117.46      | 112.39   |
| 45  | 1L    | 704 | 3PE  | O21-C21-O22 | -2.80 | 117.16      | 123.70   |
| 45  | 1L    | 704 | 3PE  | C2-O21-C21  | 2.62  | 124.07      | 117.80   |
| 45  | 1L    | 704 | 3PE  | O21-C2-C3   | 2.23  | 116.34      | 108.34   |
| 45  | 1L    | 704 | 3PE  | O21-C2-C1   | 2.07  | 115.77      | 108.34   |
| 48  | 1F    | 501 | FMN  | C4-N3-C2    | -2.07 | 121.97      | 125.64   |

There are no chirality outliers.

All (142) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | 1L    | 703 | 3PE  | C1-O11-P-O14    |
| 45  | 1L    | 703 | 3PE  | O32-C31-O31-C3  |
| 45  | 1L    | 703 | 3PE  | C32-C31-O31-C3  |
| 45  | 1L    | 703 | 3PE  | O22-C21-O21-C2  |
| 45  | 1L    | 703 | 3PE  | C22-C21-O21-C2  |
| 45  | 1L    | 704 | 3PE  | C1-O11-P-O14    |
| 45  | 1L    | 704 | 3PE  | O22-C21-O21-C2  |
| 45  | 1L    | 704 | 3PE  | C22-C21-O21-C2  |
| 45  | 1N    | 401 | 3PE  | C1-O11-P-O14    |
| 45  | 1Y    | 201 | 3PE  | C1-O11-P-O14    |
| 50  | 1I    | 203 | PC1  | C11-O13-P-O14   |
| 50  | 1I    | 203 | PC1  | C11-O13-P-O11   |
| 50  | 1J    | 201 | PC1  | C1-O11-P-O14    |
| 50  | 1J    | 201 | PC1  | C1-O11-P-O13    |
| 50  | 1M    | 502 | PC1  | C1-O11-P-O14    |
| 50  | 1f    | 101 | PC1  | O32-C31-O31-C3  |
| 50  | 1f    | 101 | PC1  | C32-C31-O31-C3  |
| 51  | 1L    | 701 | MYR  | O1-C1-C2-C3     |
| 52  | 1M    | 501 | PGT  | O31-C31-O2-C2   |
| 52  | 1M    | 501 | PGT  | C1-O3P-P-O1P    |
| 52  | 1M    | 501 | PGT  | C4-O4P-P-O3P    |
| 52  | 1M    | 501 | PGT  | C5-C4-O4P-P     |
| 52  | 1M    | 501 | PGT  | C4-C5-C6-O6     |
| 52  | 1M    | 501 | PGT  | O5-C5-C6-O6     |
| 52  | 1M    | 501 | PGT  | O11-C11-O3-C3   |
| 52  | 1M    | 501 | PGT  | C12-C11-O3-C3   |
| 53  | 1a    | 101 | CDL  | CA3-OA5-PA1-OA3 |
| 53  | 1a    | 101 | CDL  | CB3-OB5-PB2-OB3 |
| 53  | 1a    | 101 | CDL  | CB4-CB3-OB5-PB2 |
| 56  | 1P    | 501 | NDP  | C5B-O5B-PA-O1A  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 56  | 1P    | 501 | NDP  | C5B-O5B-PA-O2A  |
| 56  | 1P    | 501 | NDP  | C4B-C5B-O5B-PA  |
| 56  | 1P    | 501 | NDP  | O4D-C1D-N1N-C6N |
| 58  | 1W    | 201 | EHZ  | C16-C17-C20-O6  |
| 58  | 1W    | 201 | EHZ  | C18-C17-C20-O6  |
| 58  | 1W    | 201 | EHZ  | C19-C17-C20-O6  |
| 58  | 1W    | 201 | EHZ  | O2-C9-S1-C10    |
| 58  | 1W    | 201 | EHZ  | C8-C9-S1-C10    |
| 58  | 1n    | 201 | EHZ  | S1-C10-C11-N1   |
| 58  | 1n    | 201 | EHZ  | N2-C15-C16-C17  |
| 58  | 1n    | 201 | EHZ  | N2-C15-C16-O5   |
| 58  | 1n    | 201 | EHZ  | O4-C15-C16-C17  |
| 58  | 1n    | 201 | EHZ  | O4-C15-C16-O5   |
| 58  | 1n    | 201 | EHZ  | C15-C16-C17-C18 |
| 58  | 1n    | 201 | EHZ  | C15-C16-C17-C19 |
| 58  | 1n    | 201 | EHZ  | C15-C16-C17-C20 |
| 58  | 1n    | 201 | EHZ  | O2-C9-S1-C10    |
| 58  | 1n    | 201 | EHZ  | C8-C9-S1-C10    |
| 52  | 1M    | 501 | PGT  | C32-C31-O2-C2   |
| 45  | 1Y    | 201 | 3PE  | C2-C1-O11-P     |
| 58  | 1n    | 201 | EHZ  | C13-C14-N2-C15  |
| 53  | 1N    | 402 | CDL  | OA6-CA4-CA6-OA8 |
| 52  | 1M    | 501 | PGT  | C15-C16-C17-C18 |
| 52  | 1M    | 501 | PGT  | C14-C15-C16-C17 |
| 50  | 1f    | 101 | PC1  | C35-C36-C37-C38 |
| 52  | 1M    | 501 | PGT  | C40-C41-C42-C43 |
| 56  | 1P    | 501 | NDP  | O4D-C4D-C5D-O5D |
| 56  | 1P    | 501 | NDP  | C3D-C4D-C5D-O5D |
| 52  | 1M    | 501 | PGT  | C34-C35-C36-C37 |
| 50  | 1I    | 203 | PC1  | O21-C2-C3-O31   |
| 52  | 1M    | 501 | PGT  | C44-C45-C46-C47 |
| 52  | 1M    | 501 | PGT  | C22-C23-C24-C25 |
| 56  | 1P    | 501 | NDP  | O4B-C4B-C5B-O5B |
| 45  | 1Y    | 201 | 3PE  | C35-C36-C37-C38 |
| 50  | 1I    | 203 | PC1  | C1-C2-C3-O31    |
| 50  | 1H    | 401 | PC1  | C24-C25-C26-C27 |
| 45  | 1L    | 704 | 3PE  | O11-C1-C2-O21   |
| 50  | 1M    | 502 | PC1  | O11-C1-C2-C3    |
| 53  | 1N    | 402 | CDL  | CA3-CA4-CA6-OA8 |
| 45  | 1Y    | 201 | 3PE  | C3C-C3D-C3E-C3F |
| 53  | 1a    | 101 | CDL  | CA4-CA3-OA5-PA1 |
| 45  | 1N    | 401 | 3PE  | O31-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 45  | 1A    | 201 | 3PE  | O21-C2-C3-O31   |
| 53  | 1N    | 402 | CDL  | C75-C76-C77-C78 |
| 52  | 1M    | 501 | PGT  | C21-C22-C23-C24 |
| 53  | 1N    | 402 | CDL  | OA5-CA3-CA4-CA6 |
| 50  | 1I    | 203 | PC1  | C32-C33-C34-C35 |
| 45  | 1Y    | 201 | 3PE  | O11-C1-C2-O21   |
| 50  | 1M    | 502 | PC1  | O11-C1-C2-O21   |
| 45  | 1N    | 401 | 3PE  | C2-C3-O31-C31   |
| 58  | 1n    | 201 | EHZ  | C2-C1-C21-C22   |
| 45  | 1Y    | 201 | 3PE  | C12-C11-O13-P   |
| 50  | 1H    | 401 | PC1  | O21-C2-C3-O31   |
| 50  | 1J    | 201 | PC1  | O21-C2-C3-O31   |
| 53  | 1a    | 101 | CDL  | OB6-CB4-CB6-OB8 |
| 50  | 1J    | 201 | PC1  | O13-C11-C12-N   |
| 53  | 1N    | 402 | CDL  | C32-C33-C34-C35 |
| 48  | 1F    | 501 | FMN  | N10-C1'-C2'-O2' |
| 52  | 1M    | 501 | PGT  | C33-C34-C35-C36 |
| 50  | 1H    | 401 | PC1  | C1-C2-C3-O31    |
| 53  | 1N    | 402 | CDL  | C55-C56-C57-C58 |
| 45  | 1N    | 401 | 3PE  | C34-C35-C36-C37 |
| 50  | 1M    | 502 | PC1  | C1-O11-P-O12    |
| 50  | 1M    | 502 | PC1  | C1-O11-P-O13    |
| 50  | 1f    | 101 | PC1  | C11-O13-P-O14   |
| 52  | 1M    | 501 | PGT  | C4-O4P-P-O1P    |
| 53  | 1a    | 101 | CDL  | CB2-OB2-PB2-OB3 |
| 56  | 1P    | 501 | NDP  | C5B-O5B-PA-O3   |
| 58  | 1n    | 201 | EHZ  | O5-C16-C17-C20  |
| 45  | 1L    | 703 | 3PE  | C31-C32-C33-C34 |
| 45  | 1N    | 401 | 3PE  | C2-C1-O11-P     |
| 53  | 1a    | 101 | CDL  | C52-C51-CB5-OB6 |
| 45  | 1L    | 704 | 3PE  | C1-C2-C3-O31    |
| 54  | 1O    | 401 | GTP  | PG-O3B-PB-O1B   |
| 50  | 1H    | 401 | PC1  | O31-C31-C32-C33 |
| 53  | 1N    | 402 | CDL  | CB2-C1-CA2-OA2  |
| 45  | 1Y    | 201 | 3PE  | O11-C1-C2-C3    |
| 45  | 1L    | 702 | 3PE  | C33-C34-C35-C36 |
| 52  | 1M    | 501 | PGT  | O2-C2-C3-O3     |
| 45  | 1A    | 201 | 3PE  | C32-C33-C34-C35 |
| 45  | 1L    | 704 | 3PE  | C1-C2-O21-C21   |
| 45  | 1N    | 401 | 3PE  | C3A-C3B-C3C-C3D |
| 50  | 1M    | 502 | PC1  | C25-C26-C27-C28 |
| 52  | 1M    | 501 | PGT  | C2-C1-O3P-P     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 53  | 1N    | 402 | CDL  | OA5-CA3-CA4-OA6 |
| 58  | 1n    | 201 | EHZ  | C12-C13-C14-N2  |
| 53  | 1N    | 402 | CDL  | C53-C54-C55-C56 |
| 54  | 1O    | 401 | GTP  | C4'-C5'-O5'-PA  |
| 45  | 1Y    | 201 | 3PE  | C24-C25-C26-C27 |
| 53  | 1a    | 101 | CDL  | CB2-C1-CA2-OA2  |
| 45  | 1A    | 201 | 3PE  | C1-C2-C3-O31    |
| 53  | 1a    | 101 | CDL  | CB3-CB4-CB6-OB8 |
| 50  | 1M    | 502 | PC1  | C31-C32-C33-C34 |
| 45  | 1N    | 401 | 3PE  | C39-C3A-C3B-C3C |
| 45  | 1L    | 702 | 3PE  | C37-C38-C39-C3A |
| 54  | 1O    | 401 | GTP  | PG-O3B-PB-O2B   |
| 56  | 1P    | 501 | NDP  | PN-O3-PA-O2A    |
| 52  | 1M    | 501 | PGT  | C19-C20-C21-C22 |
| 45  | 1N    | 401 | 3PE  | O11-C1-C2-O21   |
| 50  | 1f    | 101 | PC1  | C3C-C3D-C3E-C3F |
| 50  | 1J    | 201 | PC1  | C1-C2-C3-O31    |
| 52  | 1M    | 501 | PGT  | C1-C2-C3-O3     |
| 45  | 1L    | 703 | 3PE  | C32-C33-C34-C35 |
| 48  | 1F    | 501 | FMN  | N10-C1'-C2'-C3' |
| 45  | 1L    | 704 | 3PE  | C22-C23-C24-C25 |
| 51  | 1L    | 701 | MYR  | C5-C6-C7-C8     |
| 50  | 1H    | 401 | PC1  | C3E-C3F-C3G-C3H |
| 50  | 1f    | 101 | PC1  | C2-C1-O11-P     |
| 53  | 1a    | 101 | CDL  | C12-C13-C14-C15 |
| 58  | 1n    | 201 | EHZ  | C4-C5-C6-C7     |
| 58  | 1W    | 201 | EHZ  | C21-C22-C23-C24 |
| 56  | 1P    | 501 | NDP  | PN-O3-PA-O1A    |

There are no ring outliers.

22 monomers are involved in 82 short contacts:

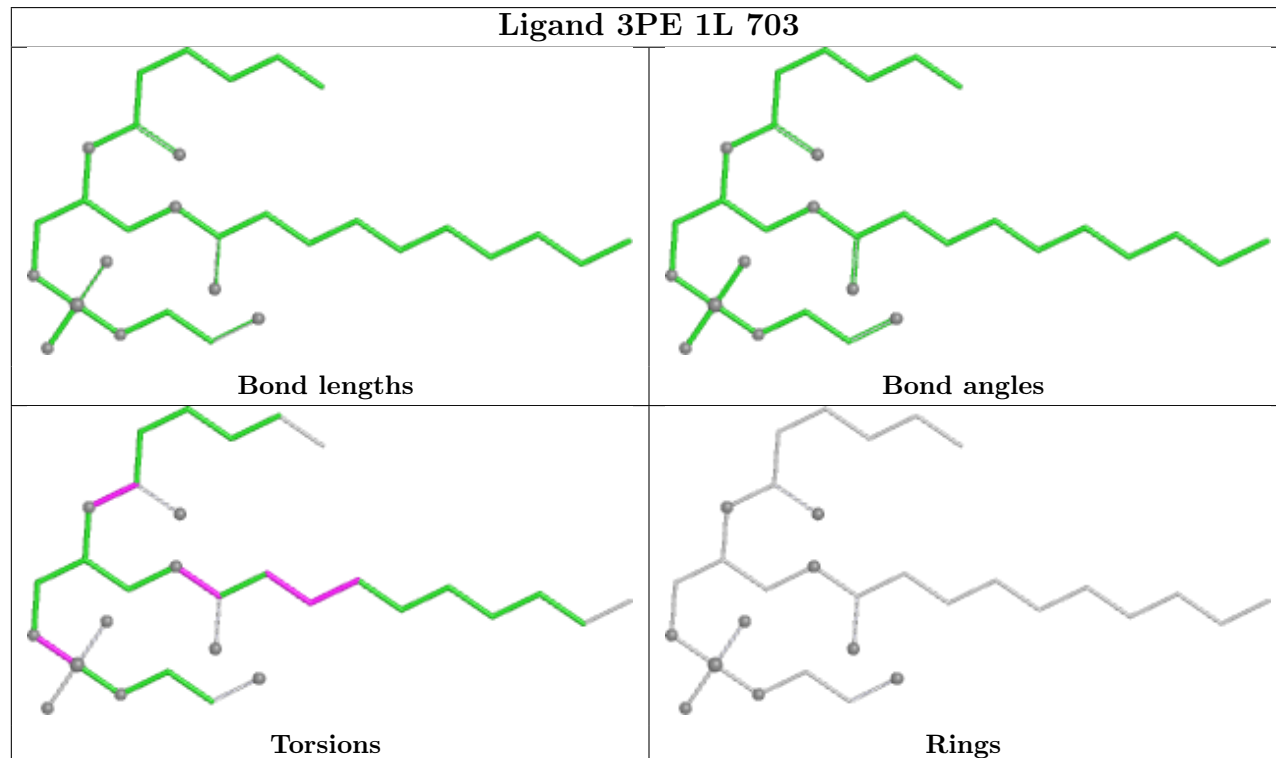
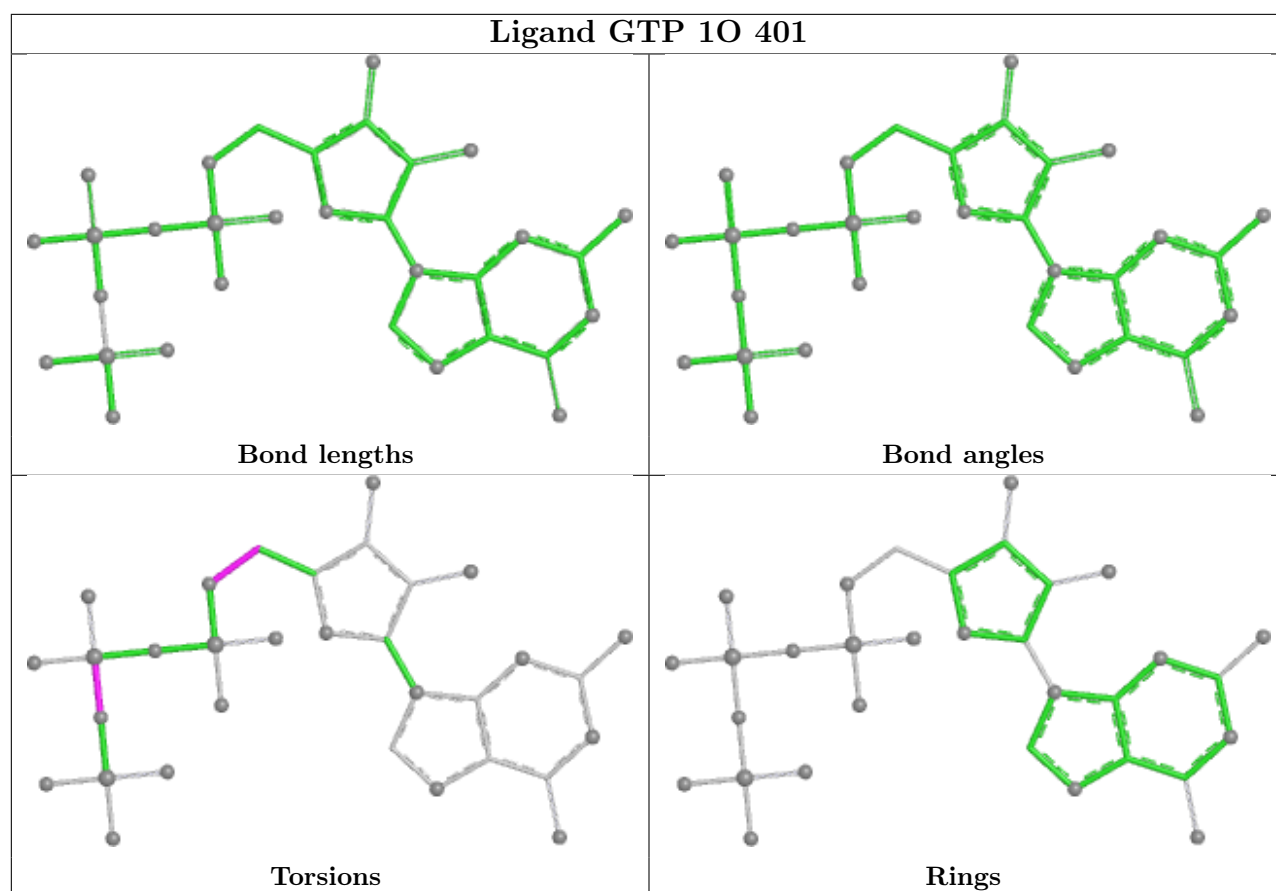
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 54  | 1O    | 401 | GTP  | 3       | 0            |
| 45  | 1L    | 703 | 3PE  | 6       | 0            |
| 45  | 1L    | 702 | 3PE  | 6       | 0            |
| 45  | 1N    | 401 | 3PE  | 6       | 0            |
| 46  | 1B    | 201 | SF4  | 2       | 0            |
| 46  | 1G    | 801 | SF4  | 1       | 0            |
| 48  | 1F    | 501 | FMN  | 4       | 0            |
| 50  | 1f    | 101 | PC1  | 6       | 0            |
| 53  | 1N    | 402 | CDL  | 2       | 0            |

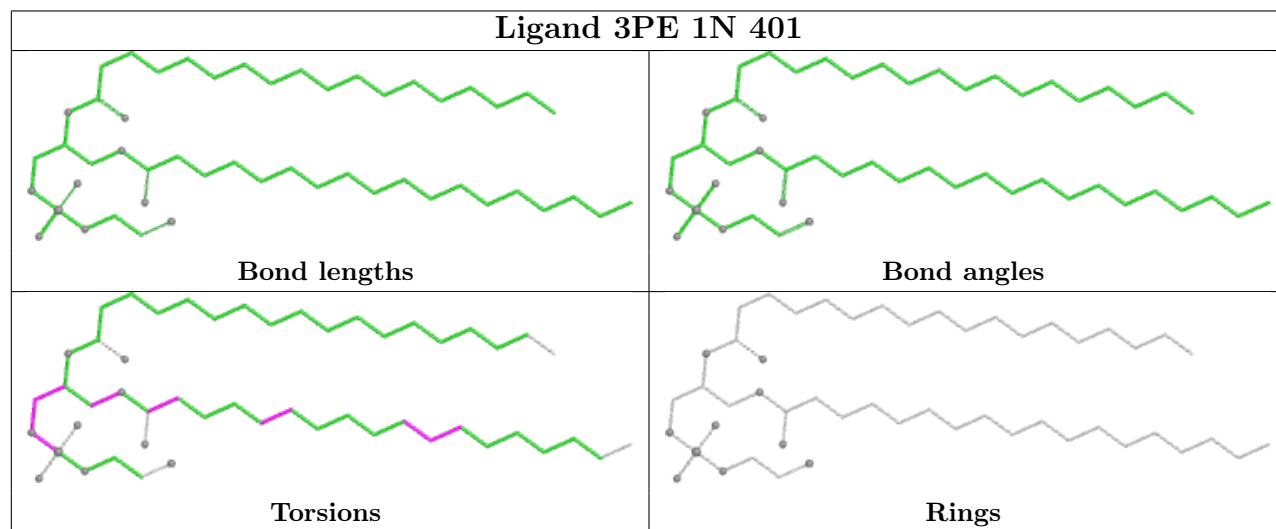
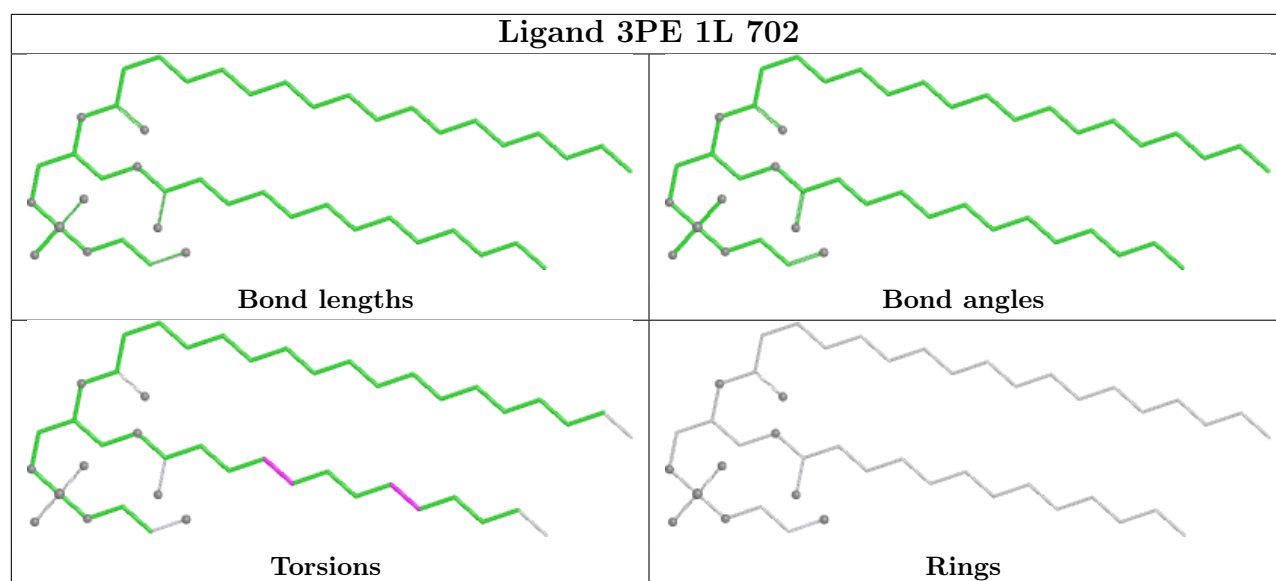
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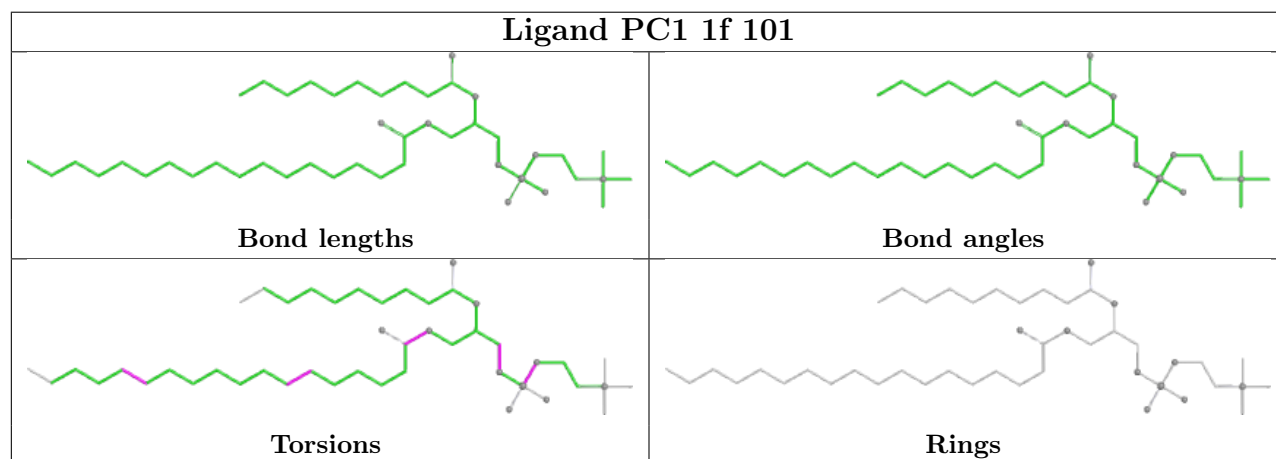
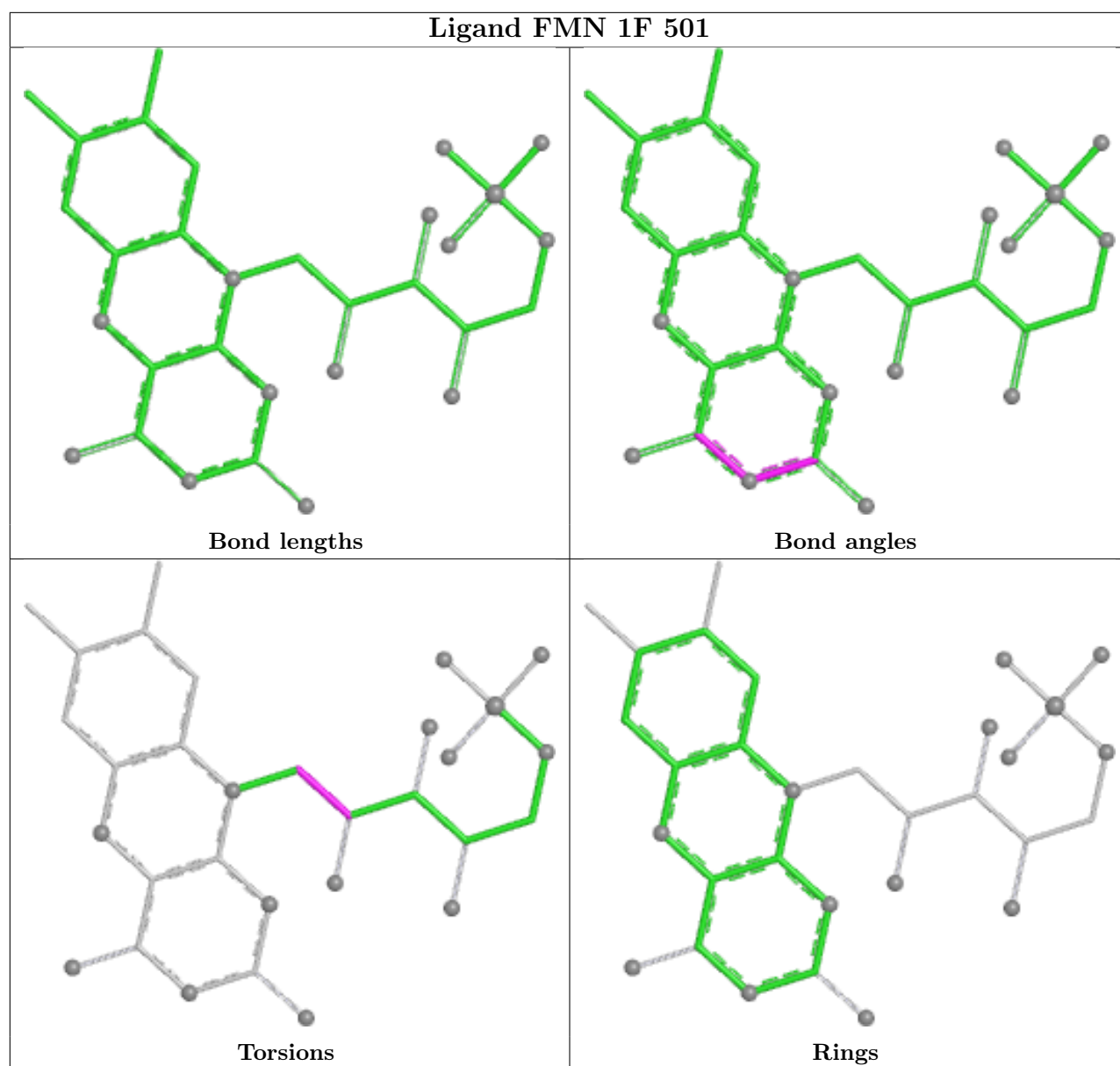
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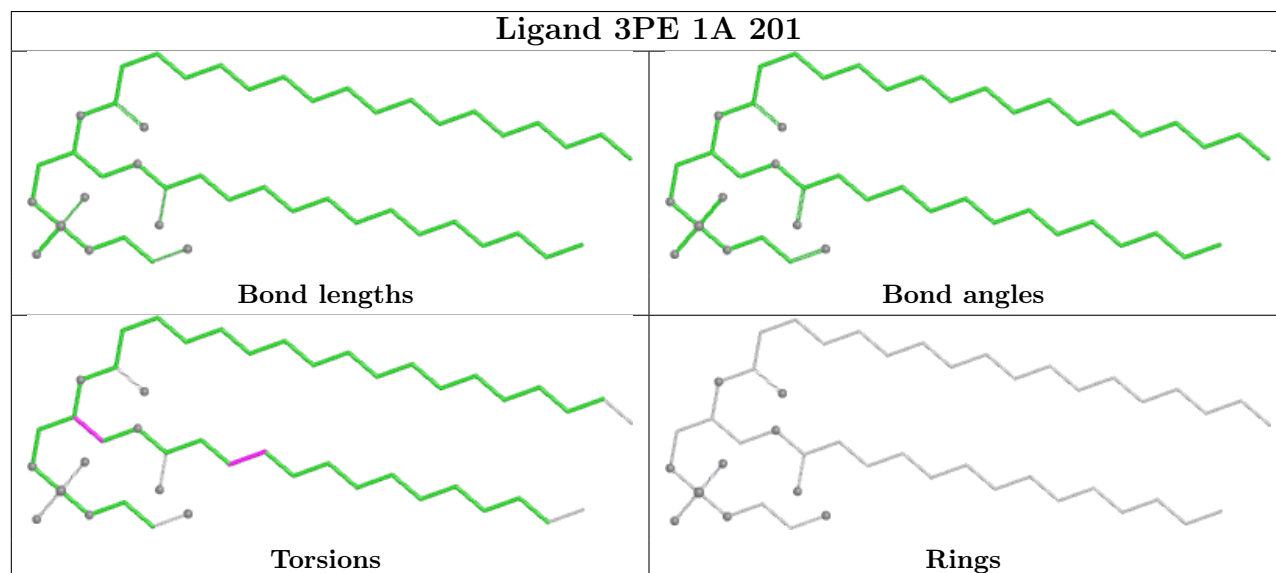
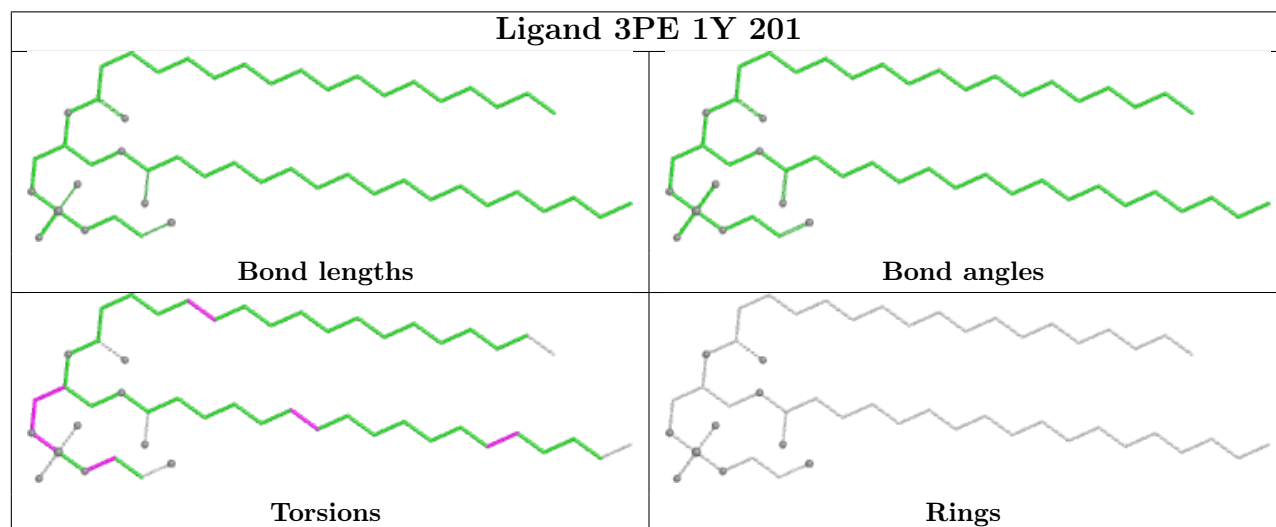
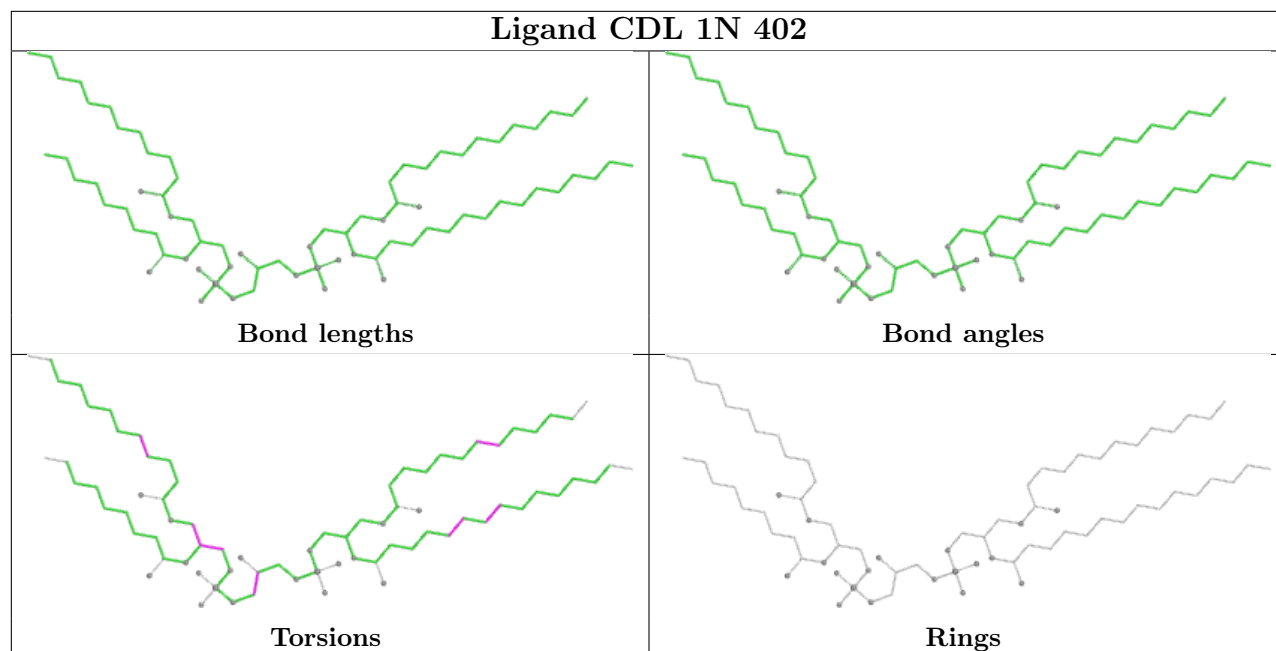
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 45  | 1Y    | 201 | 3PE  | 1       | 0            |
| 45  | 1A    | 201 | 3PE  | 4       | 0            |
| 50  | 1H    | 401 | PC1  | 7       | 0            |
| 56  | 1P    | 501 | NDP  | 5       | 0            |
| 45  | 1L    | 704 | 3PE  | 6       | 0            |
| 50  | 1M    | 502 | PC1  | 2       | 0            |
| 52  | 1M    | 501 | PGT  | 8       | 0            |
| 53  | 1a    | 101 | CDL  | 4       | 0            |
| 46  | 1I    | 201 | SF4  | 2       | 0            |
| 46  | 1F    | 502 | SF4  | 1       | 0            |
| 50  | 1J    | 201 | PC1  | 2       | 0            |
| 50  | 1I    | 203 | PC1  | 2       | 0            |
| 51  | 1L    | 701 | MYR  | 2       | 0            |

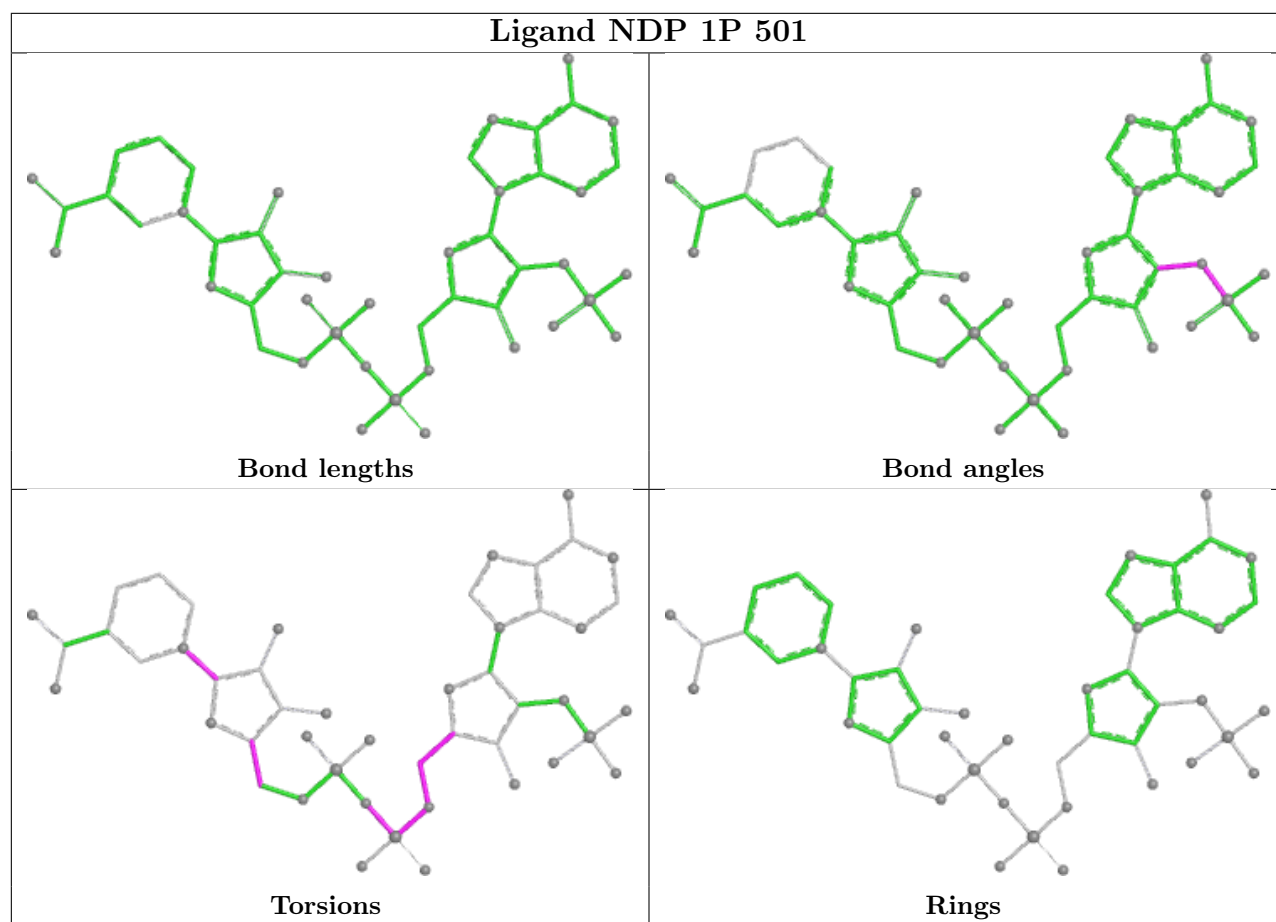
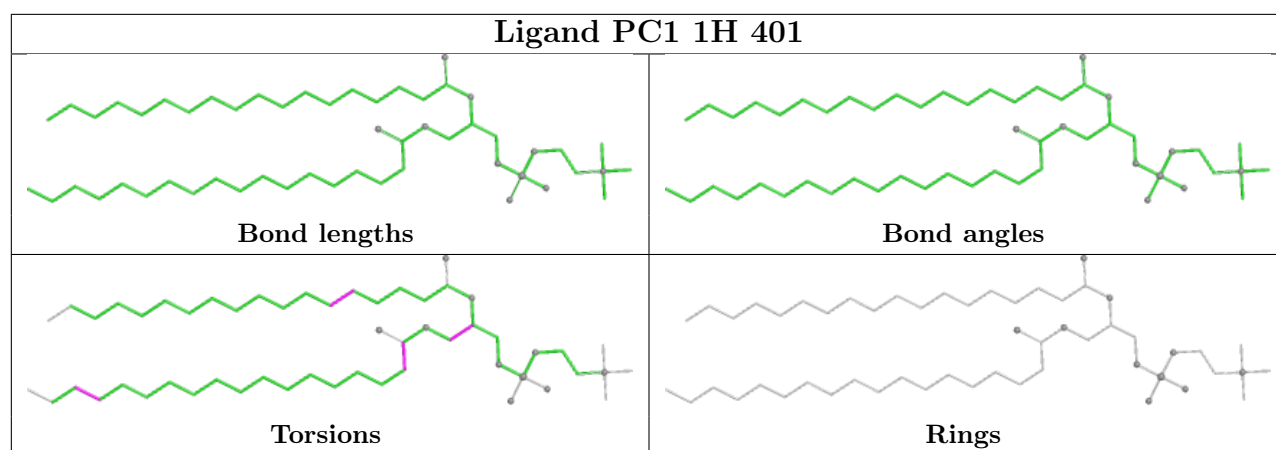
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

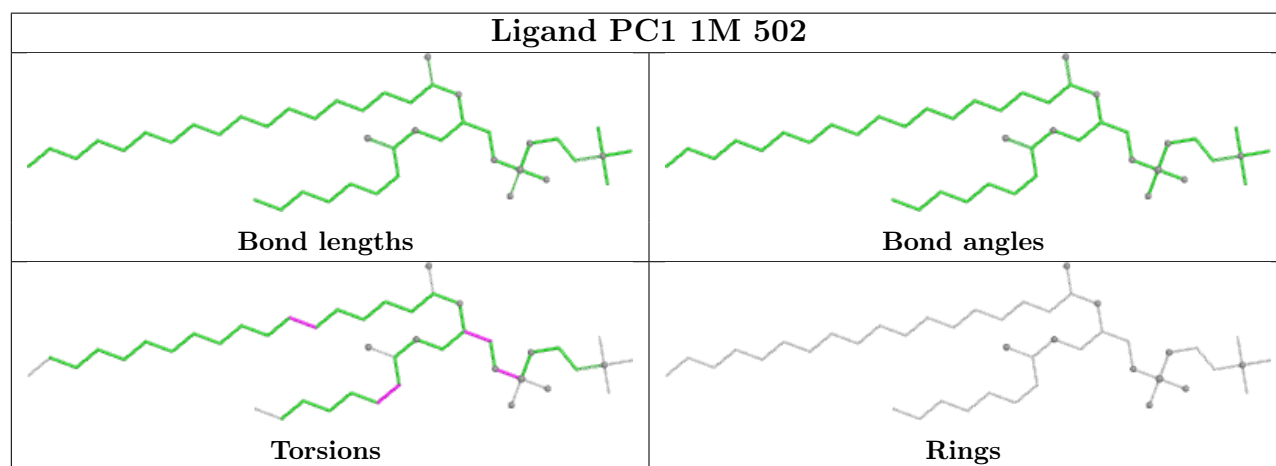
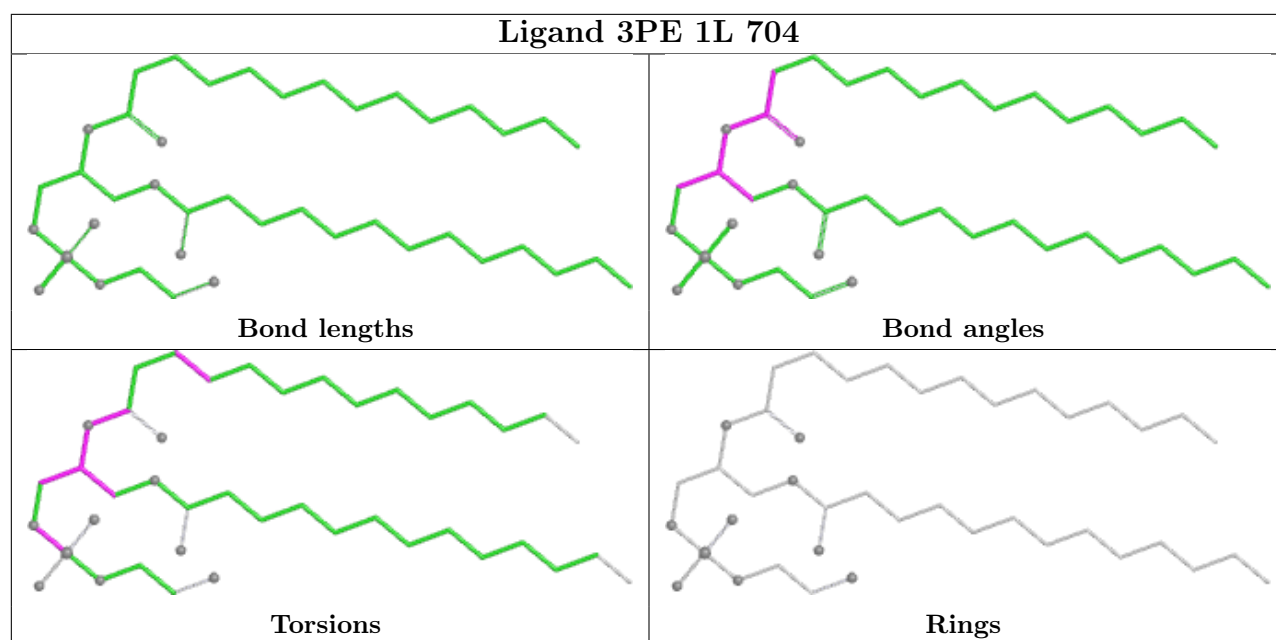


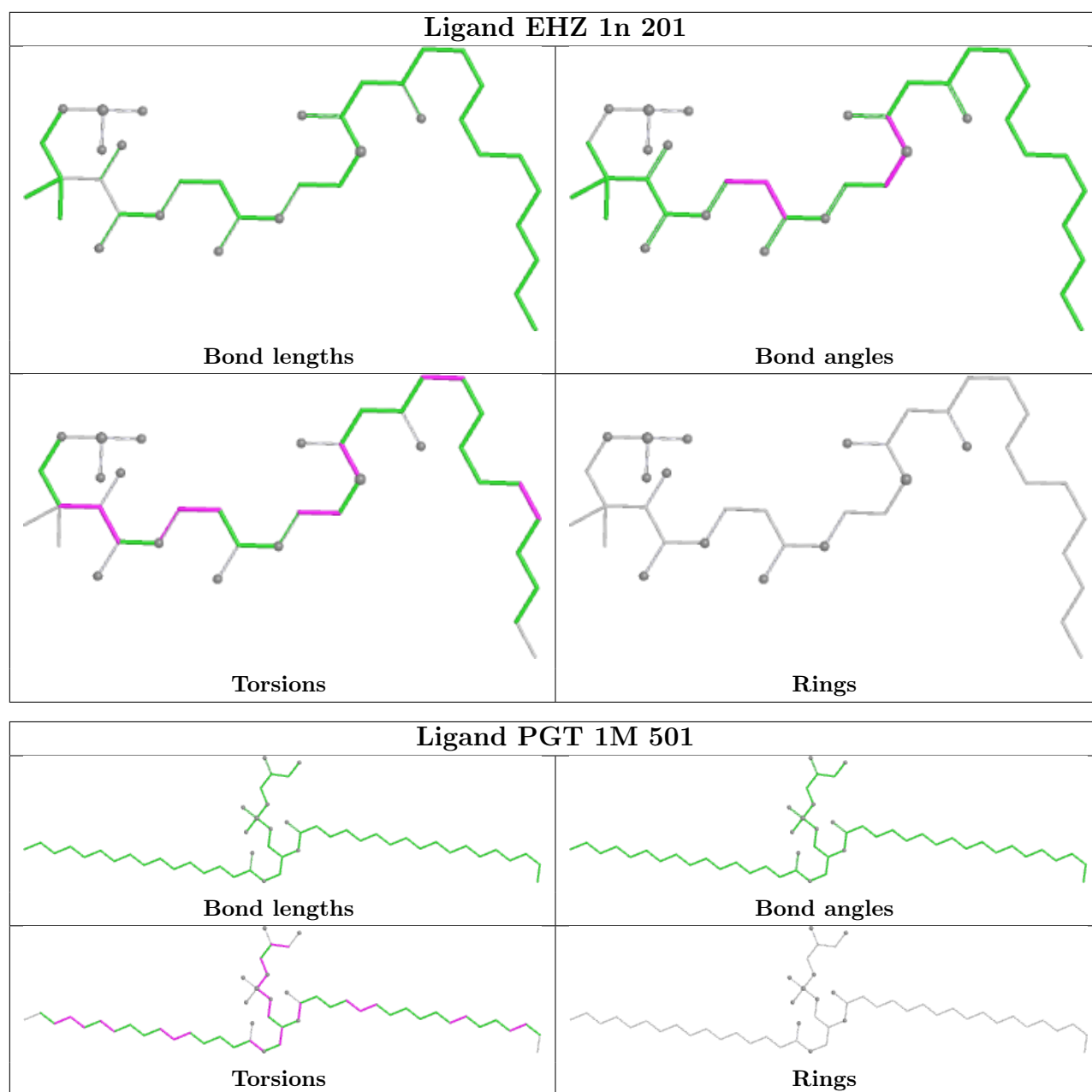


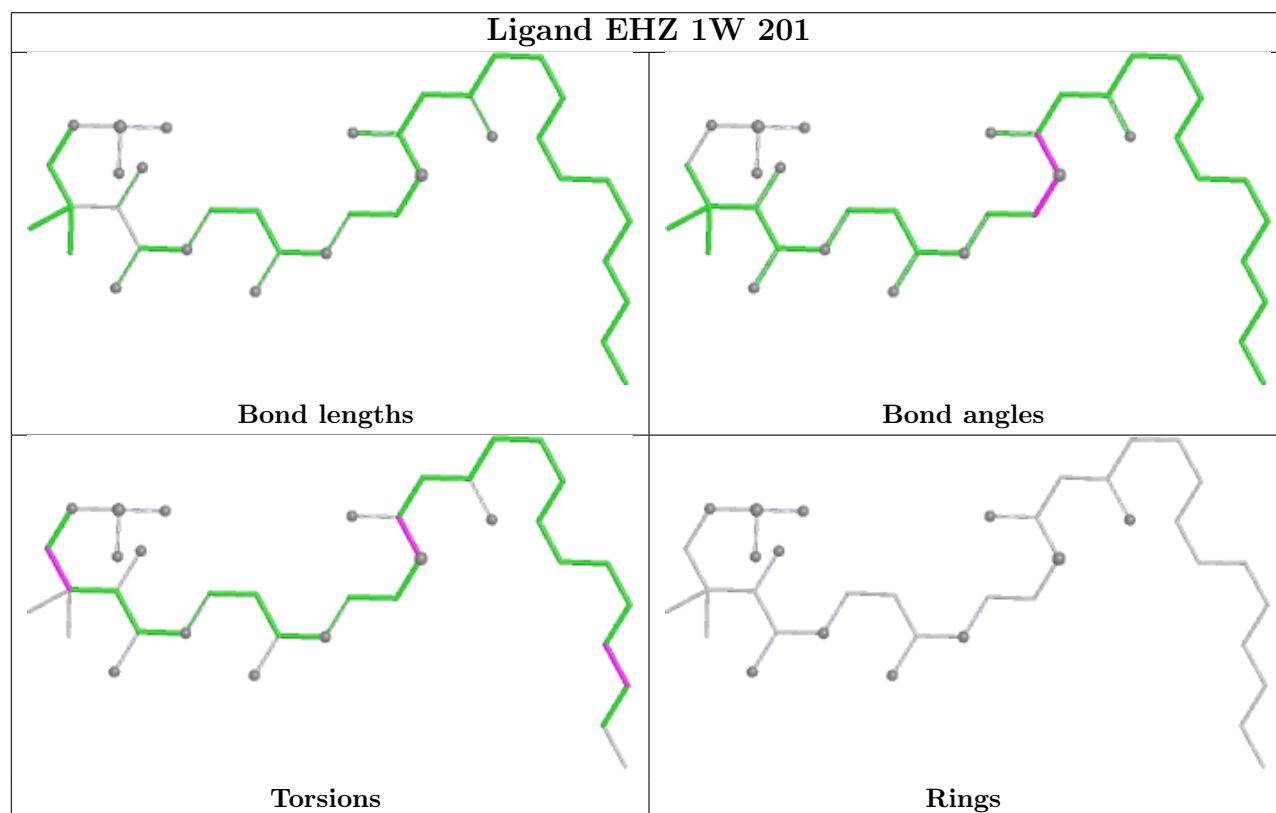
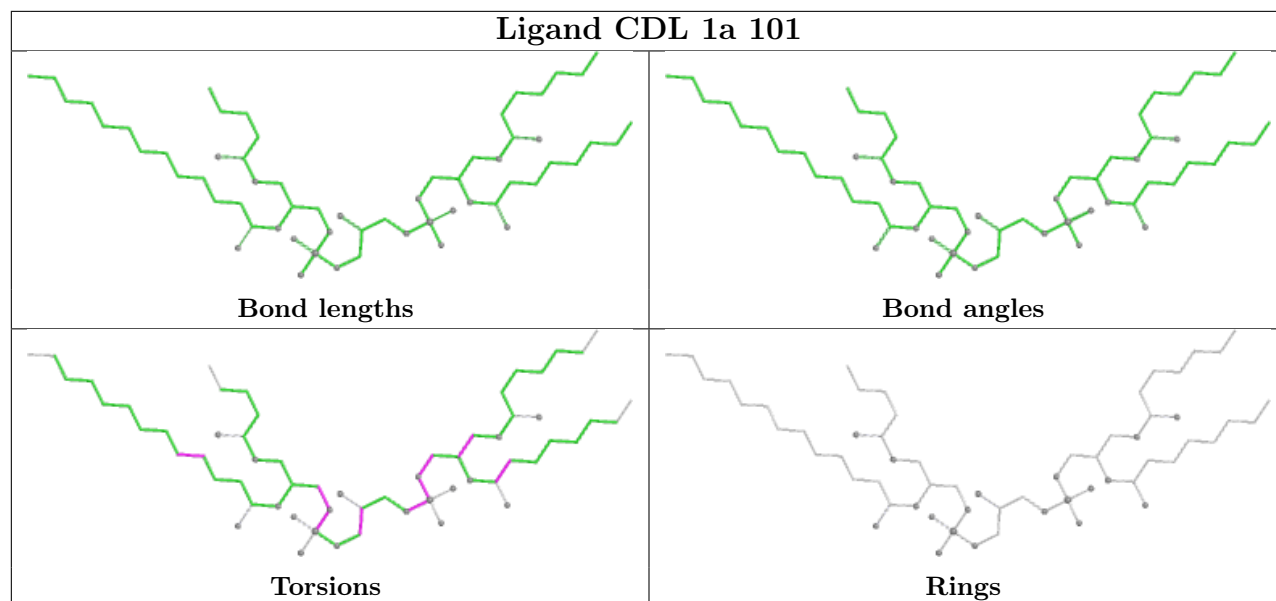


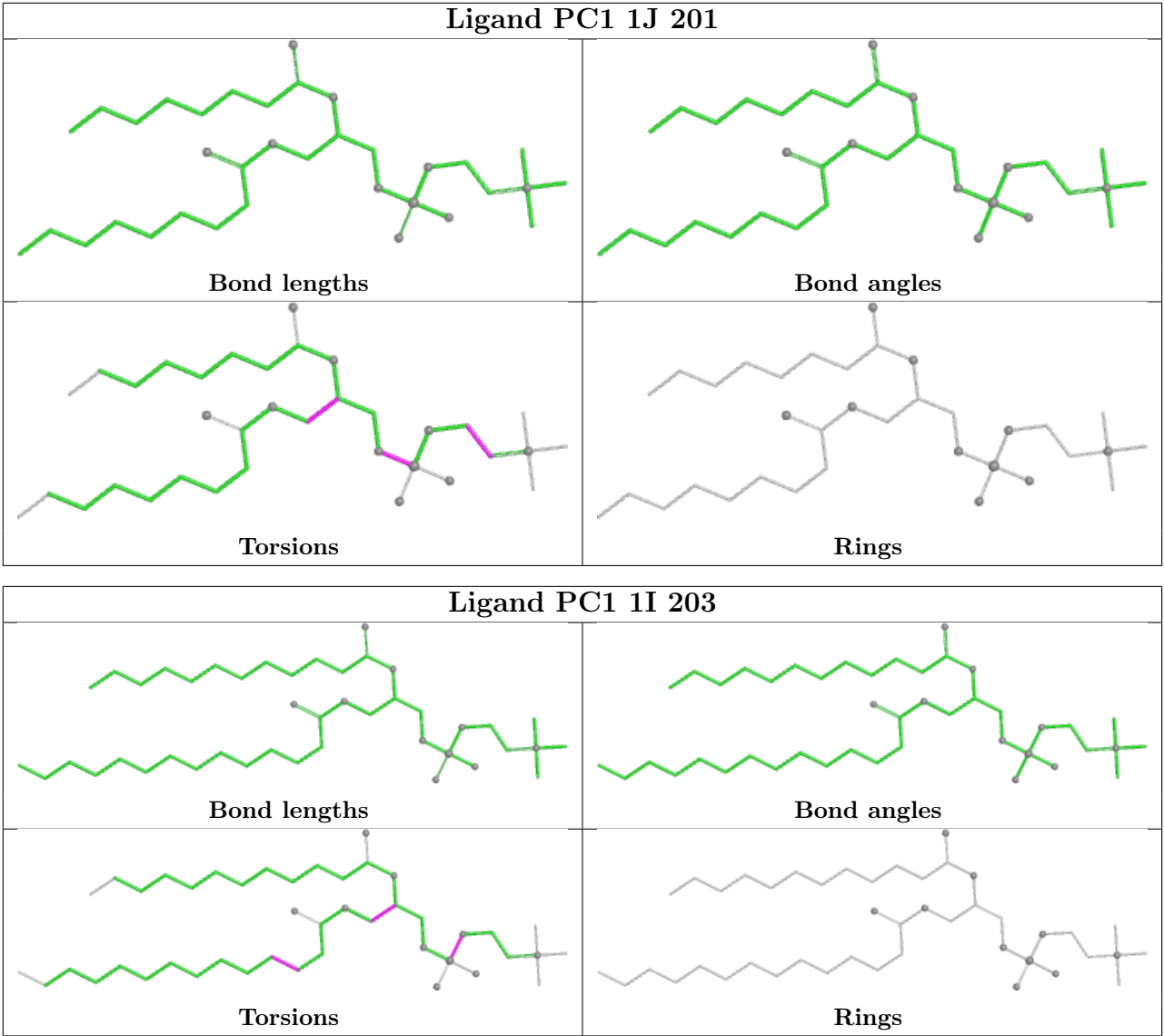












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 34  | 1i    | 1                |
| 43  | 1r    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | 1i    | 1:SAC     | C      | 2:GLY     | N      | 3.33         |
| 1     | 1r    | 1:ALA     | C      | 2:SER     | N      | 2.79         |

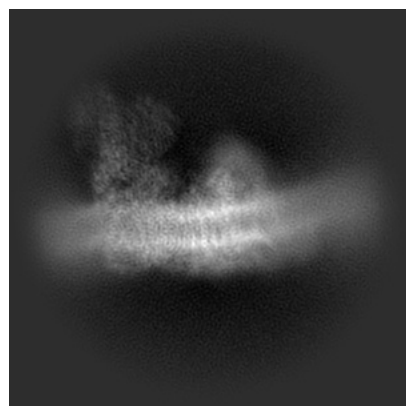
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42170. These allow visual inspection of the internal detail of the map and identification of artifacts.

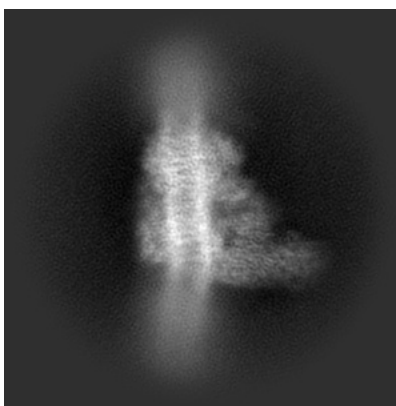
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

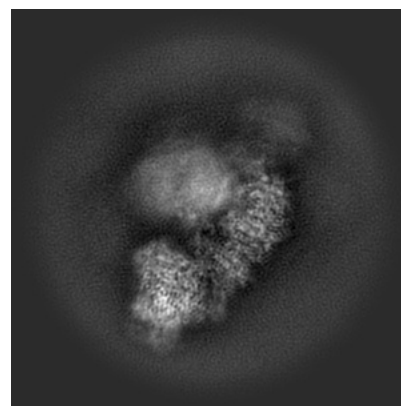
#### 6.1.1 Primary map



X

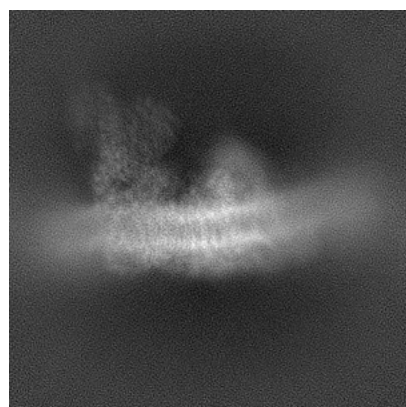


Y

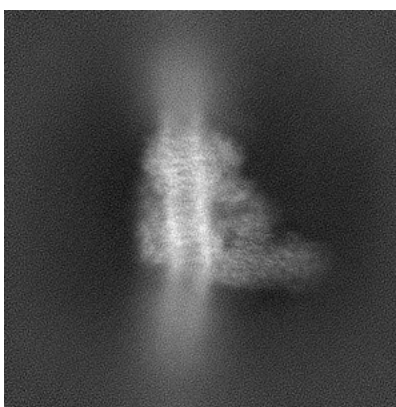


Z

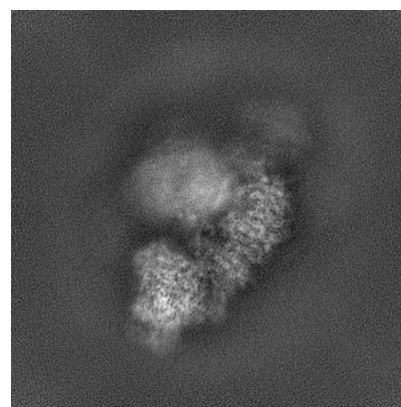
#### 6.1.2 Raw map



X



Y

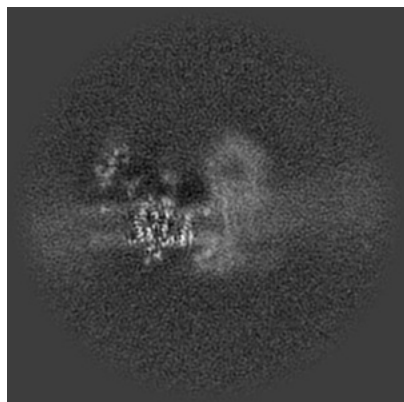


Z

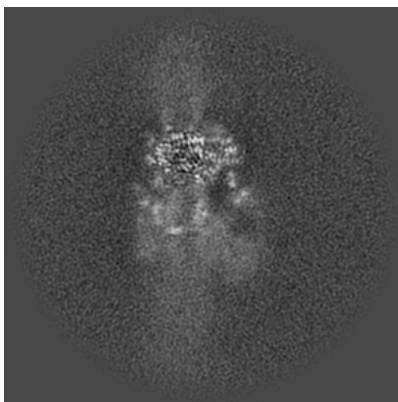
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

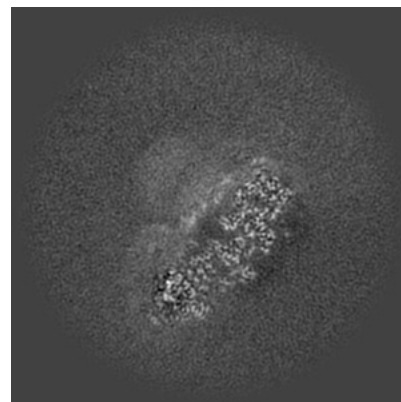
### 6.2.1 Primary map



X Index: 160



Y Index: 160

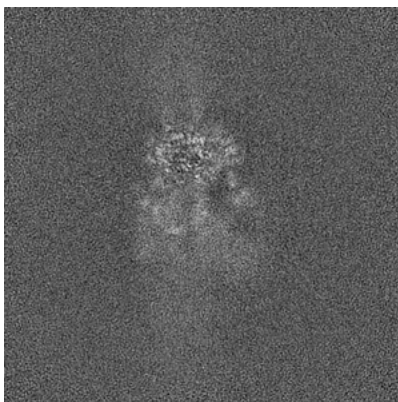


Z Index: 160

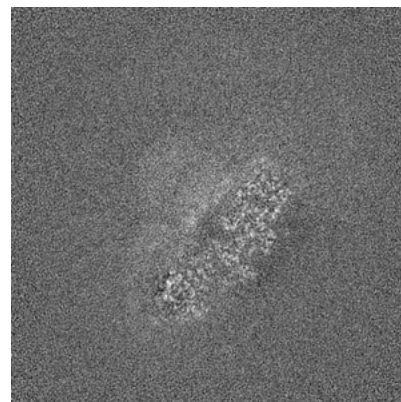
### 6.2.2 Raw map



X Index: 160



Y Index: 160

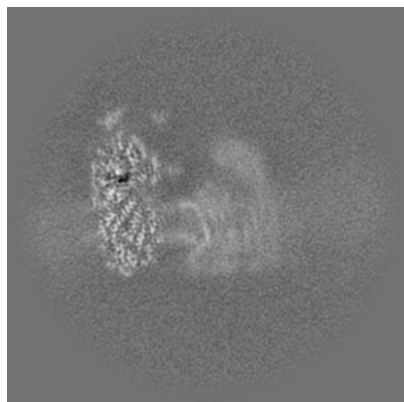


Z Index: 160

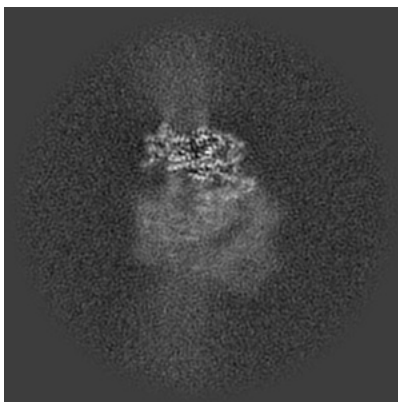
The images above show central slices of the map in three orthogonal directions.

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

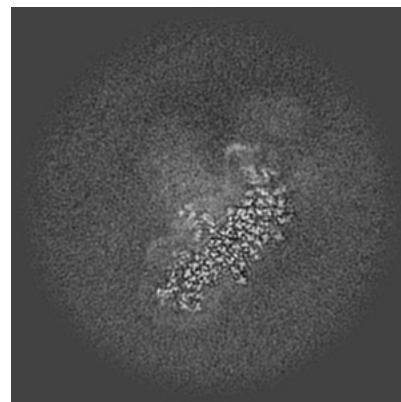
### 6.3.1 Primary map



X Index: 140

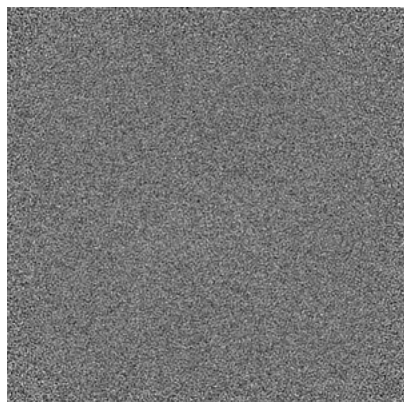


Y Index: 172

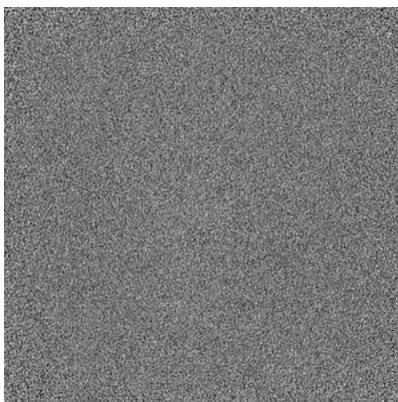


Z Index: 134

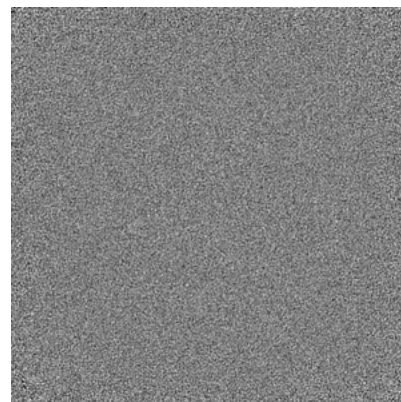
### 6.3.2 Raw map



X Index: 0



Y Index: 0

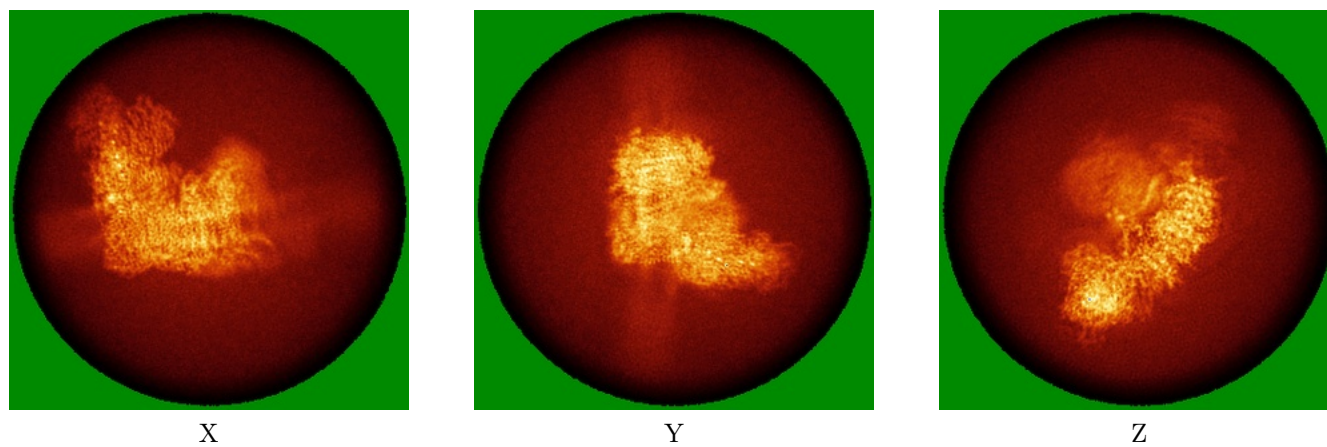


Z Index: 0

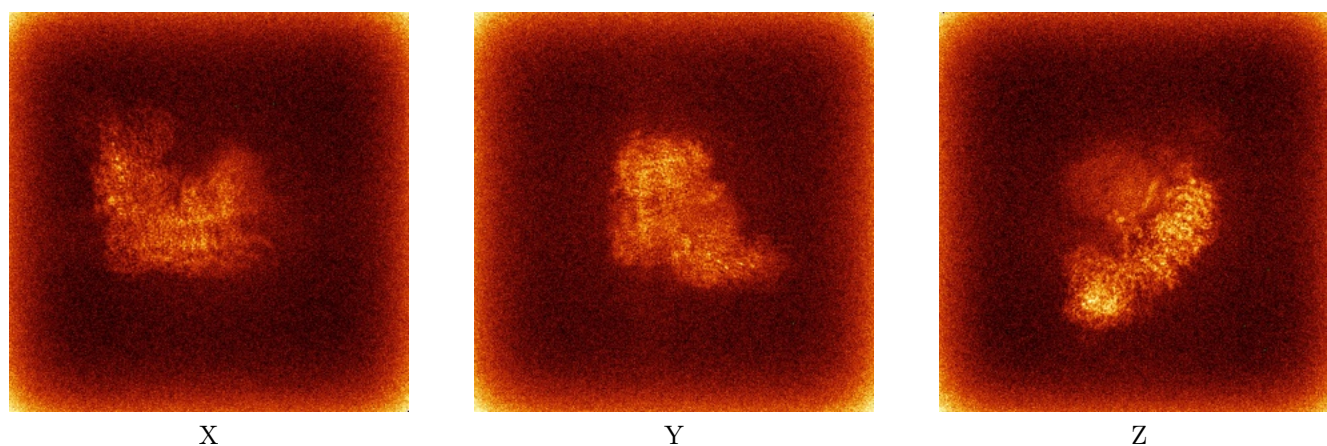
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

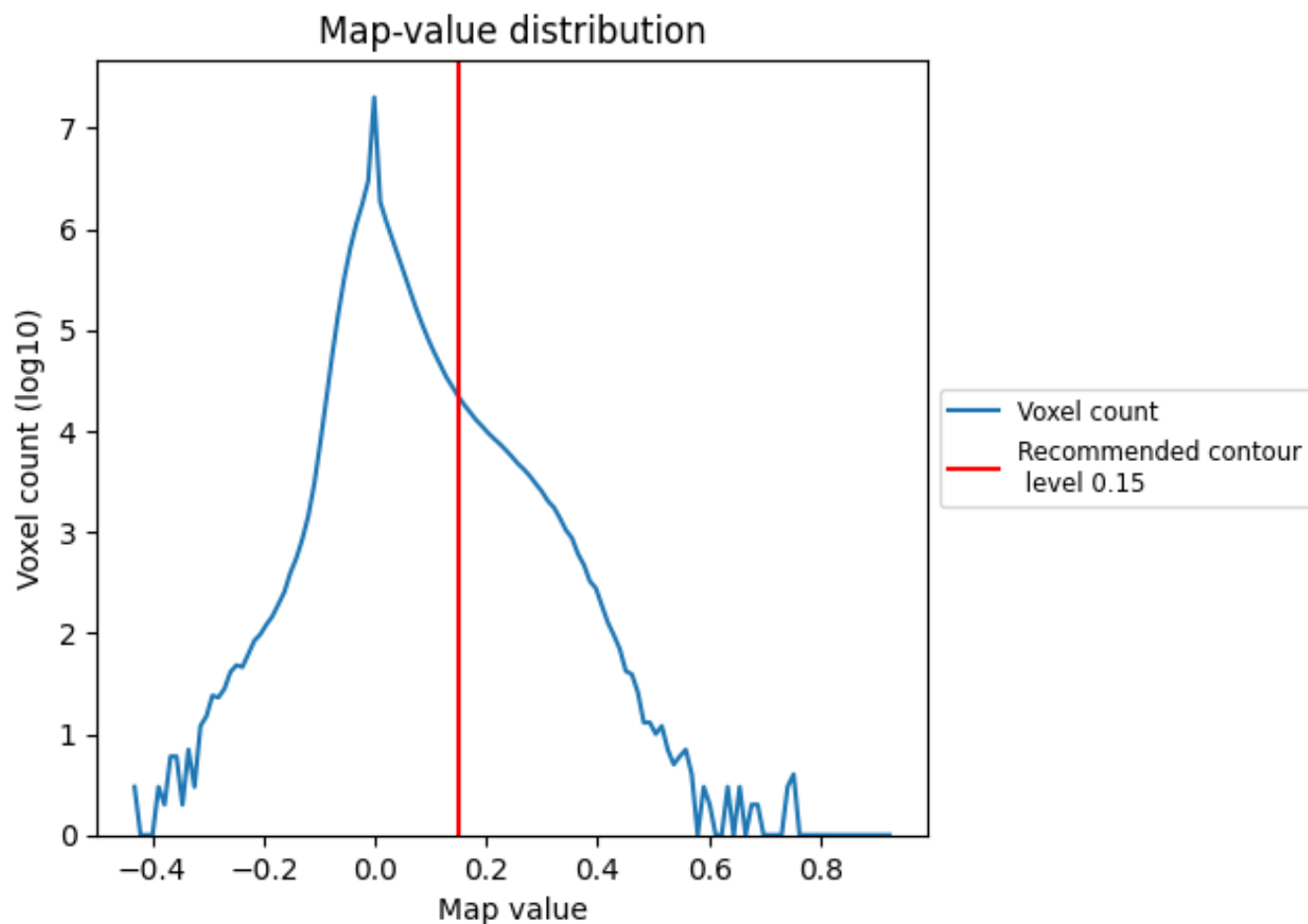
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

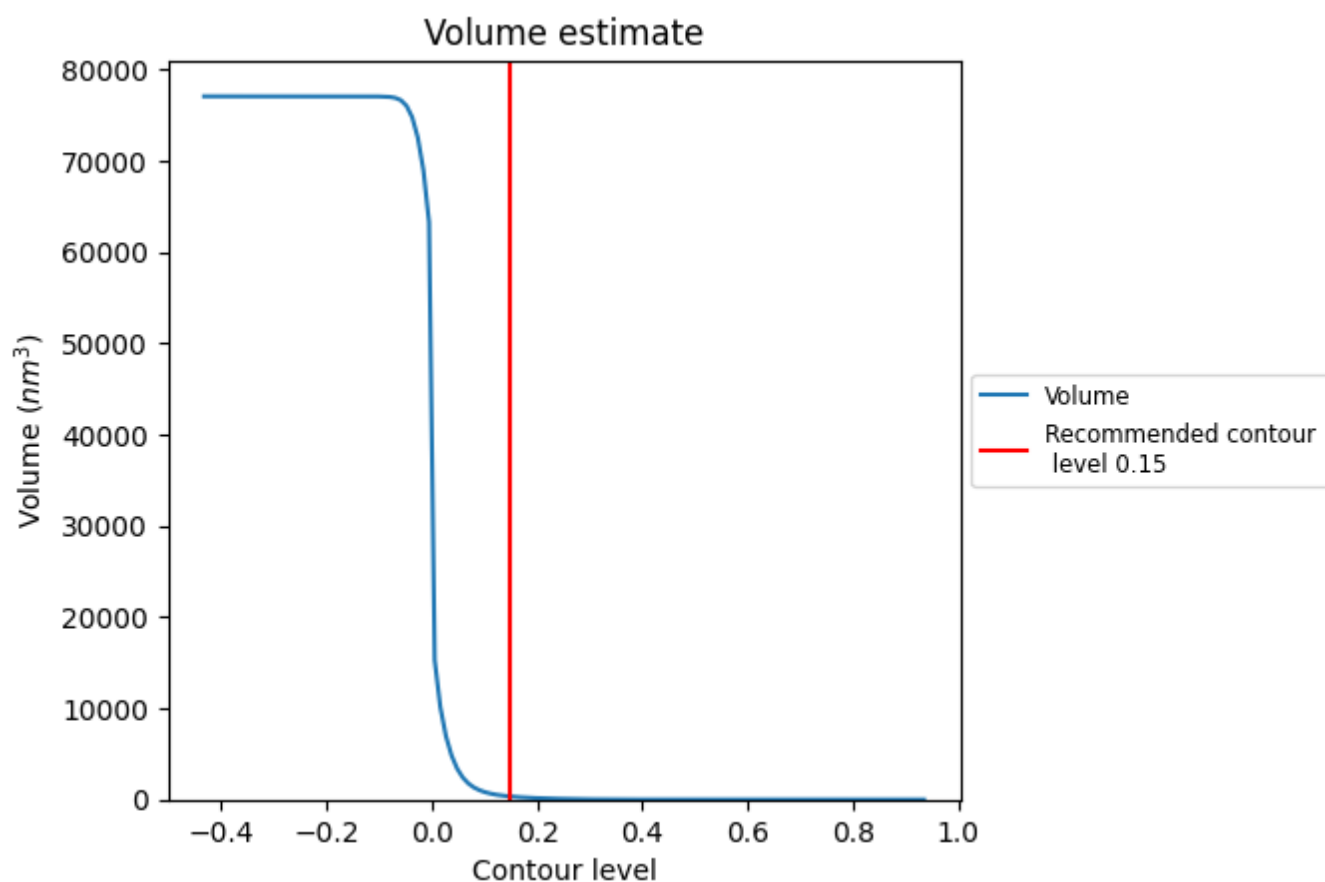
This section contains the results of statistical analysis of the map.

### 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.

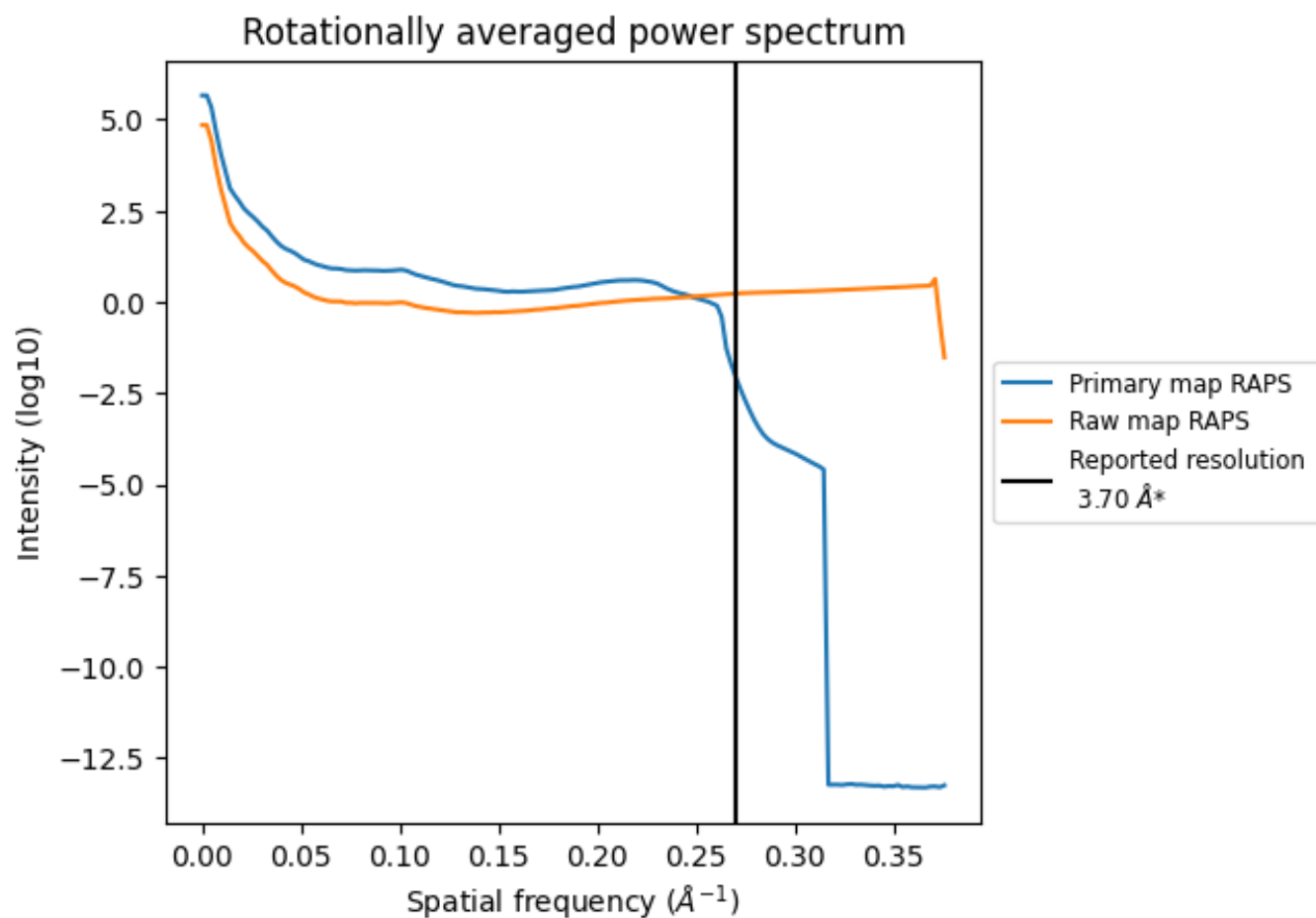
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm<sup>3</sup>; this corresponds to an approximate mass of 304 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 ⓘ

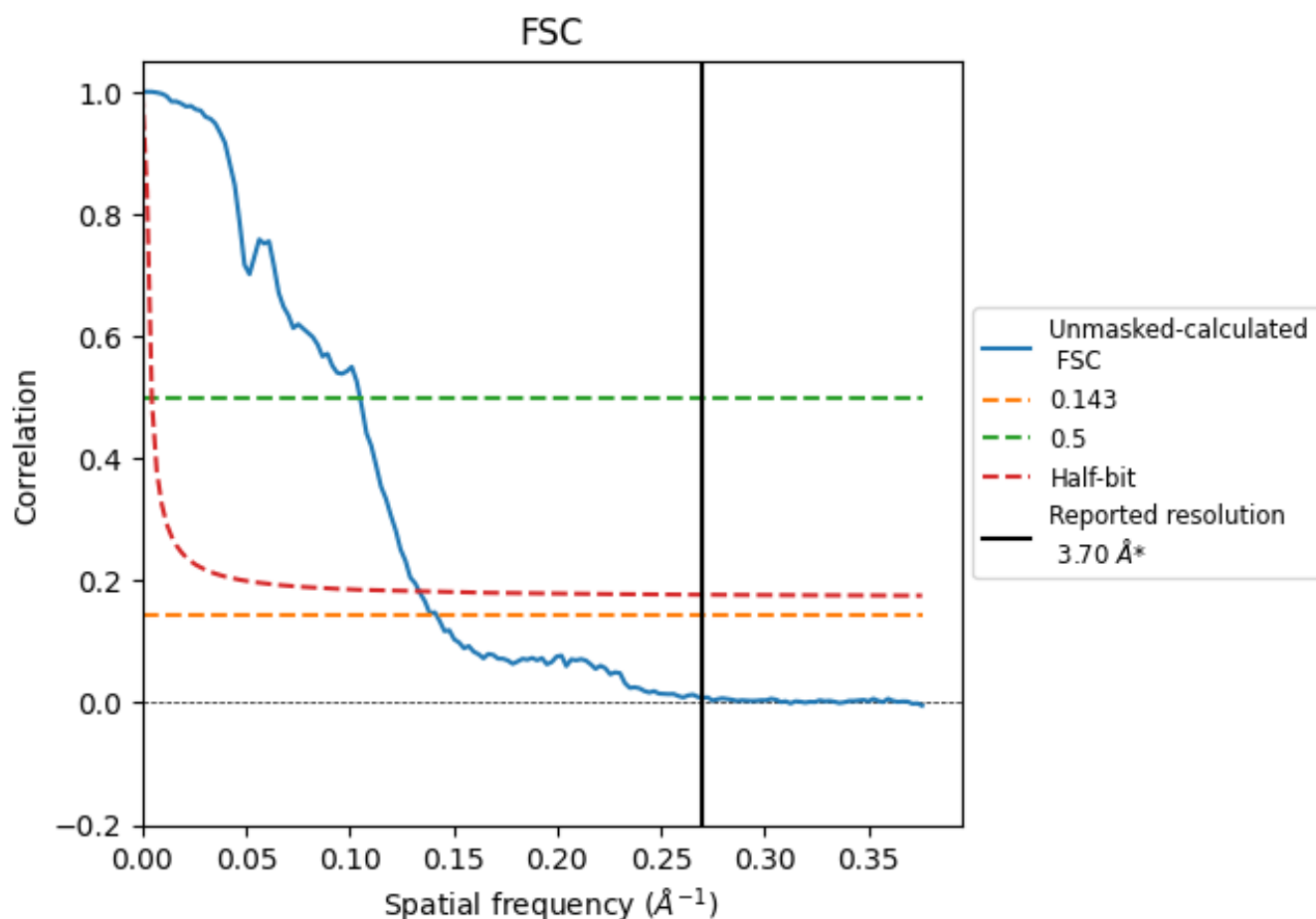


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 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 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

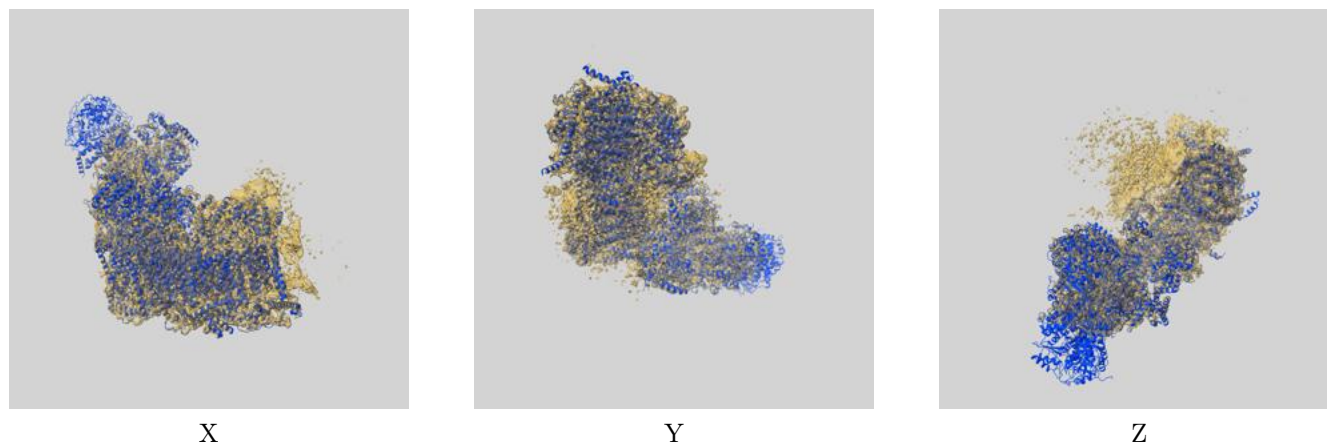
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 7.05                               | 9.53 | 7.49     |

\*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 7.05 differs from the reported value 3.7 by more than 10 %

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

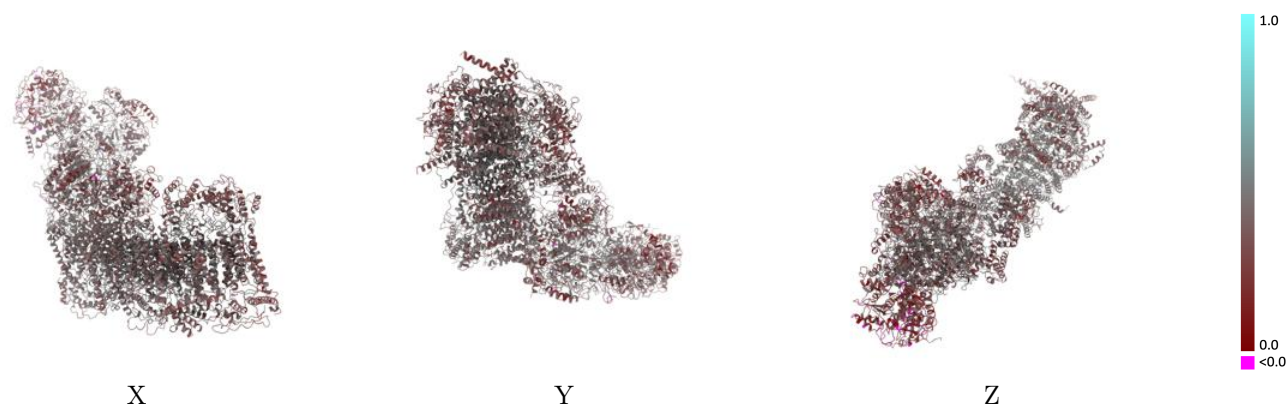
This section contains information regarding the fit between EMDB map EMD-42170 and PDB model 8UET. Per-residue inclusion information can be found in section 3 on page 21.

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



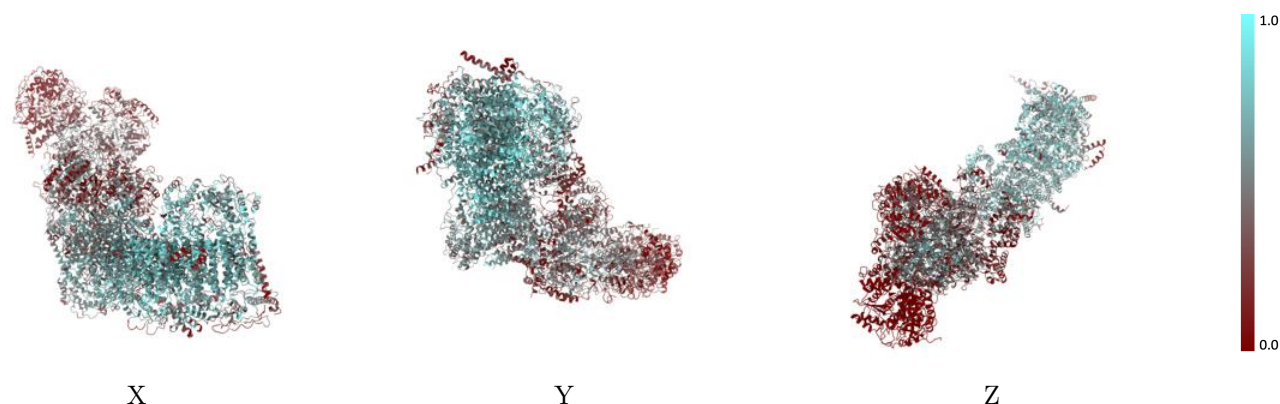
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



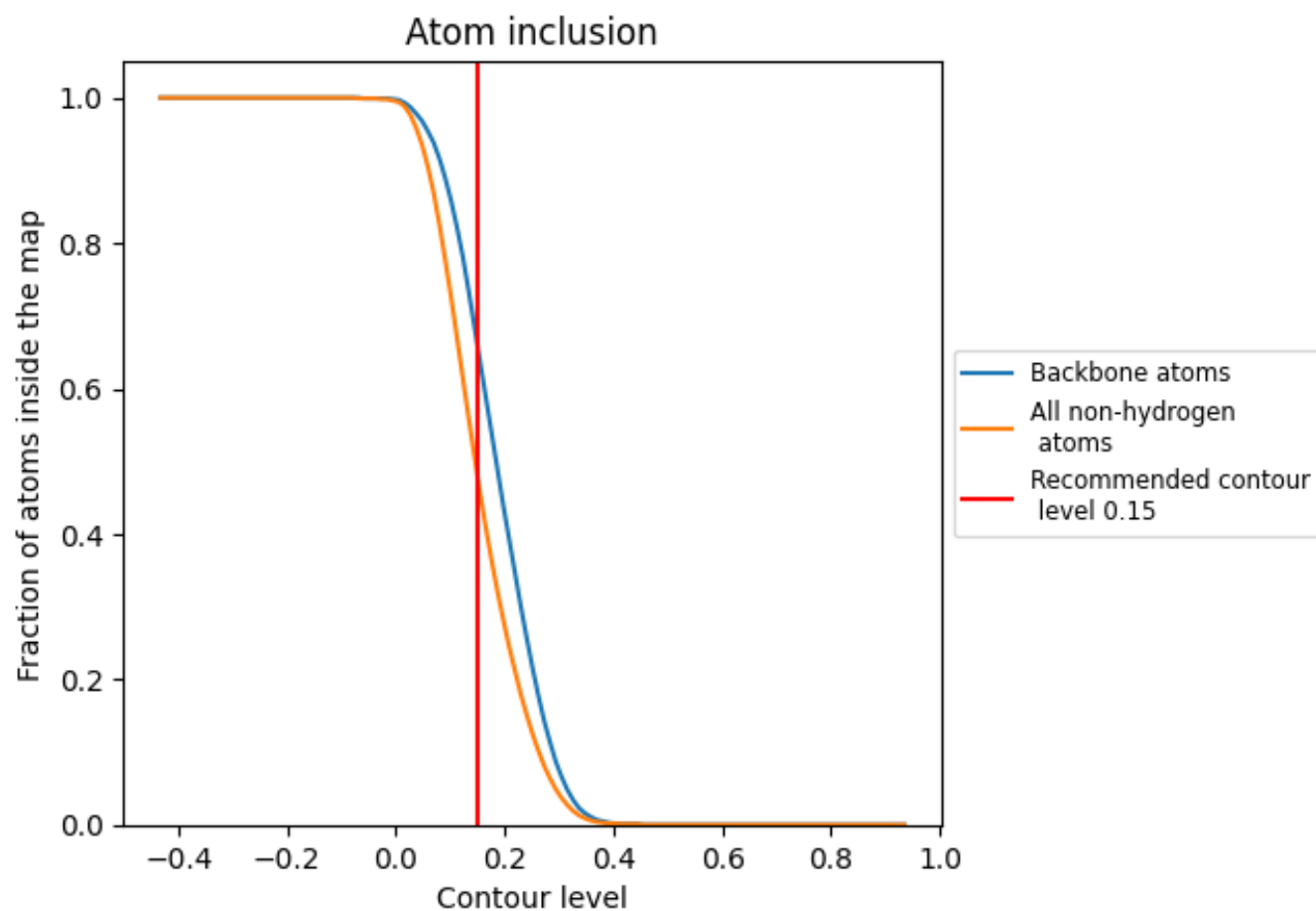
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4800   |  0.3770   |
| 1A    |  0.4830   |  0.4010   |
| 1B    |  0.5470   |  0.4180   |
| 1C    |  0.3960   |  0.4030   |
| 1D    |  0.4800   |  0.3900   |
| 1E    |  0.0280   |  0.2870   |
| 1F    |  0.0360   |  0.2590   |
| 1G    |  0.2840   |  0.3580   |
| 1H    |  0.6170   |  0.4070   |
| 1I    |  0.5820   |  0.4160   |
| 1J    |  0.5090   |  0.3870   |
| 1K    |  0.6140   |  0.4060   |
| 1L    |  0.7190   |  0.4070   |
| 1M    |  0.7590   |  0.4370   |
| 1N    |  0.6800  |  0.4280  |
| 1O    |  0.3880 |  0.3560 |
| 1P    |  0.2990 |  0.3370 |
| 1Q    |  0.3150 |  0.3830 |
| 1R    |  0.2950 |  0.4120 |
| 1S    |  0.1410 |  0.2900 |
| 1T    |  0.2340 |  0.2780 |
| 1U    |  0.6150 |  0.3370 |
| 1V    |  0.2060 |  0.3380 |
| 1W    |  0.3060 |  0.3340 |
| 1X    |  0.5480 |  0.4050 |
| 1Y    |  0.6740 |  0.3790 |
| 1Z    |  0.5480 |  0.4150 |
| 1a    |  0.6110 |  0.4090 |
| 1b    |  0.5370 |  0.4110 |
| 1c    |  0.4680 |  0.3690 |
| 1d    |  0.6670 |  0.4240 |
| 1e    |  0.5960 |  0.4280 |
| 1f    |  0.4620 |  0.3840 |
| 1g    |  0.6020 |  0.3950 |
| 1h    |  0.6730 |  0.4090 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| 1i    |  0.3890 |  0.3470 |
| 1j    |  0.5240 |  0.3740 |
| 1k    |  0.5120 |  0.3590 |
| 1l    |  0.6540 |  0.3980 |
| 1m    |  0.7090 |  0.3890 |
| 1n    |  0.6720 |  0.3670 |
| 1o    |  0.5030 |  0.3170 |
| 1p    |  0.6070 |  0.3830 |
| 1q    |  0.4470 |  0.4090 |
| 1r    |  0.3790 |  0.4020 |
| 1s    |  0.0000 |  0.2520 |