



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 06:37 AM EST

PDB ID : 7KZQ  
EMDB ID : EMD-23086  
Title : Structure of the human Fanconi anaemia Core-ID complex  
Authors : Wang, S.L.; Pavletich, N.P.  
Deposited on : 2020-12-10  
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

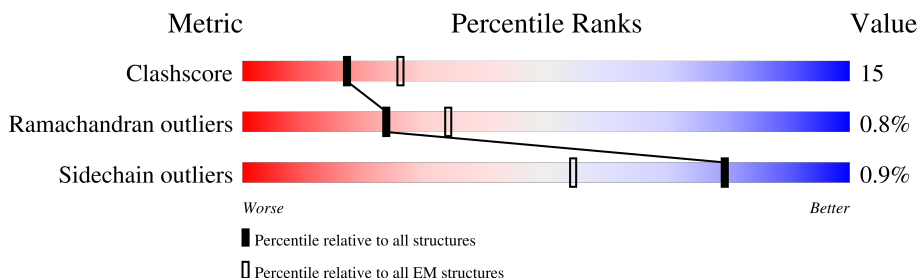
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

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







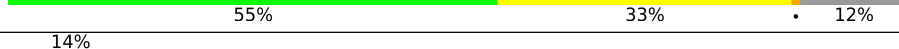
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 158937                      | 4297                        |
| Ramachandran outliers | 154571                      | 4023                        |
| Sidechain outliers    | 154315                      | 3826                        |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 1477   | <div> <div>9%</div> <div>52%</div> <div>28%</div> <div>•</div> <div>20%</div> </div> |
| 1   | S     | 1477   | <div> <div>10%</div> <div>54%</div> <div>31%</div> <div>15%</div> </div>             |
| 2   | B     | 884    | <div> <div>•</div> <div>51%</div> <div>27%</div> <div>•</div> <div>21%</div> </div>  |
| 2   | O     | 884    | <div> <div>•</div> <div>51%</div> <div>27%</div> <div>•</div> <div>21%</div> </div>  |
| 3   | C     | 583    | <div> <div>•</div> <div>68%</div> <div>25%</div> <div>•</div> <div>6%</div> </div>   |
| 4   | E     | 555    | <div> <div>•</div> <div>52%</div> <div>23%</div> <div>•</div> <div>25%</div> </div>  |
| 5   | F     | 399    | <div> <div>•</div> <div>65%</div> <div>20%</div> <div>15%</div> </div>               |
| 6   | G     | 641    | <div> <div>•</div> <div>63%</div> <div>27%</div> <div>•</div> <div>10%</div> </div>  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 6   | H     | 641    |  |
| 7   | L     | 394    |  |
| 7   | M     | 394    |  |
| 8   | P     | 906    |  |
| 8   | Q     | 906    |  |
| 9   | W     | 39     |  |
| 10  | U     | 1328   |  |
| 11  | V     | 1451   |  |

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 172709 atoms, of which 87163 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 Fanconi anemia group A protein.

| Mol | Chain | Residues | Atoms |      |       |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-------|------|------|----|---------|-------|
| 1   | A     | 1186     | Total | C    | H     | N    | O    | S  | 0       | 0     |
|     |       |          | 18889 | 6001 | 9487  | 1650 | 1692 | 59 |         |       |
| 1   | S     | 1250     | Total | C    | H     | N    | O    | S  | 0       | 0     |
|     |       |          | 19961 | 6345 | 10028 | 1747 | 1780 | 61 |         |       |

There are 44 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1456    | ALA      | -      | expression tag | UNP O15360 |
| A     | 1457    | ALA      | -      | expression tag | UNP O15360 |
| A     | 1458    | ALA      | -      | expression tag | UNP O15360 |
| A     | 1459    | LYS      | -      | expression tag | UNP O15360 |
| A     | 1460    | LEU      | -      | expression tag | UNP O15360 |
| A     | 1461    | VAL      | -      | expression tag | UNP O15360 |
| A     | 1462    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1463    | GLU      | -      | expression tag | UNP O15360 |
| A     | 1464    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1465    | LEU      | -      | expression tag | UNP O15360 |
| A     | 1466    | TYR      | -      | expression tag | UNP O15360 |
| A     | 1467    | PHE      | -      | expression tag | UNP O15360 |
| A     | 1468    | GLN      | -      | expression tag | UNP O15360 |
| A     | 1469    | SER      | -      | expression tag | UNP O15360 |
| A     | 1470    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1471    | TYR      | -      | expression tag | UNP O15360 |
| A     | 1472    | LYS      | -      | expression tag | UNP O15360 |
| A     | 1473    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1474    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1475    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1476    | ASP      | -      | expression tag | UNP O15360 |
| A     | 1477    | LYS      | -      | expression tag | UNP O15360 |
| S     | 1456    | ALA      | -      | expression tag | UNP O15360 |
| S     | 1457    | ALA      | -      | expression tag | UNP O15360 |
| S     | 1458    | ALA      | -      | expression tag | UNP O15360 |
| S     | 1459    | LYS      | -      | expression tag | UNP O15360 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| S     | 1460    | LEU      | -      | expression tag | UNP O15360 |
| S     | 1461    | VAL      | -      | expression tag | UNP O15360 |
| S     | 1462    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1463    | GLU      | -      | expression tag | UNP O15360 |
| S     | 1464    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1465    | LEU      | -      | expression tag | UNP O15360 |
| S     | 1466    | TYR      | -      | expression tag | UNP O15360 |
| S     | 1467    | PHE      | -      | expression tag | UNP O15360 |
| S     | 1468    | GLN      | -      | expression tag | UNP O15360 |
| S     | 1469    | SER      | -      | expression tag | UNP O15360 |
| S     | 1470    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1471    | TYR      | -      | expression tag | UNP O15360 |
| S     | 1472    | LYS      | -      | expression tag | UNP O15360 |
| S     | 1473    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1474    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1475    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1476    | ASP      | -      | expression tag | UNP O15360 |
| S     | 1477    | LYS      | -      | expression tag | UNP O15360 |

- Molecule 2 is a protein called Fanconi anemia group B protein.

| Mol | Chain | Residues | Atoms |      |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|------|----|---------|-------|
| 2   | B     | 701      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 11395 | 3619 | 5790 | 934 | 1013 | 39 |         |       |
| 2   | O     | 699      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 11353 | 3622 | 5759 | 926 | 1010 | 36 |         |       |

There are 50 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -24     | MET      | -      | initiating methionine | UNP Q8NB91 |
| B     | -23     | ASP      | -      | expression tag        | UNP Q8NB91 |
| B     | -22     | TYR      | -      | expression tag        | UNP Q8NB91 |
| B     | -21     | LYS      | -      | expression tag        | UNP Q8NB91 |
| B     | -20     | ASP      | -      | expression tag        | UNP Q8NB91 |
| B     | -19     | ASP      | -      | expression tag        | UNP Q8NB91 |
| B     | -18     | ASP      | -      | expression tag        | UNP Q8NB91 |
| B     | -17     | ASP      | -      | expression tag        | UNP Q8NB91 |
| B     | -16     | LYS      | -      | expression tag        | UNP Q8NB91 |
| B     | -15     | GLU      | -      | expression tag        | UNP Q8NB91 |
| B     | -14     | ASN      | -      | expression tag        | UNP Q8NB91 |
| B     | -13     | LEU      | -      | expression tag        | UNP Q8NB91 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| B     | -12     | TYR      | -      | expression tag        | UNP Q8NB91 |
| B     | -11     | PHE      | -      | expression tag        | UNP Q8NB91 |
| B     | -10     | GLN      | -      | expression tag        | UNP Q8NB91 |
| B     | -9      | GLY      | -      | expression tag        | UNP Q8NB91 |
| B     | -8      | GLY      | -      | expression tag        | UNP Q8NB91 |
| B     | -7      | GLY      | -      | expression tag        | UNP Q8NB91 |
| B     | -6      | ARG      | -      | expression tag        | UNP Q8NB91 |
| B     | -5      | LYS      | -      | expression tag        | UNP Q8NB91 |
| B     | -4      | LEU      | -      | expression tag        | UNP Q8NB91 |
| B     | -3      | GLY      | -      | expression tag        | UNP Q8NB91 |
| B     | -2      | THR      | -      | expression tag        | UNP Q8NB91 |
| B     | -1      | GLY      | -      | expression tag        | UNP Q8NB91 |
| B     | 0       | SER      | -      | expression tag        | UNP Q8NB91 |
| O     | -24     | MET      | -      | initiating methionine | UNP Q8NB91 |
| O     | -23     | ASP      | -      | expression tag        | UNP Q8NB91 |
| O     | -22     | TYR      | -      | expression tag        | UNP Q8NB91 |
| O     | -21     | LYS      | -      | expression tag        | UNP Q8NB91 |
| O     | -20     | ASP      | -      | expression tag        | UNP Q8NB91 |
| O     | -19     | ASP      | -      | expression tag        | UNP Q8NB91 |
| O     | -18     | ASP      | -      | expression tag        | UNP Q8NB91 |
| O     | -17     | ASP      | -      | expression tag        | UNP Q8NB91 |
| O     | -16     | LYS      | -      | expression tag        | UNP Q8NB91 |
| O     | -15     | GLU      | -      | expression tag        | UNP Q8NB91 |
| O     | -14     | ASN      | -      | expression tag        | UNP Q8NB91 |
| O     | -13     | LEU      | -      | expression tag        | UNP Q8NB91 |
| O     | -12     | TYR      | -      | expression tag        | UNP Q8NB91 |
| O     | -11     | PHE      | -      | expression tag        | UNP Q8NB91 |
| O     | -10     | GLN      | -      | expression tag        | UNP Q8NB91 |
| O     | -9      | GLY      | -      | expression tag        | UNP Q8NB91 |
| O     | -8      | GLY      | -      | expression tag        | UNP Q8NB91 |
| O     | -7      | GLY      | -      | expression tag        | UNP Q8NB91 |
| O     | -6      | ARG      | -      | expression tag        | UNP Q8NB91 |
| O     | -5      | LYS      | -      | expression tag        | UNP Q8NB91 |
| O     | -4      | LEU      | -      | expression tag        | UNP Q8NB91 |
| O     | -3      | GLY      | -      | expression tag        | UNP Q8NB91 |
| O     | -2      | THR      | -      | expression tag        | UNP Q8NB91 |
| O     | -1      | GLY      | -      | expression tag        | UNP Q8NB91 |
| O     | 0       | SER      | -      | expression tag        | UNP Q8NB91 |

- Molecule 3 is a protein called Fanconi anemia group C protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | C     | 550      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8838  | 2826 | 4442 | 749 | 791 | 30 |         |       |

There are 25 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| C     | -24     | MET      | -      | initiating methionine | UNP Q00597 |
| C     | -23     | ASP      | -      | expression tag        | UNP Q00597 |
| C     | -22     | TYR      | -      | expression tag        | UNP Q00597 |
| C     | -21     | LYS      | -      | expression tag        | UNP Q00597 |
| C     | -20     | ASP      | -      | expression tag        | UNP Q00597 |
| C     | -19     | ASP      | -      | expression tag        | UNP Q00597 |
| C     | -18     | ASP      | -      | expression tag        | UNP Q00597 |
| C     | -17     | ASP      | -      | expression tag        | UNP Q00597 |
| C     | -16     | LYS      | -      | expression tag        | UNP Q00597 |
| C     | -15     | GLU      | -      | expression tag        | UNP Q00597 |
| C     | -14     | ASN      | -      | expression tag        | UNP Q00597 |
| C     | -13     | LEU      | -      | expression tag        | UNP Q00597 |
| C     | -12     | TYR      | -      | expression tag        | UNP Q00597 |
| C     | -11     | PHE      | -      | expression tag        | UNP Q00597 |
| C     | -10     | GLN      | -      | expression tag        | UNP Q00597 |
| C     | -9      | GLY      | -      | expression tag        | UNP Q00597 |
| C     | -8      | GLY      | -      | expression tag        | UNP Q00597 |
| C     | -7      | GLY      | -      | expression tag        | UNP Q00597 |
| C     | -6      | ARG      | -      | expression tag        | UNP Q00597 |
| C     | -5      | LYS      | -      | expression tag        | UNP Q00597 |
| C     | -4      | LEU      | -      | expression tag        | UNP Q00597 |
| C     | -3      | GLY      | -      | expression tag        | UNP Q00597 |
| C     | -2      | THR      | -      | expression tag        | UNP Q00597 |
| C     | -1      | GLY      | -      | expression tag        | UNP Q00597 |
| C     | 0       | SER      | -      | expression tag        | UNP Q00597 |

- Molecule 4 is a protein called Fanconi anemia group E protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 4   | E     | 419      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6614  | 2048 | 3390 | 560 | 592 | 24 |         |       |

There are 19 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| E     | -18     | MET      | -      | initiating methionine | UNP Q9HB96 |
| E     | -17     | ASP      | -      | expression tag        | UNP Q9HB96 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| E     | -16     | TYR      | -      | expression tag | UNP Q9HB96 |
| E     | -15     | LYS      | -      | expression tag | UNP Q9HB96 |
| E     | -14     | ASP      | -      | expression tag | UNP Q9HB96 |
| E     | -13     | ASP      | -      | expression tag | UNP Q9HB96 |
| E     | -12     | ASP      | -      | expression tag | UNP Q9HB96 |
| E     | -11     | ASP      | -      | expression tag | UNP Q9HB96 |
| E     | -10     | LYS      | -      | expression tag | UNP Q9HB96 |
| E     | -9      | GLU      | -      | expression tag | UNP Q9HB96 |
| E     | -8      | ASN      | -      | expression tag | UNP Q9HB96 |
| E     | -7      | LEU      | -      | expression tag | UNP Q9HB96 |
| E     | -6      | TYR      | -      | expression tag | UNP Q9HB96 |
| E     | -5      | PHE      | -      | expression tag | UNP Q9HB96 |
| E     | -4      | GLN      | -      | expression tag | UNP Q9HB96 |
| E     | -3      | GLY      | -      | expression tag | UNP Q9HB96 |
| E     | -2      | GLY      | -      | expression tag | UNP Q9HB96 |
| E     | -1      | GLY      | -      | expression tag | UNP Q9HB96 |
| E     | 0       | ARG      | -      | expression tag | UNP Q9HB96 |

- Molecule 5 is a protein called Fanconi anemia group F protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 5   | F     | 340      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 5466  | 1730 | 2740 | 506 | 483 | 7 |         |       |

There are 25 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| F     | -24     | MET      | -      | initiating methionine | UNP Q9NPI8 |
| F     | -23     | ASP      | -      | expression tag        | UNP Q9NPI8 |
| F     | -22     | TYR      | -      | expression tag        | UNP Q9NPI8 |
| F     | -21     | LYS      | -      | expression tag        | UNP Q9NPI8 |
| F     | -20     | ASP      | -      | expression tag        | UNP Q9NPI8 |
| F     | -19     | ASP      | -      | expression tag        | UNP Q9NPI8 |
| F     | -18     | ASP      | -      | expression tag        | UNP Q9NPI8 |
| F     | -17     | ASP      | -      | expression tag        | UNP Q9NPI8 |
| F     | -16     | LYS      | -      | expression tag        | UNP Q9NPI8 |
| F     | -15     | GLU      | -      | expression tag        | UNP Q9NPI8 |
| F     | -14     | ASN      | -      | expression tag        | UNP Q9NPI8 |
| F     | -13     | LEU      | -      | expression tag        | UNP Q9NPI8 |
| F     | -12     | TYR      | -      | expression tag        | UNP Q9NPI8 |
| F     | -11     | PHE      | -      | expression tag        | UNP Q9NPI8 |
| F     | -10     | GLN      | -      | expression tag        | UNP Q9NPI8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | -9      | GLY      | -      | expression tag | UNP Q9NPI8 |
| F     | -8      | GLY      | -      | expression tag | UNP Q9NPI8 |
| F     | -7      | GLY      | -      | expression tag | UNP Q9NPI8 |
| F     | -6      | ARG      | -      | expression tag | UNP Q9NPI8 |
| F     | -5      | LYS      | -      | expression tag | UNP Q9NPI8 |
| F     | -4      | LEU      | -      | expression tag | UNP Q9NPI8 |
| F     | -3      | GLY      | -      | expression tag | UNP Q9NPI8 |
| F     | -2      | THR      | -      | expression tag | UNP Q9NPI8 |
| F     | -1      | GLY      | -      | expression tag | UNP Q9NPI8 |
| F     | 0       | SER      | -      | expression tag | UNP Q9NPI8 |

- Molecule 6 is a protein called Fanconi anemia group G protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | G     | 577      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 9020  | 2843 | 4537 | 778 | 844 | 18 |         |       |
| 6   | H     | 544      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 8504  | 2676 | 4288 | 734 | 790 | 16 |         |       |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| G     | -18     | MET      | -      | initiating methionine | UNP O15287 |
| G     | -17     | ASP      | -      | expression tag        | UNP O15287 |
| G     | -16     | TYR      | -      | expression tag        | UNP O15287 |
| G     | -15     | LYS      | -      | expression tag        | UNP O15287 |
| G     | -14     | ASP      | -      | expression tag        | UNP O15287 |
| G     | -13     | ASP      | -      | expression tag        | UNP O15287 |
| G     | -12     | ASP      | -      | expression tag        | UNP O15287 |
| G     | -11     | ASP      | -      | expression tag        | UNP O15287 |
| G     | -10     | LYS      | -      | expression tag        | UNP O15287 |
| G     | -9      | GLU      | -      | expression tag        | UNP O15287 |
| G     | -8      | ASN      | -      | expression tag        | UNP O15287 |
| G     | -7      | LEU      | -      | expression tag        | UNP O15287 |
| G     | -6      | TYR      | -      | expression tag        | UNP O15287 |
| G     | -5      | PHE      | -      | expression tag        | UNP O15287 |
| G     | -4      | GLN      | -      | expression tag        | UNP O15287 |
| G     | -3      | GLY      | -      | expression tag        | UNP O15287 |
| G     | -2      | GLY      | -      | expression tag        | UNP O15287 |
| G     | -1      | GLY      | -      | expression tag        | UNP O15287 |
| G     | 0       | ARG      | -      | expression tag        | UNP O15287 |
| H     | -18     | MET      | -      | initiating methionine | UNP O15287 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | -17     | ASP      | -      | expression tag | UNP O15287 |
| H     | -16     | TYR      | -      | expression tag | UNP O15287 |
| H     | -15     | LYS      | -      | expression tag | UNP O15287 |
| H     | -14     | ASP      | -      | expression tag | UNP O15287 |
| H     | -13     | ASP      | -      | expression tag | UNP O15287 |
| H     | -12     | ASP      | -      | expression tag | UNP O15287 |
| H     | -11     | ASP      | -      | expression tag | UNP O15287 |
| H     | -10     | LYS      | -      | expression tag | UNP O15287 |
| H     | -9      | GLU      | -      | expression tag | UNP O15287 |
| H     | -8      | ASN      | -      | expression tag | UNP O15287 |
| H     | -7      | LEU      | -      | expression tag | UNP O15287 |
| H     | -6      | TYR      | -      | expression tag | UNP O15287 |
| H     | -5      | PHE      | -      | expression tag | UNP O15287 |
| H     | -4      | GLN      | -      | expression tag | UNP O15287 |
| H     | -3      | GLY      | -      | expression tag | UNP O15287 |
| H     | -2      | GLY      | -      | expression tag | UNP O15287 |
| H     | -1      | GLY      | -      | expression tag | UNP O15287 |
| H     | 0       | ARG      | -      | expression tag | UNP O15287 |

- Molecule 7 is a protein called E3 ubiquitin-protein ligase FANCL.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 7   | L     | 370      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 5951  | 1914 | 2977 | 496 | 542 | 22 |         |       |
| 7   | M     | 370      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 5951  | 1914 | 2977 | 496 | 542 | 22 |         |       |

There are 38 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| L     | -18     | MET      | -      | initiating methionine | UNP Q9NW38 |
| L     | -17     | ASP      | -      | expression tag        | UNP Q9NW38 |
| L     | -16     | TYR      | -      | expression tag        | UNP Q9NW38 |
| L     | -15     | LYS      | -      | expression tag        | UNP Q9NW38 |
| L     | -14     | ASP      | -      | expression tag        | UNP Q9NW38 |
| L     | -13     | ASP      | -      | expression tag        | UNP Q9NW38 |
| L     | -12     | ASP      | -      | expression tag        | UNP Q9NW38 |
| L     | -11     | ASP      | -      | expression tag        | UNP Q9NW38 |
| L     | -10     | LYS      | -      | expression tag        | UNP Q9NW38 |
| L     | -9      | GLU      | -      | expression tag        | UNP Q9NW38 |
| L     | -8      | ASN      | -      | expression tag        | UNP Q9NW38 |
| L     | -7      | LEU      | -      | expression tag        | UNP Q9NW38 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| L     | -6      | TYR      | -      | expression tag        | UNP Q9NW38 |
| L     | -5      | PHE      | -      | expression tag        | UNP Q9NW38 |
| L     | -4      | GLN      | -      | expression tag        | UNP Q9NW38 |
| L     | -3      | GLY      | -      | expression tag        | UNP Q9NW38 |
| L     | -2      | GLY      | -      | expression tag        | UNP Q9NW38 |
| L     | -1      | GLY      | -      | expression tag        | UNP Q9NW38 |
| L     | 0       | ARG      | -      | expression tag        | UNP Q9NW38 |
| M     | -18     | MET      | -      | initiating methionine | UNP Q9NW38 |
| M     | -17     | ASP      | -      | expression tag        | UNP Q9NW38 |
| M     | -16     | TYR      | -      | expression tag        | UNP Q9NW38 |
| M     | -15     | LYS      | -      | expression tag        | UNP Q9NW38 |
| M     | -14     | ASP      | -      | expression tag        | UNP Q9NW38 |
| M     | -13     | ASP      | -      | expression tag        | UNP Q9NW38 |
| M     | -12     | ASP      | -      | expression tag        | UNP Q9NW38 |
| M     | -11     | ASP      | -      | expression tag        | UNP Q9NW38 |
| M     | -10     | LYS      | -      | expression tag        | UNP Q9NW38 |
| M     | -9      | GLU      | -      | expression tag        | UNP Q9NW38 |
| M     | -8      | ASN      | -      | expression tag        | UNP Q9NW38 |
| M     | -7      | LEU      | -      | expression tag        | UNP Q9NW38 |
| M     | -6      | TYR      | -      | expression tag        | UNP Q9NW38 |
| M     | -5      | PHE      | -      | expression tag        | UNP Q9NW38 |
| M     | -4      | GLN      | -      | expression tag        | UNP Q9NW38 |
| M     | -3      | GLY      | -      | expression tag        | UNP Q9NW38 |
| M     | -2      | GLY      | -      | expression tag        | UNP Q9NW38 |
| M     | -1      | GLY      | -      | expression tag        | UNP Q9NW38 |
| M     | 0       | ARG      | -      | expression tag        | UNP Q9NW38 |

- Molecule 8 is a protein called Fanconi anemia core complex-associated protein 100.

| Mol | Chain | Residues | Atoms |      |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|------|----|---------|-------|
| 8   | P     | 748      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 11279 | 3520 | 5681 | 972 | 1058 | 48 |         |       |
| 8   | Q     | 754      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 11355 | 3548 | 5724 | 978 | 1058 | 47 |         |       |

There are 50 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| P     | -24     | MET      | -      | initiating methionine | UNP Q0VG06 |
| P     | -23     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -22     | TYR      | -      | expression tag        | UNP Q0VG06 |
| P     | -21     | LYS      | -      | expression tag        | UNP Q0VG06 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| P     | -20     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -19     | HIS      | -      | expression tag        | UNP Q0VG06 |
| P     | -18     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -17     | GLY      | -      | expression tag        | UNP Q0VG06 |
| P     | -16     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -15     | TYR      | -      | expression tag        | UNP Q0VG06 |
| P     | -14     | LYS      | -      | expression tag        | UNP Q0VG06 |
| P     | -13     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -12     | HIS      | -      | expression tag        | UNP Q0VG06 |
| P     | -11     | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -10     | ILE      | -      | expression tag        | UNP Q0VG06 |
| P     | -9      | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -8      | TYR      | -      | expression tag        | UNP Q0VG06 |
| P     | -7      | LYS      | -      | expression tag        | UNP Q0VG06 |
| P     | -6      | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -5      | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -4      | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -3      | ASP      | -      | expression tag        | UNP Q0VG06 |
| P     | -2      | LYS      | -      | expression tag        | UNP Q0VG06 |
| P     | -1      | GLY      | -      | expression tag        | UNP Q0VG06 |
| P     | 0       | SER      | -      | expression tag        | UNP Q0VG06 |
| Q     | -24     | MET      | -      | initiating methionine | UNP Q0VG06 |
| Q     | -23     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -22     | TYR      | -      | expression tag        | UNP Q0VG06 |
| Q     | -21     | LYS      | -      | expression tag        | UNP Q0VG06 |
| Q     | -20     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -19     | HIS      | -      | expression tag        | UNP Q0VG06 |
| Q     | -18     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -17     | GLY      | -      | expression tag        | UNP Q0VG06 |
| Q     | -16     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -15     | TYR      | -      | expression tag        | UNP Q0VG06 |
| Q     | -14     | LYS      | -      | expression tag        | UNP Q0VG06 |
| Q     | -13     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -12     | HIS      | -      | expression tag        | UNP Q0VG06 |
| Q     | -11     | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -10     | ILE      | -      | expression tag        | UNP Q0VG06 |
| Q     | -9      | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -8      | TYR      | -      | expression tag        | UNP Q0VG06 |
| Q     | -7      | LYS      | -      | expression tag        | UNP Q0VG06 |
| Q     | -6      | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -5      | ASP      | -      | expression tag        | UNP Q0VG06 |
| Q     | -4      | ASP      | -      | expression tag        | UNP Q0VG06 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| Q     | -3      | ASP      | -      | expression tag | UNP Q0VG06 |
| Q     | -2      | LYS      | -      | expression tag | UNP Q0VG06 |
| Q     | -1      | GLY      | -      | expression tag | UNP Q0VG06 |
| Q     | 0       | SER      | -      | expression tag | UNP Q0VG06 |

- Molecule 9 is a protein called Fanconi anemia core complex-associated protein 20.

| Mol | Chain | Residues | Atoms |     |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---------|-------|
| 9   | W     | 39       | Total | C   | H   | N  | O  | 0       | 0     |
|     |       |          | 513   | 179 | 242 | 42 | 50 |         |       |

- Molecule 10 is a protein called Fanconi anemia, complementation group I.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 10  | U     | 1168     | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 18882 | 5933 | 9626 | 1549 | 1720 | 54 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| U     | 877     | LEU      | ILE    | conflict | UNP B7ZMF2 |
| U     | 1235    | VAL      | ALA    | conflict | UNP B7ZMF2 |
| U     | 1274    | SER      | ASN    | conflict | UNP B7ZMF2 |

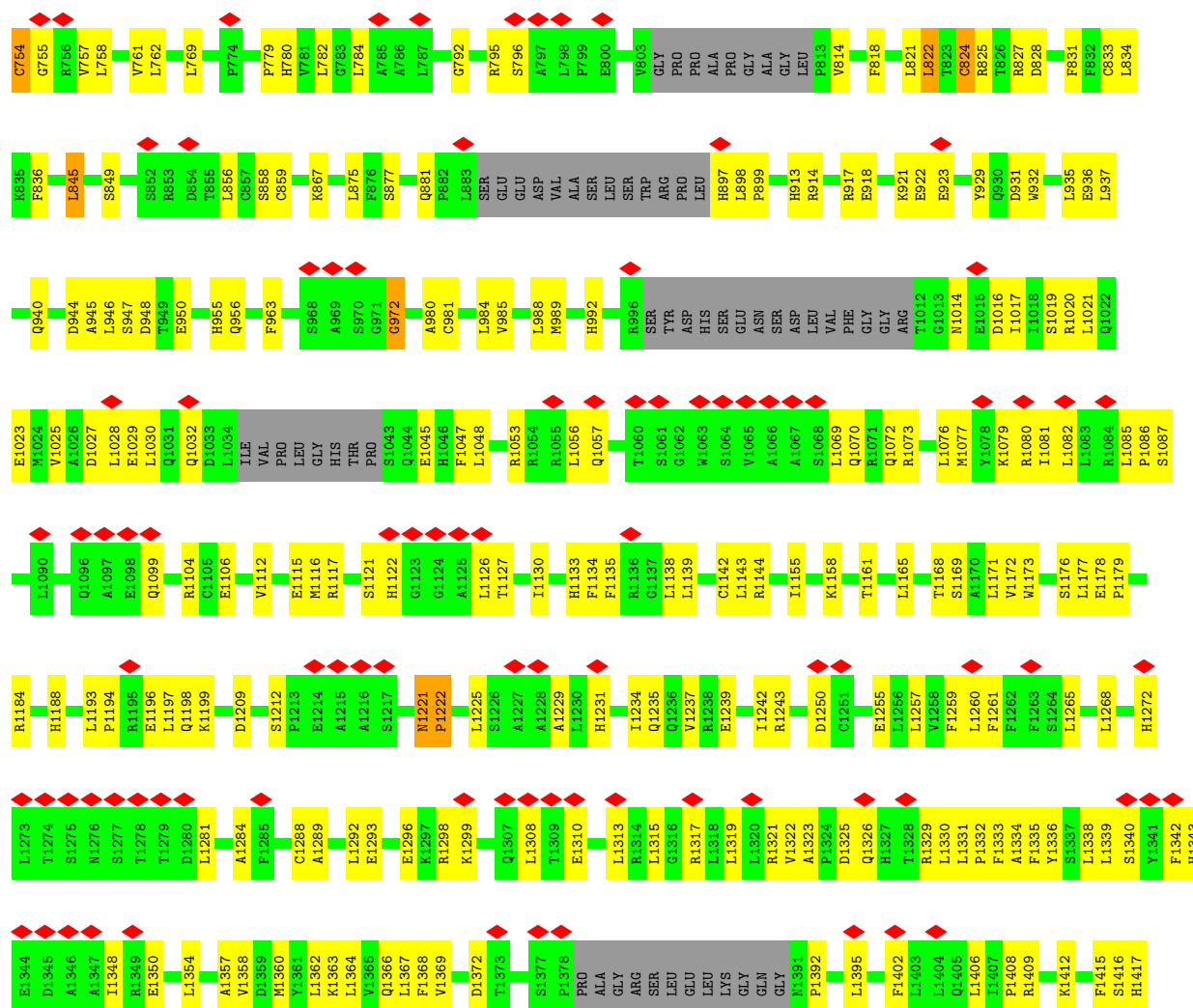
- Molecule 11 is a protein called Fanconi anemia group D2 protein.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 11  | V     | 1153     | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 18733 | 5970 | 9475 | 1527 | 1709 | 52 |         |       |

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 12  | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 12  | L     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 12  | M     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |





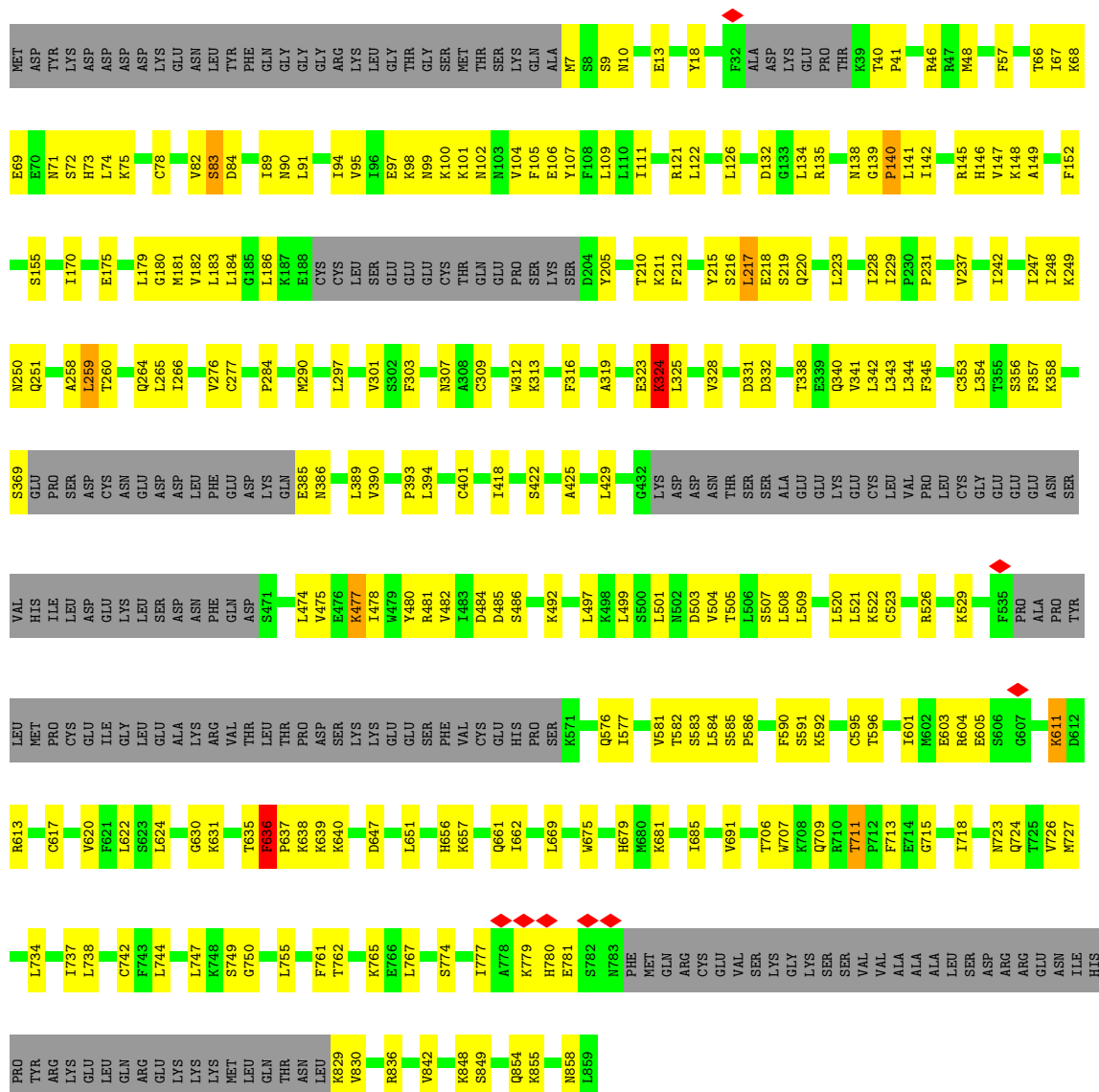
• Molecule 1: Fanconi anemia group A protein



|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| S1264 | L1265 | H1272 | S1275 | N1276 | S1277 | T1278 | T1279 | H1286 | V1287 | I1291 | L1292 | E1293 | C1294 | L1295 | E1296 | K1297 | R1298 | K1299 | W1302 | L1303 | A1304 | L1305 | F1306 | Q1307 | L1308 | T1309 | E1310 | S1311 | D1312 | L1313 | G1316 | R1317 | L1318 | L1319 | L1320 | R1321 | V1322 | D1325 | Q1326 | H1327 | T1328 | R1329 | L1330 | L1331 | P1332 | F1333 | A1334 | F1335 | F1336 | S1337 | L1338 | L1339 |
| T1161 | K1162 | C1163 | S1169 | W1173 | W1174 | S1175 | S1176 | L1177 | E1178 | R1186 | H1187 | H1188 | C1189 | Q1190 | S1191 | P1192 | L1193 | F1194 | R1195 | E1196 | L1197 | L1200 | F1210 | E1214 | A1215 | A1216 | S1217 | D1218 | T1219 | I1230 | H1233 | F1134 | F1135 | R1136 | M1140 | L1143 | R1144 | S1145 | P1148 | M1151 | V1152 | D1153 | F1154 | T1155 | L1156 | A1157 | K1158 | L1260 | F1261 | F1262 | F1263 |       |
| S1087 | L1090 | C1091 | S1094 | Q1099 | P1100 | I1101 | T1102 | A1103 | R1104 | C1105 | Q1107 | F1108 | F1109 | H1110 | L1111 | V1112 | N1113 | S1114 | E1115 | M1116 | R1117 | N1118 | H1122 | G1123 | G1124 | A1125 | L1126 | T1127 | Q1128 | D1129 | T1130 | H1133 | F1134 | F1135 | R1136 | M1140 | L1143 | R1144 | S1145 | P1148 | M1151 | V1152 | D1153 | F1154 | T1155 | L1156 | A1157 | K1158 | L1260 | F1261 | F1262 | F1263 |
| V1007 | T1012 | G1013 | N1014 | I1018 | S1019 | R1020 | L1021 | Q1022 | E1023 | M1024 | D1027 | L1028 | E1029 | L1030 | Q1031 | Q1032 | D1033 | LEU   | I1034 | VAL   | PRO   | LEU   | HIS   | THR   | PRO   | S1043 | Q1044 | E1045 | F1052 | R1053 | L1056 | S1061 | G1062 | W1063 | S1064 | V1065 | A1066 | L1069 | Q1070 | R1071 | Q1072 | E1073 | L1075 | L1076 | R1080 | T1081 | L1082 | R1084 |       |       |       |       |
| V925  | T928  | Y929  | Q930  | D931  | W932  | H933  | H934  | L935  | E936  | L937  | E938  | I939  | Q940  | D944  | A945  | L946  | S947  | D948  | T949  | E950  | R951  | Q952  | H955  | L964  | P965  | E966  | S967  | S968  | G971  | G972  | C973  | D974  | G975  | D976  | L977  | C981  | T982  | I983  | L984  | V985  | N986  | H992  | S995  | Y998  | S1001 | E1002 | N1003 |       |       |       |       |       |
| S844  | L845  | C846  | S849  | S850  | Q851  | S852  | R853  | D854  | T855  | S861  | R862  | C863  | L864  | I865  | K866  | K867  | F868  | R874  | S877  | R880  | Q881  | P882  | LEU   | SER   | GLU   | GLU   | ASP   | VAL   | ALA   | SER   | LEU   | TRP   | PRO   | LEU   | H897  | L898  | P899  | S900  | A901  | Q904  | R905  | W911  | T915  | F916  | R917  | E918  | Y919  | L920  | K921  |       |       |       |
| V761  | L762  | T763  | R764  | L765  | C766  | Q767  | L768  | L769  | L776  | H780  | L781  | G783  | L784  | L787  | A788  | V789  | H790  | L791  | R795  | L798  | V801  | V803  | G804  | PRO   | ALA   | PRO   | GLY   | ALA   | GLY   | ALA   | GLY   | LEU   | P813  | V814  | P815  | P818  | D819  | S820  | L821  | L822  | T823  | C824  | R825  | T826  | S829  | C833  | S842  | Y843  |       |       |       |       |
| A678  | V679  | L680  | R683  | S606  | K608  | R609  | A610  | D611  | K612  | I613  | P614  | F615  | S616  | L617  | T620  | A627  | ALA   | GLU   | GLU   | LYS   | PRO   | GLU   | ALA   | ALA   | GLY   | VAL   | L730  | W731  | A732  | A733  | S734  | S735  | V736  | P739  | E740  | L652  | T654  | A655  | A656  | L657  | L660  | R670  | L673  | S674  | A675  | Q676  | V677  |       |       |       |       |       |
| S524  | I525  | GLU   | ASN   | MET   | GLY   | LEU   | TTR   | ASP   | LEU   | SER   | SER   | ALA   | GLY   | ILE   | THR   | E542  | D550  | V551  | K552  | K553  | I555  | M556  | V557  | F558  | E559  | H560  | N563  | I564  | P565  | V566  | L567  | V568  | M569  | E570  | A571  | S572  | R576  | P577  | F583  | L584  | L587  | L588  | L593  | P594  | K595  | V596  | D598  | S599  | R600  |       |       |       |
| PRO   | ALA   | PHE   | LYS   | MET   | PRO   | GLN   | V265  | T266  | L270  | L278  | L281  | G284  | V285  | Q286  | E287  | E288  | S289  | T291  | H292  | K293  | I294  | V295  | R296  | F299  | S303  | G304  | H305  | L306  | L307  | G308  | S309  | V310  | I311  | S312  | T313  | D314  | P315  | L316  | K317  | F320  | S321  | L324  | T325  | Q326  | I327  | L328  | S331  | P332  |       |       |       |       |
| K335  | A336  | S337  | Q341  | W346  | L358  | Y359  | R360  | F361  | L362  | F363  | V364  | M365  | L366  | L371  | V372  | L375  | Q376  | E377  | E380  | T381  | Q382  | E383  | V384  | Q387  | V393  | L396  | C399  | E402  | Q405  | V411  | L414  | M415  | L424  | D425  | S426  | M427  | V428  | T429  | R517  | A430  | L439  | GLU   | GLY   |       |       |       |       |       |       |       |       |       |

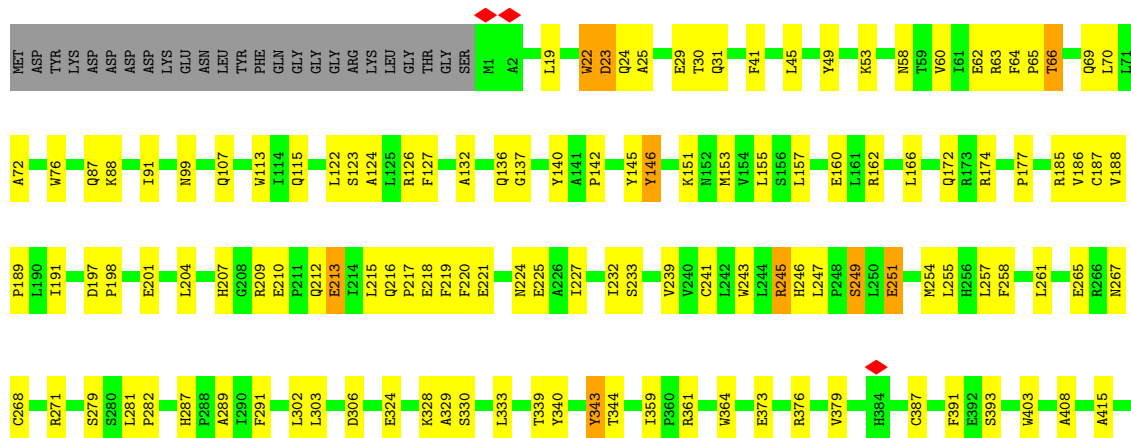


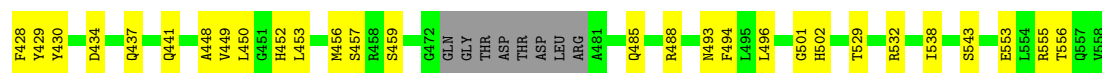




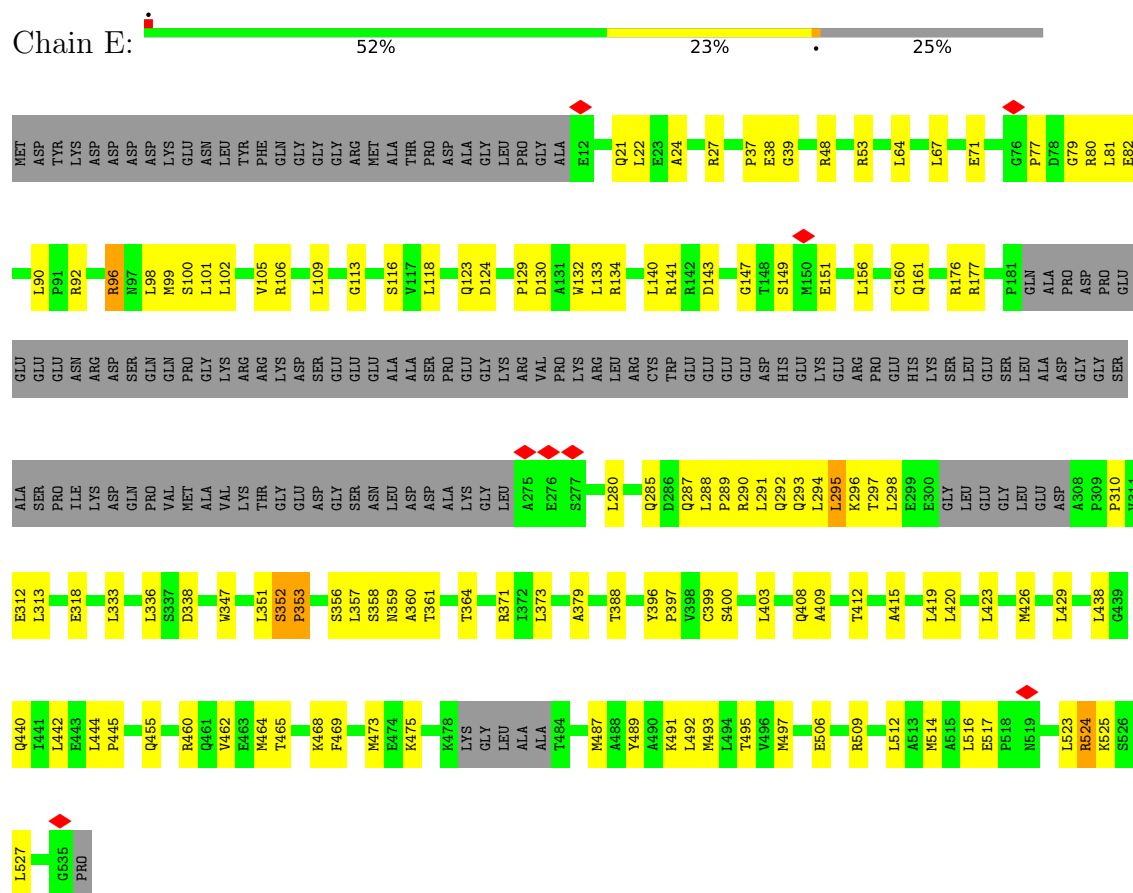
• Molecule 3: Fanconi anemia group C protein

Chain C: 68% 25% 6%

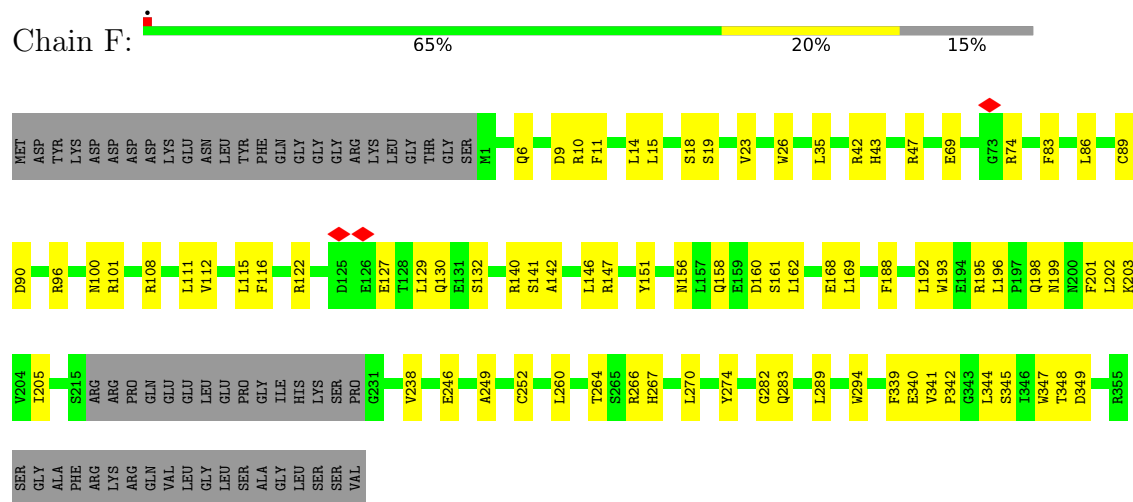




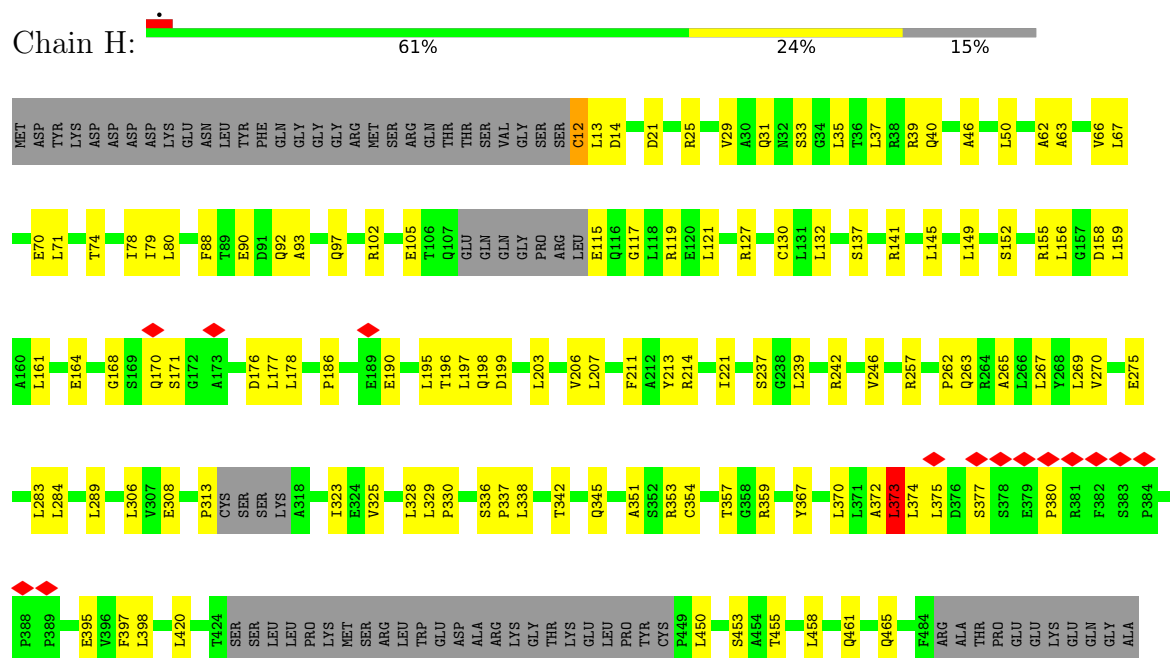
• Molecule 4: Fanconi anemia group E protein

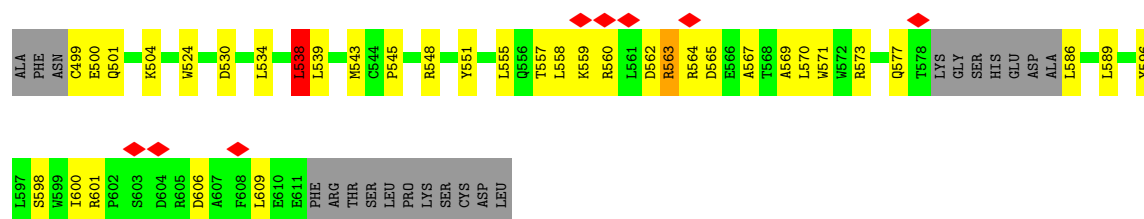


• Molecule 5: Fanconi anemia group F protein



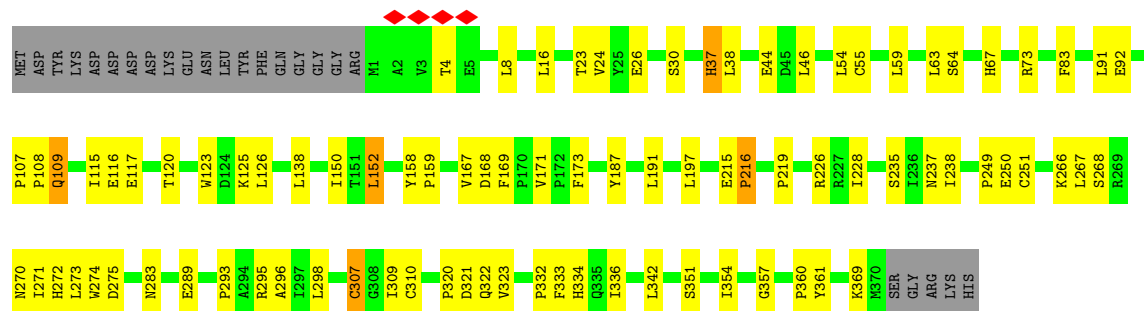
• Molecule 6: Fanconi anemia group G protein





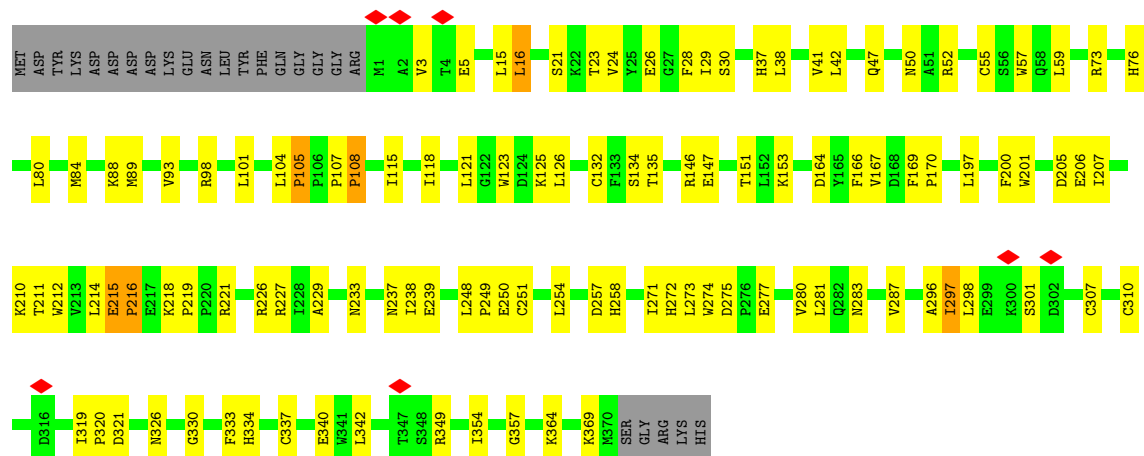
• Molecule 7: E3 ubiquitin-protein ligase FANCL

Chain L: 72% 21% 6%



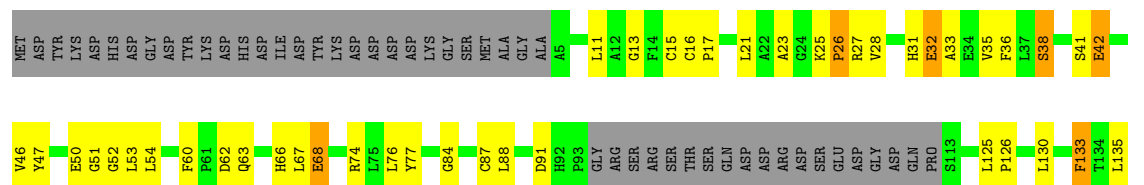
• Molecule 7: E3 ubiquitin-protein ligase FANCL

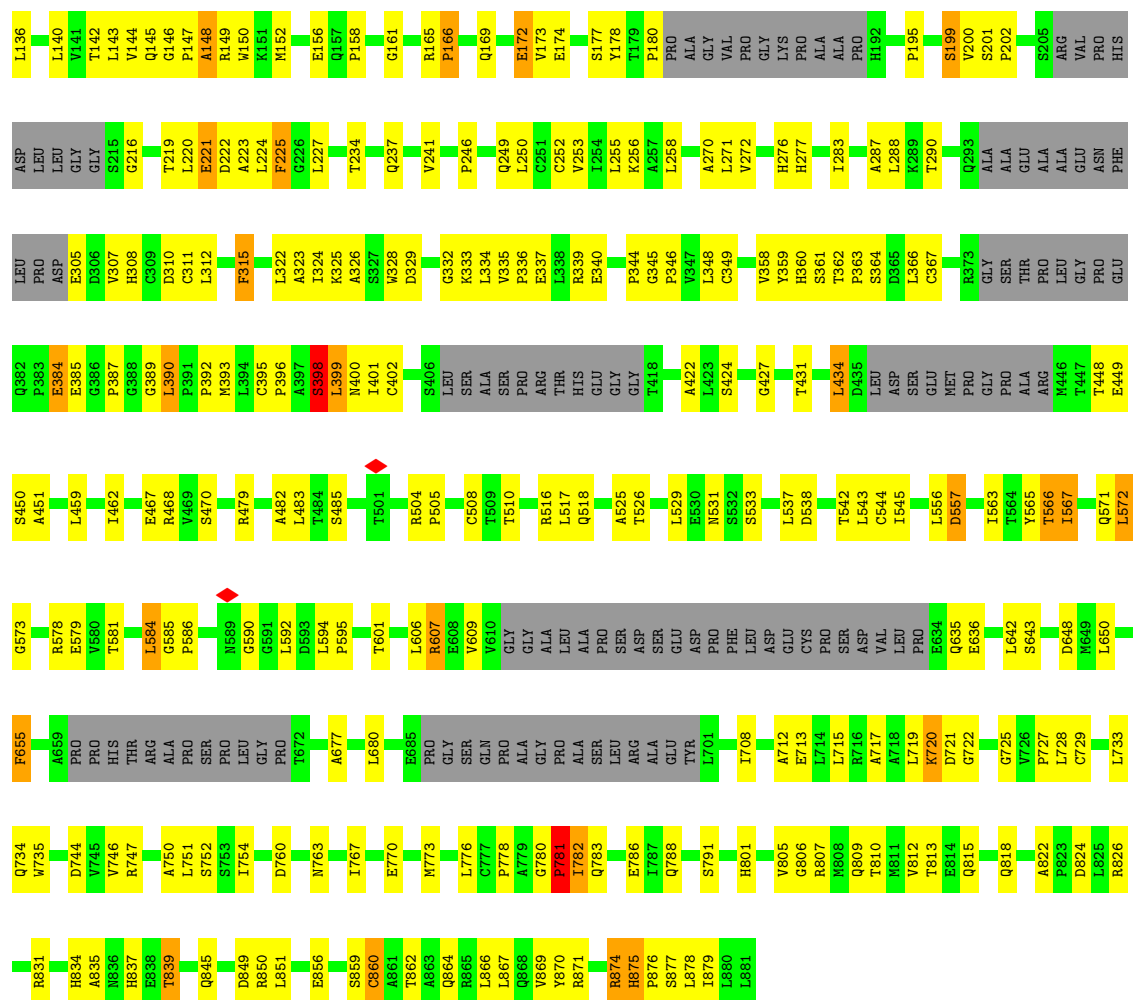
Chain M: 65% 27% 6%



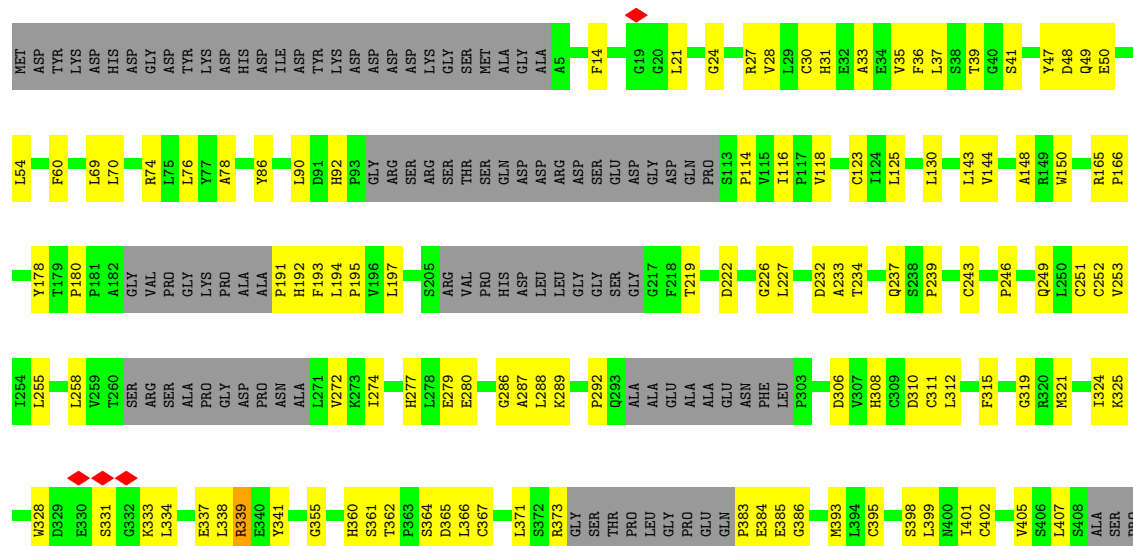
• Molecule 8: Fanconi anemia core complex-associated protein 100

Chain P: 50% 29% 17%

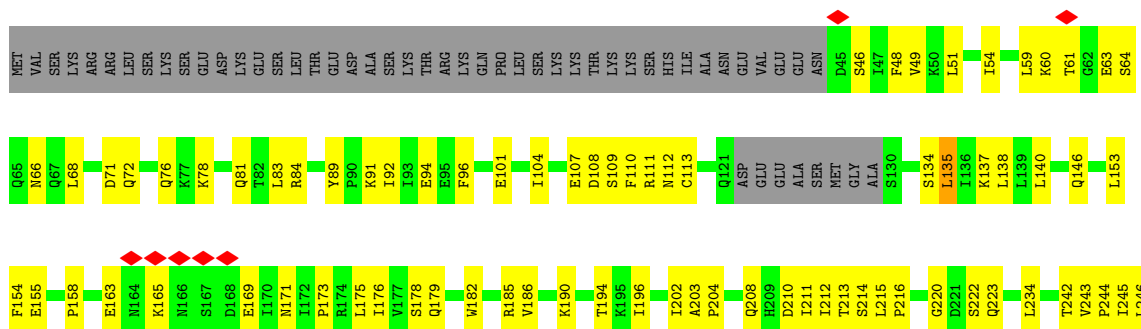
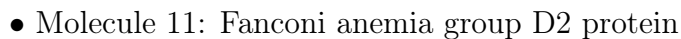




● Molecule 8: Fanconi anemia core complex-associated protein 100









|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| S1287 | H1288 | P1289 | V1290 | L1291 | H1292 | V1293 | L1294 | L1295 | R1299 | L1300 | F1301 | V1302 | E1303 | A1304 | F1306 | L1306 | K1307 | Q1308 | C1309 | M1310 | P1311 | L1312 | L1313 | D1314 | F1315 | S1316 | F1317 | R1318 | K1319 | H1320 | R1321 | E1322 | D1323 | L1324 | S1325 | S1326 | L1327 | L1328 | E1329 | F1331 | L1332 | D1334 | T1335 | R1336 | L1337 | L1338 | H1339 | H1340 | L1341 | C1342 | G1343 | H1344 | S1345 | K1346 | I1347 | H1348 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASP   | ALA   | SER   | S1220 | S1221 | T1222 | L1226 | T1227 | R1228 | H1229 | F1301 | T1230 | F1231 | V1232 | F1233 | F1234 | F1235 | R1236 | V1237 | M1238 | K1244 | T1245 | V1246 | K1247 | I1249 | E1250 | P1251 | G1252 | T1253 | A1254 | A1255 | D1256 | S1257 | Q1258 | Q1259 | I1260 | H1261 | E1262 | K1264 | L1265 | L1266 | M1269 | M1270 | R1273 | I1277 | M1280 | L1281 | K1282 | V1284 | F1285 | D1286 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| L1134 | I1135 | L1138 | M1139 | V1140 | I1141 | L1142 | E1143 | K1144 | S1145 | THR   | ALA   | SER   | ALA   | Q1150 | T1155 | L1158 | C1164 | R1165 | V1166 | W1167 | P1168 | S1169 | G1170 | D1171 | K1172 | E1173 | K1174 | S1175 | M1176 | I1177 | S1178 | M1179 | D1180 | Q1181 | A1184 | L1185 | L1186 | S1195 | I1196 | L1197 | A1204 | G1205 | V1206 | G1207 | V1208 | P1209 | E1210 | L1211 | I1212 | N1213 | S1214 | P1215 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASN   | GLY   | ARG   | ASN   | ILE   | GLY   | F1001 | L1004 | Q1005 | Q1006 | R1007 | S1008 | A1009 | Q1010 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| Y1062 | Q1063 | R1064 | L1065 | I1068 | G1071 | W1075 | S1076 | G1077 | F1078 | S1079 | Q1080 | P1081 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| L1134 | I1135 | L1138 | M1139 | V1140 | I1141 | L1142 | E1143 | K1144 | S1145 | THR   | ALA   | SER   | ALA   | Q1150 | T1155 | L1158 | C1164 | R1165 | V1166 | W1167 | P1168 | S1169 | G1170 | D1171 | K1172 | E1173 | K1174 | S1175 | M1176 | I1177 | S1178 | M1179 | D1180 | Q1181 | A1184 | L1185 | L1186 | S1195 | I1196 | L1197 | A1204 | G1205 | V1206 | G1207 | V1208 | P1209 | E1210 | L1211 | I1212 | N1213 | S1214 | P1215 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASN   | GLY   | ARG   | ASN   | ILE   | GLY   | F1001 | L1004 | Q1005 | Q1006 | R1007 | S1008 | A1009 | Q1010 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| Y1062 | Q1063 | R1064 | L1065 | I1068 | G1071 | W1075 | S1076 | G1077 | F1078 | S1079 | Q1080 | P1081 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| L1134 | I1135 | L1138 | M1139 | V1140 | I1141 | L1142 | E1143 | K1144 | S1145 | THR   | ALA   | SER   | ALA   | Q1150 | T1155 | L1158 | C1164 | R1165 | V1166 | W1167 | P1168 | S1169 | G1170 | D1171 | K1172 | E1173 | K1174 | S1175 | M1176 | I1177 | S1178 | M1179 | D1180 | Q1181 | A1184 | L1185 | L1186 | S1195 | I1196 | L1197 | A1204 | G1205 | V1206 | G1207 | V1208 | P1209 | E1210 | L1211 | I1212 | N1213 | S1214 | P1215 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASP   | ALA   | SER   | S1220 | S1221 | T1222 | L1226 | T1227 | R1228 | H1229 | T1230 | F1231 | V1232 | F1233 | F1234 | F1235 | R1236 | V1237 | M1238 | K1244 | T1245 | V1246 | K1247 | I1249 | E1250 | P1251 | G1252 | T1253 | A1254 | A1255 | D1256 | S1257 | Q1258 | Q1259 | I1260 | H1261 | E1262 | K1264 | L1265 | L1266 | M1269 | M1270 | R1273 | I1277 | M1280 | L1281 | K1282 | V1284 | F1285 | D1286 |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| D255  | F258  | V262  | R263  | Q264  | L265  | D268  | K269  | I273  | R274  | L278  | P279  | V280  | I281  | I282  | K283  | F284  | I285  | L286  | H287  | S288  | D293  | E296  | V297  | I298  | S299  | R302  | E303  | K304  | D306  | L307  | Q308  | H309  | C310  | V311  | LEU   | PRO   | SER   | ARG   | LEU   | GLN   | ALA   | SER   | GLN   | VAL   | LYS   | LEU   | LYS   | SER   | LYS   |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| GLY   | ARG   | ALA   | SER   | SER   | GLY   | ASN   | GLN   | GLU   | S337  | S338  | G339  | Q340  | S341  | C342  | I343  | L344  | L345  | L346  | F347  | D348  | V349  | K350  | K351  | S352  | R355  | Y356  | E357  | K358  | T359  | E362  | A363  | W364  | I365  | K366  | E369  | T370  | T371  | Q372  | H377  | K378  | V379  | F380  | D381  | L382  | V383  | M384  | I387  | T391  | N392  | L393  | Q394  | LYS   |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| K397  | Y398  | R401  | K406  | I412  | Q413  | Q415  | L416  | L417  | V423  | H424  | K429  | D430  | M431  | L436  | L442  | L443  | I450  | I451  | F452  | F453  | L456  | Y460  | L477  | I481  | C482  | S483  | G484  | M485  | T491  | V500  | M507  | M508  | V514  | K515  | G516  | I517  | P526  | Q527  | Q528  | I529  | R530  |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| K531  | L532  | L536  | F541  | S542  | N545  | E546  | I551  | M555  | V558  | I559  | R560  | K561  | Q562  | S565  | F568  | K569  | Y570  | K571  | T580  | A582  | G583  | M585  | A586  | A587  | ASP   | ARG   | SER   | GLU   | SER   | PRO   | SER   | LEU   | THR   | GLN   | GLU   | ARG   | ALA   | ASN   | LEU   | SER   | D604  | C607  | V610  | L613  | I695  |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| V617  | H618  | S619  | C620  | E621  | E622  | Q623  | S624  | A627  | L630  | E634  | N637  | L638  | H641  | K642  | E643  | L644  | D645  | P646  | K647  | L649  | E650  | T650  | M651  | V652  | I656  | D659  | V665  | S668  | E673  | G674  | D675  | P676  | F677  | V678  | P679  | V680  | K681  | A682  | L686  | E687  | E688  | Y689  | D690  | T691  | Q692  | D693  | G694  |       |       |       |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| A696  | Q706  | D707  | PHE   | ALA   | LYS   | ASP   | GLY   | GLY   | PRD   | VAL   | THR   | SER   | GLN   | GLU   | SER   | GLY   | L728  | C729  | Y733  | L736  | L737  | R738  | E742  | H745  | N746  | G747  | N748  | I762  | D763  | G764  | L765  | E766  | P767  | G768  | E769  | K770  | L771  | E772  | L786  | T787  | N791  | W792  | F793  | R794  | E795  | I796  | Y797  | A799  | Q802  | E803  | T804  | E807  | M808  | T814  | R815  | L816  | K817 | V820 | L826 | E827 | K828 | Y829 | L830 | A831 | L833 | T833 | L840 | G841 | N842 | F843 | D844 | V845 | E846 | T847 | L848 | D849 | I850 | T851 | PRO |
| LYS   | THR   | VAL   | THR   | ALA   | ILE   | SER   | ALA   | ASN   | THR   | GLY   | ILE   | GLY   | THR   | GLN   | GLU   | ILE   | GLY   | ARG   | LYS   | GLY   | THR   | LYS   | THR   | THR   | GLY   | ASP   | GLY   | LYS   | THR   | GLY   | GLU   | GLU   | GLU   | LYS   | THR   | THR   | THR   | GLN   | GLN   | ASN   | LYS   | GLY   | LEU   | LEU   | GLY   | THR   | GLY   | LYS   | GLY   | VAL   | PRO   | PHE   | LEU   |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | THR   | SER   | L916  | N920  | S921  | H922  | A923  | F924  | F925  | A926  | E927  | D929  | E930  | L931  | V932  | F933  | H937  | C938  | R943  | F944  | I945  | L946  | ASP   | THR   | GLU   | THR   | MET   | HIS   | THR   | GLU   | ALA   | ALA   | THR   | VAL   | VAL   | L960  | L969  | L972  | K975  | L976  | T981  | PRO   | PRO   | ILE   | ALA   | ARG   | ARG   | VAL   | PRO   | PHE   | LEU   |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASN   | GLY   | SER   | ARG   | ASN   | ILE   | GLY   | F1001 | L1004 | Q1005 | Q1006 | R1007 | S1008 | A1009 | Q1010 | E1011 | I1012 | V1013 | H1014 | C1015 | V1016 | F1017 | Q1018 | L1019 | L1020 | P1021 | P1022 | M1023 | C1024 | N1025 | H1026 | H1031 | L1037 | A1038 | E1039 | E1040 | N1041 | H1042 | GLY   | VAL   | VAL   | ASP   | GLY   | PRO   | GLY   | VAL   | K1051 | V1052 | Q1053 | E1054 | Y1055 | H1056 | I1057 | M1058 | S1059 |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| Y1062 | Q1063 | R1064 | L1065 | I1068 | G1071 | W1075 | S1076 | G1077 | F1078 | S1079 | Q1080 | P1081 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| L1134 | I1135 | L1138 | M1139 | V1140 | I1141 | L1142 | E1143 | K1144 | S1145 | THR   | ALA   | SER   | ALA   | Q1150 | T1155 | L1158 | C1164 | R1165 | V1166 | W1167 | P1168 | S1169 | G1170 | D1171 | K1172 | E1173 | K1174 | S1175 | M1176 | I1177 | S1178 | M1179 | D1180 | Q1181 | A1184 | L1185 | L1186 | S1195 | I1196 | L1197 | A1204 | G1205 | V1206 | G1207 | V1208 | P1209 | E1210 | L1211 | I1212 | N1213 | S1214 | P1215 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASN   | GLY   | ARG   | ASN   | ILE   | GLY   | F1001 | L1004 | Q1005 | Q1006 | R1007 | S1008 | A1009 | Q1010 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| Y1062 | Q1063 | R1064 | L1065 | I1068 | G1071 | W1075 | S1076 | G1077 | F1078 | S1079 | Q1080 | P1081 | E1082 | M1083 | Q1084 | M1085 | L1086 | L1087 | Y1088 | S1089 | A1090 | L1091 | H1092 | V1093 | L1094 | R1097 | L1098 | K1099 | Q1100 | G1101 | E1102 | H1103 | S1104 | Q1105 | P1106 | L1107 | E1108 | L1109 | L1110 | L1111 | S1112 | Q1113 | S1114 | V1115 | H1122 | Q1123 | S1124 | I1125 | F1128 | M1058 | S1059 |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| L1134 | I1135 | L1138 | M1139 | V1140 | I1141 | L1142 | E1143 | K1144 | S1145 | THR   | ALA   | SER   | ALA   | Q1150 | T1155 | L1158 | C1164 | R1165 | V1166 | W1167 | P1168 | S1169 | G1170 | D1171 | K1172 | E1173 | K1174 | S1175 | M1176 | I1177 | S1178 | M1179 | D1180 | Q1181 | A1184 | L1185 | L1186 | S1195 | I1196 | L1197 | A1204 | G1205 | V1206 | G1207 | V1208 | P1209 | E1210 | L1211 | I1212 | N1213 | S1214 | P1215 |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| LYS   | ASP   | ALA   | SER   | S1220 | S1221 | T1222 | L1226 | T1227 | R1228 | H1229 | T1230 | F1231 | V1232 | F1233 | F1234 | F1235 | R1236 | V1237 | M1238 | K1244 | T1245 | V1246 | K1247 | I1249 | E1250 | P1251 | G1252 | T1253 | A1254 | A1255 | D1256 | S1257 | Q1258 | Q1259 | I1260 | H1261 | E1262 | K1264 | L1265 | L1266 | M1269 | M1270 | R1273 | I1277 | M1280 | L1281 | K1282 | V1284 | F1285 | D1286 |       |       |       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
| S1287 | H1288 | P1289 | V1290 | L1291 | H1292 | V1293 | L1294 | L1295 | R1299 | L1300 | F1301 | V1302 | E1303 | A1304 | F1306 | L1306 | K1307 | Q1308 | C1309 | M1310 | P1311 | L1312 | L1313 | D1314 | F1315 | S1316 | F1317 | R1318 | K1319 | H1320 | R1321 | E1322 | D1323 | L1324 | S1325 | S1326 | L1327 | L1328 | E1329 | F1331 | L1332 | D1334 | T1335 | R1336 | L1337 | L1338 | H1339 | H1340 | L1341 | C1342 | G1343 | H1344 | S1345 | K1346 | I1347 | H1348 |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | ASP | GLU | GLU | GLU | ASP | ASP | MET | SER | SER | GLN | ALA | SER | LYS | SER | LYS | ALA | THR | GLU | ASP | GLY | GLY | GLU | GLU | ASP | GLU | VAL | SER | ALA | ALA | GLY | GLU | LYS | GLU | GLN | ASP | SER | ASP | GLU | TYR | ASP | ASP | SER | ASP | ASP |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 76111                                   | 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 ( $e^-/\text{\AA}^2$ ) | 65                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.071                                   | Depositor |
| Minimum map value                    | -0.039                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.0055                                  | Depositor |
| Map size (Å)                         | 487.63455, 487.63455, 487.63455         | wwPDB     |
| Map dimensions                       | 448, 448, 448                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.08847, 1.08847, 1.08847               | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$     | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.40         | 0/9605          | 0.55        | 2/13008 (0.0%)   |
| 1   | S     | 0.37         | 0/10153         | 0.43        | 0/13749          |
| 2   | B     | 0.82         | 9/5707 (0.2%)   | 0.90        | 4/7686 (0.1%)    |
| 2   | O     | 0.49         | 0/5701          | 0.69        | 1/7686 (0.0%)    |
| 3   | C     | 0.79         | 12/4497 (0.3%)  | 0.79        | 2/6103 (0.0%)    |
| 4   | E     | 0.62         | 4/3274 (0.1%)   | 0.73        | 1/4438 (0.0%)    |
| 5   | F     | 0.66         | 3/2791 (0.1%)   | 0.73        | 0/3790           |
| 6   | G     | 0.63         | 2/4568 (0.0%)   | 0.71        | 1/6215 (0.0%)    |
| 6   | H     | 0.44         | 0/4293          | 0.60        | 2/5840 (0.0%)    |
| 7   | L     | 0.73         | 3/3050 (0.1%)   | 0.80        | 2/4143 (0.0%)    |
| 7   | M     | 0.48         | 0/3050          | 0.67        | 2/4143 (0.0%)    |
| 8   | P     | 0.98         | 21/5697 (0.4%)  | 1.01        | 11/7752 (0.1%)   |
| 8   | Q     | 0.46         | 0/5737          | 0.67        | 0/7810           |
| 9   | W     | 0.34         | 0/202           | 0.44        | 0/281            |
| 10  | U     | 0.42         | 0/9400          | 0.55        | 0/12676          |
| 11  | V     | 0.42         | 0/9433          | 0.55        | 0/12760          |
| All | All   | 0.57         | 54/87158 (0.1%) | 0.67        | 28/118080 (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 |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 9                   |
| 1   | S     | 0                   | 4                   |
| 2   | B     | 0                   | 8                   |
| 2   | O     | 0                   | 4                   |
| 3   | C     | 0                   | 2                   |
| 4   | E     | 0                   | 1                   |
| 6   | G     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | H     | 0                   | 3                   |
| 7   | L     | 0                   | 2                   |
| 7   | M     | 0                   | 2                   |
| 8   | P     | 0                   | 12                  |
| 8   | Q     | 0                   | 6                   |
| 10  | U     | 0                   | 4                   |
| 11  | V     | 0                   | 7                   |
| All | All   | 0                   | 66                  |

All (54) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | P     | 68  | GLU  | CD-OE1 | 9.56  | 1.36        | 1.25     |
| 8   | P     | 68  | GLU  | CD-OE2 | 8.94  | 1.35        | 1.25     |
| 8   | P     | 222 | ASP  | CG-OD1 | 8.80  | 1.45        | 1.25     |
| 3   | C     | 201 | GLU  | CD-OE2 | 8.49  | 1.34        | 1.25     |
| 3   | C     | 225 | GLU  | CD-OE2 | 8.34  | 1.34        | 1.25     |
| 5   | F     | 141 | SER  | CA-CB  | -8.10 | 1.40        | 1.52     |
| 3   | C     | 221 | GLU  | CD-OE1 | 8.10  | 1.34        | 1.25     |
| 8   | P     | 133 | PHE  | CG-CD1 | -7.62 | 1.27        | 1.38     |
| 2   | B     | 507 | SER  | CA-CB  | -7.57 | 1.41        | 1.52     |
| 8   | P     | 216 | GLY  | C-O    | 7.26  | 1.35        | 1.23     |
| 5   | F     | 168 | GLU  | CD-OE1 | 7.22  | 1.33        | 1.25     |
| 2   | B     | 416 | GLU  | CD-OE1 | 7.20  | 1.33        | 1.25     |
| 2   | B     | 314 | GLU  | CD-OE1 | 7.16  | 1.33        | 1.25     |
| 2   | B     | 314 | GLU  | CD-OE2 | 7.02  | 1.33        | 1.25     |
| 3   | C     | 251 | GLU  | CD-OE2 | 6.79  | 1.33        | 1.25     |
| 4   | E     | 100 | SER  | CA-CB  | -6.78 | 1.42        | 1.52     |
| 8   | P     | 222 | ASP  | CG-OD2 | 6.63  | 1.40        | 1.25     |
| 2   | B     | 407 | GLU  | CD-OE2 | 6.61  | 1.32        | 1.25     |
| 2   | B     | 407 | GLU  | CD-OE1 | 6.52  | 1.32        | 1.25     |
| 8   | P     | 38  | SER  | CA-CB  | -6.51 | 1.43        | 1.52     |
| 4   | E     | 99  | MET  | CG-SD  | -6.43 | 1.64        | 1.81     |
| 2   | B     | 336 | SER  | CA-CB  | -6.39 | 1.43        | 1.52     |
| 3   | C     | 213 | GLU  | CD-OE2 | 6.35  | 1.32        | 1.25     |
| 8   | P     | 398 | SER  | CA-CB  | -6.33 | 1.43        | 1.52     |
| 2   | B     | 339 | GLU  | CD-OE2 | 6.32  | 1.32        | 1.25     |
| 3   | C     | 249 | SER  | CA-CB  | -6.32 | 1.43        | 1.52     |
| 7   | L     | 307 | CYS  | CB-SG  | -6.03 | 1.72        | 1.82     |
| 3   | C     | 218 | GLU  | CD-OE2 | 5.97  | 1.32        | 1.25     |
| 6   | G     | 344 | SER  | CA-CB  | -5.93 | 1.44        | 1.52     |
| 3   | C     | 221 | GLU  | CD-OE2 | 5.92  | 1.32        | 1.25     |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 8   | P     | 172 | GLU  | CD-OE2 | 5.86  | 1.32        | 1.25     |
| 3   | C     | 213 | GLU  | CD-OE1 | 5.86  | 1.32        | 1.25     |
| 5   | F     | 340 | GLU  | CD-OE1 | 5.83  | 1.32        | 1.25     |
| 8   | P     | 359 | TYR  | CG-CD2 | -5.78 | 1.31        | 1.39     |
| 3   | C     | 201 | GLU  | CD-OE1 | 5.73  | 1.31        | 1.25     |
| 2   | B     | 339 | GLU  | CD-OE1 | 5.70  | 1.31        | 1.25     |
| 6   | G     | 418 | GLU  | CD-OE1 | 5.60  | 1.31        | 1.25     |
| 8   | P     | 358 | VAL  | CB-CG1 | -5.56 | 1.41        | 1.52     |
| 4   | E     | 38  | GLU  | CD-OE1 | 5.50  | 1.31        | 1.25     |
| 8   | P     | 133 | PHE  | CB-CG  | -5.50 | 1.42        | 1.51     |
| 3   | C     | 160 | GLU  | CD-OE1 | 5.48  | 1.31        | 1.25     |
| 4   | E     | 71  | GLU  | CD-OE2 | 5.38  | 1.31        | 1.25     |
| 8   | P     | 42  | GLU  | CD-OE1 | 5.35  | 1.31        | 1.25     |
| 8   | P     | 225 | PHE  | CG-CD1 | -5.30 | 1.30        | 1.38     |
| 8   | P     | 172 | GLU  | CD-OE1 | 5.27  | 1.31        | 1.25     |
| 8   | P     | 360 | HIS  | CG-ND1 | -5.27 | 1.27        | 1.38     |
| 8   | P     | 310 | ASP  | CG-OD1 | 5.26  | 1.37        | 1.25     |
| 8   | P     | 398 | SER  | CB-OG  | -5.25 | 1.35        | 1.42     |
| 3   | C     | 204 | LEU  | C-O    | -5.22 | 1.13        | 1.23     |
| 7   | L     | 92  | GLU  | CD-OE1 | 5.16  | 1.31        | 1.25     |
| 7   | L     | 37  | HIS  | C-O    | -5.14 | 1.13        | 1.23     |
| 8   | P     | 156 | GLU  | CD-OE1 | 5.09  | 1.31        | 1.25     |
| 8   | P     | 348 | LEU  | C-O    | -5.01 | 1.13        | 1.23     |
| 8   | P     | 13  | GLY  | C-O    | -5.00 | 1.15        | 1.23     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 8   | P     | 359 | TYR  | CB-CG-CD2 | -7.40 | 116.56      | 121.00   |
| 3   | C     | 245 | ARG  | NE-CZ-NH2 | -7.01 | 116.79      | 120.30   |
| 8   | P     | 315 | PHE  | CB-CA-C   | -6.79 | 96.82       | 110.40   |
| 2   | B     | 324 | LYS  | CB-CG-CD  | 6.61  | 128.80      | 111.60   |
| 8   | P     | 874 | ARG  | NE-CZ-NH1 | 6.46  | 123.53      | 120.30   |
| 6   | G     | 417 | CYS  | CA-CB-SG  | -6.42 | 102.45      | 114.00   |
| 8   | P     | 359 | TYR  | CB-CG-CD1 | 6.37  | 124.82      | 121.00   |
| 8   | P     | 874 | ARG  | NE-CZ-NH2 | -6.21 | 117.19      | 120.30   |
| 2   | B     | 406 | ARG  | NE-CZ-NH1 | -6.21 | 117.19      | 120.30   |
| 4   | E     | 96  | ARG  | NE-CZ-NH2 | 6.17  | 123.38      | 120.30   |
| 8   | P     | 542 | THR  | CA-CB-OG1 | -6.04 | 96.31       | 109.00   |
| 2   | O     | 474 | LEU  | CA-CB-CG  | 5.94  | 128.96      | 115.30   |
| 2   | B     | 480 | TYR  | CB-CG-CD1 | -5.92 | 117.45      | 121.00   |
| 8   | P     | 434 | LEU  | CB-CG-CD2 | -5.88 | 101.01      | 111.00   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 8   | P     | 222 | ASP  | CB-CG-OD2  | -5.77 | 113.11      | 118.30   |
| 8   | P     | 566 | THR  | CB-CA-C    | -5.72 | 96.16       | 111.60   |
| 8   | P     | 26  | PRO  | N-CD-CG    | -5.68 | 94.67       | 103.20   |
| 7   | L     | 26  | GLU  | OE1-CD-OE2 | -5.61 | 116.57      | 123.30   |
| 7   | M     | 16  | LEU  | CA-CB-CG   | 5.53  | 128.01      | 115.30   |
| 8   | P     | 221 | GLU  | CB-CA-C    | -5.46 | 99.48       | 110.40   |
| 6   | H     | 538 | LEU  | CA-CB-CG   | 5.41  | 127.75      | 115.30   |
| 3   | C     | 245 | ARG  | NE-CZ-NH1  | 5.37  | 122.98      | 120.30   |
| 6   | H     | 373 | LEU  | CA-CB-CG   | 5.36  | 127.63      | 115.30   |
| 1   | A     | 822 | LEU  | CA-CB-CG   | -5.24 | 103.25      | 115.30   |
| 7   | M     | 16  | LEU  | CB-CG-CD1  | -5.16 | 102.23      | 111.00   |
| 1   | A     | 736 | VAL  | C-N-CA     | -5.10 | 108.96      | 121.70   |
| 7   | L     | 91  | LEU  | CB-CG-CD2  | -5.05 | 102.41      | 111.00   |
| 2   | B     | 336 | SER  | CB-CA-C    | -5.00 | 100.59      | 110.10   |

There are no chirality outliers.

All (66) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1221 | ASN  | Peptide |
| 1   | A     | 1350 | GLU  | Peptide |
| 1   | A     | 138  | THR  | Peptide |
| 1   | A     | 313  | THR  | Peptide |
| 1   | A     | 484  | GLU  | Peptide |
| 1   | A     | 824  | CYS  | Peptide |
| 1   | A     | 899  | PRO  | Peptide |
| 1   | A     | 922  | GLU  | Peptide |
| 1   | A     | 923  | GLU  | Peptide |
| 2   | B     | 139  | GLY  | Peptide |
| 2   | B     | 145  | ARG  | Peptide |
| 2   | B     | 146  | HIS  | Peptide |
| 2   | B     | 191  | LEU  | Peptide |
| 2   | B     | 259  | LEU  | Peptide |
| 2   | B     | 324  | LYS  | Peptide |
| 2   | B     | 618  | GLY  | Peptide |
| 2   | B     | 636  | PHE  | Peptide |
| 3   | C     | 172  | GLN  | Peptide |
| 3   | C     | 22   | TRP  | Peptide |
| 4   | E     | 352  | SER  | Peptide |
| 6   | G     | 496  | ALA  | Peptide |
| 6   | G     | 563  | ARG  | Peptide |
| 6   | H     | 132  | LEU  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 6   | H     | 186  | PRO  | Peptide |
| 6   | H     | 563  | ARG  | Peptide |
| 7   | L     | 109  | GLN  | Peptide |
| 7   | L     | 215  | GLU  | Peptide |
| 7   | M     | 215  | GLU  | Peptide |
| 7   | M     | 296  | ALA  | Peptide |
| 2   | O     | 259  | LEU  | Peptide |
| 2   | O     | 324  | LYS  | Peptide |
| 2   | O     | 636  | PHE  | Peptide |
| 2   | O     | 711  | THR  | Peptide |
| 8   | P     | 146  | GLY  | Peptide |
| 8   | P     | 329  | ASP  | Peptide |
| 8   | P     | 345  | GLY  | Peptide |
| 8   | P     | 389  | GLY  | Peptide |
| 8   | P     | 398  | SER  | Peptide |
| 8   | P     | 584  | LEU  | Peptide |
| 8   | P     | 594  | LEU  | Peptide |
| 8   | P     | 62   | ASP  | Peptide |
| 8   | P     | 725  | GLY  | Peptide |
| 8   | P     | 780  | GLY  | Peptide |
| 8   | P     | 781  | PRO  | Peptide |
| 8   | P     | 878  | LEU  | Peptide |
| 8   | Q     | 584  | LEU  | Peptide |
| 8   | Q     | 594  | LEU  | Peptide |
| 8   | Q     | 647  | VAL  | Peptide |
| 8   | Q     | 720  | LYS  | Peptide |
| 8   | Q     | 726  | VAL  | Peptide |
| 8   | Q     | 781  | PRO  | Peptide |
| 1   | S     | 1221 | ASN  | Peptide |
| 1   | S     | 1222 | PRO  | Peptide |
| 1   | S     | 29   | ARG  | Peptide |
| 1   | S     | 484  | GLU  | Peptide |
| 10  | U     | 224  | GLY  | Peptide |
| 10  | U     | 492  | PRO  | Peptide |
| 10  | U     | 717  | GLU  | Peptide |
| 10  | U     | 802  | ASP  | Peptide |
| 11  | V     | 1169 | SER  | Peptide |
| 11  | V     | 204  | PRO  | Peptide |
| 11  | V     | 391  | THR  | Peptide |
| 11  | V     | 483  | SER  | Peptide |
| 11  | V     | 484  | GLY  | Peptide |
| 11  | V     | 541  | PHE  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 11  | V     | 842 | ASN  | 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   | A     | 9402  | 9487     | 9431     | 310     | 0            |
| 1   | S     | 9933  | 10028    | 9969     | 345     | 0            |
| 2   | B     | 5605  | 5790     | 5768     | 186     | 0            |
| 2   | O     | 5594  | 5759     | 5740     | 182     | 0            |
| 3   | C     | 4396  | 4442     | 4427     | 128     | 0            |
| 4   | E     | 3224  | 3390     | 3384     | 107     | 0            |
| 5   | F     | 2726  | 2740     | 2729     | 66      | 0            |
| 6   | G     | 4483  | 4537     | 4523     | 126     | 0            |
| 6   | H     | 4216  | 4288     | 4273     | 105     | 0            |
| 7   | L     | 2974  | 2977     | 2972     | 60      | 0            |
| 7   | M     | 2974  | 2977     | 2972     | 97      | 0            |
| 8   | P     | 5598  | 5681     | 5652     | 227     | 0            |
| 8   | Q     | 5631  | 5724     | 5694     | 191     | 0            |
| 9   | W     | 271   | 242      | 195      | 16      | 0            |
| 10  | U     | 9256  | 9626     | 9595     | 315     | 0            |
| 11  | V     | 9258  | 9475     | 9422     | 329     | 0            |
| 12  | G     | 1     | 0        | 0        | 0       | 0            |
| 12  | L     | 2     | 0        | 0        | 0       | 0            |
| 12  | M     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 85546 | 87163    | 86746    | 2627    | 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 15.

All (2627) 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) |
|------------------|------------------|--------------------------|-------------------|
| 11:V:586:ALA:HB1 | 11:V:645:ASP:CB  | 1.70                     | 1.20              |
| 11:V:586:ALA:CB  | 11:V:645:ASP:HB2 | 1.76                     | 1.15              |
| 11:V:637:ASN:O   | 11:V:641:HIS:ND1 | 1.85                     | 1.09              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:362:LEU:O     | 8:P:468:ARG:NH2    | 1.94                     | 1.01              |
| 10:U:261:SER:O    | 10:U:265:ARG:HG2   | 1.62                     | 0.99              |
| 11:V:647:LYS:O    | 11:V:650:GLU:HG3   | 1.62                     | 0.98              |
| 7:M:107:PRO:HG3   | 2:O:401:CYS:SG     | 2.09                     | 0.92              |
| 11:V:930:ILE:HG22 | 11:V:1019:LEU:HD21 | 1.51                     | 0.92              |
| 2:B:523:CYS:HG    | 2:B:582:THR:HG1    | 1.09                     | 0.91              |
| 3:C:224:ASN:OD1   | 3:C:243:TRP:HH2    | 1.54                     | 0.89              |
| 8:P:544:CYS:SG    | 8:P:601:THR:OG1    | 2.28                     | 0.89              |
| 8:P:467:GLU:O     | 8:P:470:SER:OG     | 1.89                     | 0.89              |
| 3:C:243:TRP:HZ3   | 3:C:249:SER:OG     | 1.57                     | 0.88              |
| 3:C:142:PRO:HA    | 3:C:145:TYR:CE2    | 2.07                     | 0.88              |
| 11:V:508:MET:SD   | 11:V:545:ASN:ND2   | 2.47                     | 0.87              |
| 10:U:729:PHE:HB2  | 10:U:788:LYS:HD2   | 1.57                     | 0.86              |
| 11:V:618:HIS:O    | 11:V:622:GLU:HG3   | 1.74                     | 0.86              |
| 2:O:277:CYS:HB2   | 2:O:316:PHE:HB3    | 1.58                     | 0.86              |
| 2:O:484:ASP:OD1   | 2:O:486:SER:OG     | 1.93                     | 0.86              |
| 7:M:107:PRO:HG2   | 7:M:108:PRO:HD3    | 1.56                     | 0.85              |
| 7:M:297:ILE:HG13  | 7:M:301:SER:HA     | 1.56                     | 0.85              |
| 2:O:522:LYS:O     | 2:O:523:CYS:SG     | 2.35                     | 0.84              |
| 8:P:720:LYS:O     | 8:P:722:GLY:N      | 2.09                     | 0.84              |
| 8:P:290:THR:OG1   | 8:P:325:LYS:NZ     | 2.10                     | 0.84              |
| 3:C:243:TRP:HZ3   | 3:C:249:SER:HG     | 0.89                     | 0.84              |
| 6:G:511:GLN:NE2   | 6:G:544:CYS:SG     | 2.50                     | 0.83              |
| 2:O:146:HIS:O     | 2:O:148:LYS:N      | 2.11                     | 0.83              |
| 7:L:266:LYS:HD3   | 7:L:289:GLU:HB2    | 1.61                     | 0.83              |
| 11:V:637:ASN:HB3  | 11:V:641:HIS:HE1   | 1.42                     | 0.82              |
| 4:E:318:GLU:HA    | 7:M:76:HIS:HE1     | 1.44                     | 0.82              |
| 1:S:1156:LEU:HD23 | 1:S:1196:GLU:HB3   | 1.60                     | 0.82              |
| 3:C:241:CYS:SG    | 4:E:37:PRO:CD      | 2.67                     | 0.82              |
| 2:B:69:GLU:OE1    | 2:B:71:ASN:ND2     | 2.13                     | 0.82              |
| 8:P:566:THR:O     | 8:P:566:THR:OG1    | 1.90                     | 0.82              |
| 2:B:88:GLY:HA2    | 8:P:15:CYS:SG      | 2.18                     | 0.82              |
| 3:C:241:CYS:SG    | 4:E:37:PRO:HG3     | 2.20                     | 0.82              |
| 6:H:559:LYS:HD2   | 6:H:563:ARG:HG2    | 1.62                     | 0.82              |
| 2:B:68:LYS:O      | 2:B:69:GLU:HG3     | 1.80                     | 0.81              |
| 2:B:423:TYR:CG    | 8:P:606:LEU:HD13   | 2.14                     | 0.81              |
| 5:F:294:TRP:NE1   | 5:F:349:ASP:OD2    | 2.13                     | 0.81              |
| 6:H:262:PRO:HB3   | 6:H:289:LEU:HD21   | 1.61                     | 0.81              |
| 4:E:356:SER:OG    | 4:E:359:ASN:ND2    | 2.13                     | 0.81              |
| 3:C:212:GLN:HE21  | 3:C:212:GLN:HA     | 1.46                     | 0.80              |
| 5:F:289:LEU:O     | 6:G:485:ARG:NH1    | 2.14                     | 0.80              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:M:215:GLU:HG2   | 7:M:319:ILE:HG13   | 1.63                     | 0.80              |
| 8:P:361:SER:OG    | 8:P:398:SER:O      | 1.99                     | 0.80              |
| 6:H:283:LEU:HB2   | 6:H:306:LEU:HD13   | 1.63                     | 0.80              |
| 2:O:509:LEU:HD22  | 8:Q:542:THR:HG21   | 1.63                     | 0.80              |
| 8:P:585:GLY:HA2   | 8:P:592:LEU:HD11   | 1.61                     | 0.80              |
| 2:B:710:ARG:HD2   | 2:B:711:THR:HG23   | 1.62                     | 0.80              |
| 3:C:140:TYR:CE2   | 5:F:169:LEU:HD22   | 2.17                     | 0.80              |
| 2:O:75:LYS:HB3    | 2:O:97:GLU:HB3     | 1.63                     | 0.80              |
| 1:S:31:LYS:HB2    | 1:S:34:LYS:HD3     | 1.64                     | 0.79              |
| 3:C:333:LEU:HD11  | 4:E:48:ARG:HE      | 1.46                     | 0.79              |
| 2:B:98:LYS:HB3    | 2:B:106:GLU:HB2    | 1.64                     | 0.78              |
| 1:S:822:LEU:HD13  | 1:S:867:LYS:HD3    | 1.66                     | 0.78              |
| 1:A:497:PRO:HB2   | 1:A:507:LEU:HD21   | 1.66                     | 0.78              |
| 2:B:309:CYS:SG    | 2:B:310:ALA:N      | 2.56                     | 0.78              |
| 4:E:80:ARG:NH2    | 4:E:81:LEU:O       | 2.16                     | 0.77              |
| 2:B:846:GLN:HE22  | 8:P:877:SER:HB3    | 1.48                     | 0.77              |
| 1:S:1155:ILE:HD13 | 1:S:1158:LYS:HZ1   | 1.48                     | 0.77              |
| 2:B:506:LEU:H     | 2:B:525:ASN:HD21   | 1.30                     | 0.77              |
| 8:Q:234:THR:O     | 8:Q:237:GLN:NE2    | 2.17                     | 0.77              |
| 1:A:650:LEU:HD21  | 1:A:714:ARG:HH22   | 1.48                     | 0.77              |
| 1:A:1082:LEU:HD11 | 1:A:1130:ILE:HG22  | 1.66                     | 0.77              |
| 2:B:257:ILE:HD11  | 2:B:287:VAL:HG21   | 1.66                     | 0.77              |
| 1:S:1336:TYR:OH   | 1:S:1357:ALA:O     | 2.01                     | 0.77              |
| 11:V:1031:HIS:NE2 | 11:V:1058:MET:O    | 2.15                     | 0.77              |
| 1:A:1422:LEU:HD12 | 1:A:1426:GLY:HA3   | 1.67                     | 0.77              |
| 8:Q:24:GLY:O      | 8:Q:27:ARG:NH1     | 2.18                     | 0.76              |
| 4:E:336:LEU:O     | 4:E:371:ARG:NH2    | 2.18                     | 0.76              |
| 8:P:571:GLN:O     | 8:P:573:GLY:N      | 2.17                     | 0.76              |
| 10:U:835:SER:CB   | 10:U:838:PHE:HB3   | 2.14                     | 0.76              |
| 3:C:224:ASN:OD1   | 3:C:243:TRP:CH2    | 2.38                     | 0.76              |
| 11:V:1264:LYS:HE3 | 11:V:1312:LEU:HD22 | 1.67                     | 0.76              |
| 7:L:150:ILE:HG13  | 7:L:167:VAL:HG22   | 1.68                     | 0.76              |
| 8:P:11:LEU:HD22   | 8:P:52:GLY:HA3     | 1.65                     | 0.76              |
| 11:V:920:ASN:HA   | 11:V:924:PHE:HB2   | 1.68                     | 0.76              |
| 2:O:829:LYS:N     | 8:Q:824:ASP:O      | 2.18                     | 0.75              |
| 3:C:241:CYS:SG    | 4:E:37:PRO:CG      | 2.74                     | 0.75              |
| 8:Q:516:ARG:NH1   | 8:Q:519:THR:O      | 2.16                     | 0.75              |
| 3:C:122:LEU:O     | 5:F:140:ARG:NE     | 2.20                     | 0.75              |
| 1:A:511:ILE:HG22  | 1:A:515:LYS:HE2    | 1.68                     | 0.74              |
| 8:Q:165:ARG:HG3   | 8:Q:166:PRO:HD2    | 1.69                     | 0.74              |
| 1:A:281:LEU:HD21  | 1:A:295:VAL:HG11   | 1.68                     | 0.74              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:H:141:ARG:HH11  | 6:H:199:ASP:HA     | 1.52                     | 0.74              |
| 10:U:340:ASP:OD2  | 10:U:357:ARG:NH2   | 2.20                     | 0.74              |
| 1:A:948:ASP:OD2   | 1:S:1080:ARG:NH1   | 2.20                     | 0.74              |
| 2:B:481:ARG:NH1   | 2:B:647:ASP:OD1    | 2.20                     | 0.74              |
| 2:B:500:SER:O     | 2:B:604:ARG:NH1    | 2.20                     | 0.74              |
| 1:S:228:ALA:HB1   | 1:S:232:ARG:HH21   | 1.52                     | 0.74              |
| 6:G:96:ILE:HG23   | 6:G:142:LEU:HD21   | 1.70                     | 0.73              |
| 11:V:586:ALA:HB1  | 11:V:645:ASP:HB2   | 0.82                     | 0.73              |
| 8:P:362:THR:HG23  | 8:P:364:SER:H      | 1.53                     | 0.73              |
| 1:S:861:SER:HB2   | 1:S:864:LEU:HD23   | 1.70                     | 0.73              |
| 4:E:293:GLN:HG3   | 4:E:294:LEU:HD12   | 1.70                     | 0.73              |
| 2:O:69:GLU:OE1    | 2:O:71:ASN:ND2     | 2.22                     | 0.73              |
| 7:M:101:LEU:HD23  | 8:Q:386:GLY:HA2    | 1.70                     | 0.73              |
| 7:M:354:ILE:HG12  | 7:M:369:LYS:HG2    | 1.69                     | 0.73              |
| 11:V:68:LEU:HD13  | 11:V:72:GLN:HE22   | 1.54                     | 0.73              |
| 1:A:309:SER:O     | 8:P:831:ARG:NH2    | 2.22                     | 0.72              |
| 2:O:590:PHE:O     | 2:O:591:SER:OG     | 2.06                     | 0.72              |
| 2:O:40:THR:OG1    | 2:O:69:GLU:O       | 2.07                     | 0.72              |
| 11:V:1174:LYS:HD3 | 11:V:1177:ILE:HD12 | 1.71                     | 0.72              |
| 8:P:165:ARG:NE    | 8:P:166:PRO:HD2    | 2.05                     | 0.72              |
| 3:C:177:PRO:HG3   | 3:C:210:GLU:OE1    | 1.89                     | 0.72              |
| 6:G:242:ARG:NH1   | 6:G:275:GLU:O      | 2.23                     | 0.72              |
| 11:V:558:VAL:HG22 | 11:V:562:GLN:HE22  | 1.54                     | 0.72              |
| 3:C:207:HIS:O     | 4:E:92:ARG:NH2     | 2.22                     | 0.72              |
| 4:E:287:GLN:OE1   | 4:E:290:ARG:NH1    | 2.23                     | 0.72              |
| 7:L:216:PRO:HB2   | 7:L:219:PRO:HB3    | 1.70                     | 0.72              |
| 10:U:115:ALA:HB1  | 10:U:121:LEU:HD21  | 1.70                     | 0.72              |
| 5:F:122:ARG:NH2   | 5:F:130:GLN:OE1    | 2.23                     | 0.72              |
| 6:H:284:LEU:HG    | 6:H:306:LEU:HD21   | 1.71                     | 0.72              |
| 8:P:362:THR:OG1   | 8:P:363:PRO:HD2    | 1.89                     | 0.72              |
| 11:V:1256:ASP:HB3 | 11:V:1260:ILE:HD11 | 1.70                     | 0.72              |
| 8:Q:709:LYS:HB2   | 8:Q:879:ILE:HG23   | 1.72                     | 0.72              |
| 2:B:277:CYS:HB2   | 2:B:316:PHE:HB3    | 1.72                     | 0.71              |
| 1:A:1313:LEU:HD13 | 1:A:1317:ARG:HG3   | 1.72                     | 0.71              |
| 4:E:525:LYS:HD2   | 11:V:155:GLU:HB3   | 1.72                     | 0.71              |
| 7:M:104:LEU:HD12  | 7:M:105:PRO:CD     | 2.19                     | 0.71              |
| 6:G:416:LEU:HD12  | 1:S:22:TRP:HZ3     | 1.56                     | 0.71              |
| 8:Q:715:LEU:O     | 8:Q:719:LEU:N      | 2.21                     | 0.71              |
| 2:O:481:ARG:NH1   | 2:O:647:ASP:OD1    | 2.23                     | 0.71              |
| 2:O:520:LEU:HD12  | 8:Q:567:ILE:HG12   | 1.70                     | 0.71              |
| 8:Q:341:TYR:OH    | 8:Q:385:GLU:O      | 2.08                     | 0.71              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:192:SER:OG     | 1:S:195:GLU:OE1    | 2.08                     | 0.71              |
| 2:B:102:ASN:HB3    | 2:B:104:VAL:HG22   | 1.72                     | 0.70              |
| 10:U:622:SER:O     | 10:U:626:THR:OG1   | 2.08                     | 0.70              |
| 1:A:415:MET:HE1    | 1:A:427:MET:HA     | 1.73                     | 0.70              |
| 1:S:557:VAL:HG13   | 1:S:565:PRO:HG2    | 1.74                     | 0.70              |
| 11:V:482:CYS:SG    | 11:V:517:ILE:HG13  | 2.31                     | 0.70              |
| 11:V:1179:ASN:HB3  | 11:V:1233:VAL:HG21 | 1.73                     | 0.70              |
| 1:A:512:SER:HA     | 1:A:515:LYS:HE3    | 1.72                     | 0.70              |
| 8:Q:654:ARG:NH2    | 8:Q:758:ALA:O      | 2.24                     | 0.70              |
| 2:B:336:SER:O      | 2:B:336:SER:OG     | 2.06                     | 0.70              |
| 1:A:1319:LEU:HA    | 1:A:1322:VAL:HG12  | 1.73                     | 0.70              |
| 6:G:431:MET:HG2    | 6:G:434:LEU:HB2    | 1.73                     | 0.70              |
| 8:Q:371:LEU:HD11   | 8:Q:384:GLU:HB2    | 1.73                     | 0.70              |
| 1:S:727:CYS:HG     | 9:W:87:TRP:HE1     | 1.36                     | 0.70              |
| 11:V:928:LEU:HD23  | 11:V:932:VAL:HG11  | 1.73                     | 0.70              |
| 4:E:516:LEU:HD22   | 4:E:527:LEU:HD13   | 1.73                     | 0.70              |
| 3:C:29:GLU:OE2     | 3:C:30:THR:HG23    | 1.91                     | 0.70              |
| 6:G:62:ALA:O       | 6:G:106:THR:OG1    | 2.09                     | 0.70              |
| 11:V:1125:ILE:HD11 | 11:V:1134:LEU:HD13 | 1.72                     | 0.70              |
| 1:A:456:PHE:HA     | 1:A:460:ARG:HB3    | 1.73                     | 0.70              |
| 2:O:492:LYS:HA     | 2:O:577:ILE:HG22   | 1.74                     | 0.70              |
| 10:U:409:SER:HA    | 10:U:412:ARG:HE    | 1.57                     | 0.70              |
| 11:V:263:ARG:NH1   | 11:V:293:ASP:OD2   | 2.25                     | 0.69              |
| 4:E:464:MET:HE3    | 4:E:468:LYS:HB3    | 1.74                     | 0.69              |
| 1:S:1422:LEU:HD12  | 1:S:1426:GLY:HA3   | 1.74                     | 0.69              |
| 2:O:781:GLU:HA     | 8:Q:826:ARG:HD3    | 1.75                     | 0.69              |
| 2:O:520:LEU:HD22   | 8:P:518:GLN:HB3    | 1.74                     | 0.69              |
| 1:A:22:TRP:O       | 1:A:26:LEU:HG      | 1.92                     | 0.69              |
| 1:S:332:PRO:HB2    | 1:S:335:LYS:HE3    | 1.73                     | 0.69              |
| 1:S:186:HIS:HD2    | 1:S:193:LEU:H      | 1.38                     | 0.69              |
| 3:C:247:LEU:HB2    | 4:E:132:TRP:NE1    | 2.08                     | 0.69              |
| 2:O:836:ARG:NH2    | 8:Q:820:SER:O      | 2.26                     | 0.69              |
| 1:S:1422:LEU:HD23  | 1:S:1437:GLN:HE21  | 1.57                     | 0.69              |
| 7:M:153:LYS:HB2    | 7:M:164:ASP:HB2    | 1.75                     | 0.68              |
| 10:U:1014:CYS:HA   | 10:U:1074:ILE:HD12 | 1.74                     | 0.68              |
| 10:U:675:LEU:HD13  | 10:U:702:LEU:HD22  | 1.74                     | 0.68              |
| 1:A:992:HIS:ND1    | 1:A:1077:MET:SD    | 2.59                     | 0.68              |
| 6:G:115:GLU:N      | 6:G:121:LEU:HD21   | 2.08                     | 0.68              |
| 7:L:295:ARG:HD2    | 7:L:298:LEU:HD21   | 1.75                     | 0.68              |
| 6:G:388:PRO:HG2    | 8:P:270:ALA:HB1    | 1.75                     | 0.68              |
| 10:U:920:GLN:O     | 10:U:924:GLN:NE2   | 2.27                     | 0.68              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 8:Q:401:ILE:HD11 | 8:Q:420:LEU:HD22  | 1.75                     | 0.68              |
| 1:A:769:LEU:HB2  | 1:A:821:LEU:HD22  | 1.76                     | 0.68              |
| 7:L:275:ASP:O    | 7:L:283:ASN:ND2   | 2.25                     | 0.68              |
| 8:P:67:LEU:O     | 8:P:68:GLU:HG2    | 1.92                     | 0.68              |
| 1:A:1336:TYR:OH  | 1:A:1357:ALA:O    | 2.12                     | 0.68              |
| 8:Q:714:LEU:HA   | 8:Q:815:GLN:HE22  | 1.59                     | 0.68              |
| 1:A:23:ALA:HA    | 1:A:26:LEU:HD12   | 1.74                     | 0.68              |
| 1:A:1045:GLU:HA  | 1:A:1104:ARG:HG2  | 1.76                     | 0.68              |
| 8:P:130:LEU:HA   | 8:P:144:VAL:HA    | 1.75                     | 0.68              |
| 3:C:265:GLU:HG2  | 3:C:271:ARG:HB2   | 1.75                     | 0.67              |
| 1:S:605:GLU:HB3  | 1:S:609:ARG:HH12  | 1.58                     | 0.67              |
| 7:L:250:GLU:CD   | 7:L:250:GLU:N     | 2.47                     | 0.67              |
| 8:Q:130:LEU:HA   | 8:Q:144:VAL:HA    | 1.76                     | 0.67              |
| 1:A:1027:ASP:O   | 1:A:1030:LEU:HG   | 1.94                     | 0.67              |
| 3:C:373:GLU:OE1  | 3:C:376:ARG:NH2   | 2.27                     | 0.67              |
| 5:F:196:LEU:HD11 | 5:F:201:PHE:HB2   | 1.76                     | 0.67              |
| 1:S:977:LEU:HB3  | 1:S:1028:LEU:HD21 | 1.75                     | 0.67              |
| 11:V:792:TRP:CE2 | 11:V:796:ILE:HD11 | 2.28                     | 0.67              |
| 2:B:517:ARG:HH12 | 2:B:589:THR:HG21  | 1.59                     | 0.67              |
| 6:H:257:ARG:HB2  | 6:H:289:LEU:HD12  | 1.77                     | 0.67              |
| 11:V:542:SER:HB2 | 11:V:545:ASN:HD21 | 1.60                     | 0.67              |
| 1:S:1161:THR:O   | 1:S:1321:ARG:NH2  | 2.28                     | 0.67              |
| 1:S:1336:TYR:HB3 | 1:S:1395:LEU:HD11 | 1.77                     | 0.67              |
| 10:U:970:LEU:O   | 10:U:1019:ARG:NH2 | 2.28                     | 0.67              |
| 11:V:1122:HIS:O  | 11:V:1165:ARG:NH1 | 2.28                     | 0.67              |
| 11:V:515:LYS:HD3 | 11:V:551:ILE:HG22 | 1.77                     | 0.67              |
| 6:H:79:ILE:HG13  | 6:H:145:LEU:HD21  | 1.76                     | 0.67              |
| 7:M:216:PRO:HB2  | 7:M:219:PRO:HB3   | 1.76                     | 0.67              |
| 10:U:417:HIS:HA  | 10:U:420:LYS:HG2  | 1.77                     | 0.67              |
| 11:V:637:ASN:C   | 11:V:641:HIS:HD1  | 1.97                     | 0.67              |
| 1:A:218:CYS:HA   | 1:A:221:MET:HG2   | 1.76                     | 0.67              |
| 2:B:678:GLU:N    | 2:B:678:GLU:OE1   | 2.28                     | 0.67              |
| 7:M:104:LEU:HD12 | 7:M:105:PRO:HD3   | 1.77                     | 0.67              |
| 1:A:39:ARG:NH2   | 6:H:308:GLU:OE1   | 2.27                     | 0.66              |
| 1:A:1336:TYR:O   | 1:A:1340:SER:OG   | 2.12                     | 0.66              |
| 8:Q:879:ILE:HG22 | 8:Q:881:LEU:HD13  | 1.76                     | 0.66              |
| 10:U:117:ARG:NH2 | 10:U:163:THR:O    | 2.28                     | 0.66              |
| 2:B:519:ARG:NH2  | 2:B:586:PRO:O     | 2.28                     | 0.66              |
| 3:C:212:GLN:HA   | 3:C:212:GLN:NE2   | 2.09                     | 0.66              |
| 1:S:313:THR:HG22 | 1:S:317:LYS:HG2   | 1.78                     | 0.66              |
| 10:U:596:SER:HA  | 10:U:602:ARG:HH21 | 1.60                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:274:LEU:HD11   | 1:A:323:THR:HG23   | 1.75                     | 0.66              |
| 1:A:460:ARG:HA     | 1:A:463:HIS:CD2    | 2.29                     | 0.66              |
| 6:G:39:ARG:NH2     | 6:G:319:PRO:O      | 2.28                     | 0.66              |
| 7:M:84:MET:HB3     | 7:M:88:LYS:HZ1     | 1.60                     | 0.66              |
| 2:O:82:VAL:O       | 2:O:138:ASN:ND2    | 2.27                     | 0.66              |
| 1:S:411:VAL:HG13   | 1:S:430:ALA:HB1    | 1.77                     | 0.66              |
| 7:M:239:GLU:HB3    | 7:M:250:GLU:HG2    | 1.77                     | 0.66              |
| 2:O:484:ASP:OD1    | 2:O:484:ASP:N      | 2.27                     | 0.66              |
| 1:A:468:LYS:HA     | 1:A:471:VAL:HG23   | 1.77                     | 0.66              |
| 8:Q:546:GLN:HB3    | 8:Q:564:THR:HG22   | 1.78                     | 0.66              |
| 11:V:1138:LEU:HD23 | 11:V:1141:ILE:HD11 | 1.77                     | 0.66              |
| 6:H:35:LEU:HD12    | 6:H:37:LEU:H       | 1.61                     | 0.66              |
| 2:O:503:ASP:OD1    | 2:O:604:ARG:NH2    | 2.29                     | 0.66              |
| 6:H:214:ARG:NH1    | 6:H:328:LEU:O      | 2.28                     | 0.66              |
| 2:O:497:LEU:HD21   | 2:O:504:VAL:HG11   | 1.77                     | 0.66              |
| 1:S:495:HIS:HB3    | 1:S:496:PRO:HD3    | 1.76                     | 0.66              |
| 7:M:115:ILE:HD11   | 2:O:394:LEU:HD11   | 1.77                     | 0.66              |
| 1:S:1305:LEU:HA    | 1:S:1308:LEU:HD21  | 1.77                     | 0.66              |
| 2:B:145:ARG:NH1    | 2:B:168:SER:O      | 2.29                     | 0.66              |
| 10:U:840:ARG:NH2   | 10:U:899:GLU:OE2   | 2.28                     | 0.66              |
| 10:U:856:THR:OG1   | 10:U:858:HIS:O     | 2.13                     | 0.66              |
| 7:M:107:PRO:CG     | 2:O:401:CYS:SG     | 2.84                     | 0.66              |
| 1:A:780:HIS:O      | 1:A:784:LEU:HD12   | 1.95                     | 0.65              |
| 2:B:520:LEU:HD12   | 8:P:567:ILE:HG23   | 1.76                     | 0.65              |
| 2:O:509:LEU:HD23   | 8:Q:566:THR:HB     | 1.78                     | 0.65              |
| 11:V:64:SER:O      | 11:V:112:ASN:ND2   | 2.29                     | 0.65              |
| 2:B:431:GLN:NE2    | 2:B:614:TYR:OH     | 2.29                     | 0.65              |
| 2:B:706:THR:HG22   | 2:B:718:ILE:HB     | 1.78                     | 0.65              |
| 6:G:19:LYS:O       | 6:G:23:LEU:HD13    | 1.95                     | 0.65              |
| 6:H:586:LEU:HA     | 6:H:589:LEU:HD13   | 1.78                     | 0.65              |
| 8:Q:769:ARG:NH1    | 8:Q:786:GLU:OE2    | 2.29                     | 0.65              |
| 2:B:617:CYS:O      | 2:B:617:CYS:SG     | 2.53                     | 0.65              |
| 7:M:342:LEU:HD22   | 7:M:357:GLY:HA3    | 1.77                     | 0.65              |
| 2:O:325:LEU:HA     | 2:O:344:LEU:O      | 1.96                     | 0.65              |
| 8:P:140:LEU:HD23   | 8:P:140:LEU:O      | 1.97                     | 0.65              |
| 1:S:456:PHE:HA     | 1:S:460:ARG:HB3    | 1.77                     | 0.65              |
| 1:S:730:LEU:HD23   | 1:S:783:GLY:HA2    | 1.77                     | 0.65              |
| 2:B:360:THR:O      | 2:B:360:THR:OG1    | 2.11                     | 0.65              |
| 3:C:243:TRP:HA     | 3:C:243:TRP:HE3    | 1.61                     | 0.65              |
| 6:H:221:ILE:HD11   | 6:H:336:SER:OG     | 1.97                     | 0.65              |
| 1:A:288:GLU:HG3    | 1:A:292:HIS:CG     | 2.32                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:305:HIS:HA     | 2:B:824:LEU:HD21   | 1.78                     | 0.65              |
| 3:C:254:MET:HE1    | 3:C:257:LEU:HD23   | 1.79                     | 0.65              |
| 11:V:263:ARG:NH2   | 11:V:288:SER:O     | 2.30                     | 0.65              |
| 11:V:586:ALA:CB    | 11:V:645:ASP:CB    | 2.54                     | 0.65              |
| 11:V:742:GLU:OE2   | 11:V:802:GLN:NE2   | 2.30                     | 0.65              |
| 7:L:270:ASN:ND2    | 7:L:289:GLU:OE2    | 2.27                     | 0.65              |
| 11:V:1115:VAL:HG13 | 11:V:1138:LEU:HD22 | 1.78                     | 0.65              |
| 2:B:325:LEU:HA     | 2:B:344:LEU:O      | 1.97                     | 0.65              |
| 3:C:127:PHE:CE1    | 5:F:147:ARG:HD3    | 2.31                     | 0.65              |
| 4:E:124:ASP:N      | 4:E:124:ASP:OD1    | 2.30                     | 0.65              |
| 1:A:653:LEU:HA     | 1:A:683:ARG:HE     | 1.62                     | 0.65              |
| 5:F:116:PHE:HA     | 5:F:130:GLN:HE21   | 1.60                     | 0.65              |
| 5:F:289:LEU:HD21   | 6:G:480:LEU:HB3    | 1.79                     | 0.65              |
| 6:H:93:ALA:O       | 6:H:97:GLN:HG3     | 1.97                     | 0.65              |
| 8:P:543:LEU:HB3    | 8:P:567:ILE:HG13   | 1.78                     | 0.65              |
| 8:Q:495:ALA:HB1    | 8:Q:505:PRO:HG3    | 1.79                     | 0.65              |
| 8:Q:781:PRO:O      | 8:Q:782:ILE:HG12   | 1.97                     | 0.65              |
| 10:U:214:VAL:HA    | 10:U:217:LEU:HD12  | 1.79                     | 0.65              |
| 10:U:506:LEU:HB3   | 10:U:513:MET:HE1   | 1.78                     | 0.65              |
| 11:V:345:LEU:O     | 11:V:349:VAL:HG23  | 1.96                     | 0.65              |
| 1:A:1144:ARG:HH22  | 1:S:1144:ARG:HH22  | 1.43                     | 0.64              |
| 3:C:243:TRP:HA     | 3:C:243:TRP:CE3    | 2.31                     | 0.64              |
| 2:O:259:LEU:HB3    | 2:O:265:LEU:HD12   | 1.79                     | 0.64              |
| 4:E:497:MET:HG2    | 4:E:512:LEU:HD13   | 1.79                     | 0.64              |
| 8:P:202:PRO:HB3    | 8:P:225:PHE:CD2    | 2.32                     | 0.64              |
| 1:A:1080:ARG:NH1   | 1:S:949:THR:O      | 2.31                     | 0.64              |
| 1:A:1143:LEU:HD13  | 1:A:1188:HIS:HD2   | 1.62                     | 0.64              |
| 8:P:169:GLN:NE2    | 8:P:172:GLU:OE2    | 2.29                     | 0.64              |
| 10:U:1026:LYS:HD3  | 10:U:1083:THR:HB   | 1.79                     | 0.64              |
| 1:S:1252:GLU:O     | 1:S:1298:ARG:NH1   | 2.30                     | 0.64              |
| 2:B:840:LEU:HD21   | 8:P:812:VAL:HG11   | 1.80                     | 0.64              |
| 4:E:123:GLN:HE22   | 4:E:130:ASP:H      | 1.44                     | 0.64              |
| 10:U:751:GLU:HA    | 10:U:754:ILE:HD12  | 1.78                     | 0.64              |
| 2:B:846:GLN:HG3    | 8:P:874:ARG:NH1    | 2.13                     | 0.64              |
| 8:P:27:ARG:C       | 8:P:400:ASN:HD21   | 2.00                     | 0.64              |
| 10:U:504:GLN:HA    | 10:U:507:LEU:HD13  | 1.79                     | 0.64              |
| 8:P:200:VAL:O      | 8:P:200:VAL:HG12   | 1.98                     | 0.64              |
| 10:U:5:ILE:HG12    | 10:U:20:PHE:CE2    | 2.33                     | 0.64              |
| 2:B:277:CYS:SG     | 2:B:278:GLN:N      | 2.70                     | 0.64              |
| 8:Q:720:LYS:C      | 8:Q:722:GLY:H      | 1.99                     | 0.64              |
| 10:U:749:VAL:O     | 10:U:753:LEU:HD23  | 1.98                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:G:524:TRP:HB2    | 6:G:533:ALA:HB2    | 1.80                     | 0.64              |
| 8:Q:734:GLN:HE21   | 8:Q:747:ARG:HG2    | 1.62                     | 0.64              |
| 1:S:612:LYS:HB2    | 1:S:613:ILE:HD12   | 1.80                     | 0.64              |
| 1:A:291:THR:HA     | 1:A:294:ILE:HD12   | 1.79                     | 0.63              |
| 8:P:746:VAL:HG13   | 8:P:751:LEU:HD23   | 1.79                     | 0.63              |
| 10:U:1095:VAL:HG11 | 10:U:1141:LEU:HD11 | 1.79                     | 0.63              |
| 1:A:1168:THR:HA    | 1:A:1171:LEU:HD12  | 1.80                     | 0.63              |
| 7:M:3:VAL:HG23     | 7:M:5:GLU:HG2      | 1.80                     | 0.63              |
| 2:O:248:ILE:O      | 2:O:249:LYS:HG3    | 1.97                     | 0.63              |
| 2:O:499:LEU:HD12   | 2:O:576:GLN:HG2    | 1.79                     | 0.63              |
| 8:Q:764:VAL:HG12   | 8:Q:791:SER:HB2    | 1.80                     | 0.63              |
| 10:U:431:LYS:HB2   | 10:U:432:ILE:HG23  | 1.80                     | 0.63              |
| 2:B:65:PHE:HB2     | 2:B:118:PHE:CD1    | 2.33                     | 0.63              |
| 2:B:657:LYS:NZ     | 8:P:557:ASP:OD1    | 2.32                     | 0.63              |
| 8:Q:249:GLN:HB2    | 8:Q:274:ILE:HD11   | 1.81                     | 0.63              |
| 8:Q:712:ALA:HB3    | 8:Q:782:ILE:HG22   | 1.80                     | 0.63              |
| 8:Q:772:ALA:HB2    | 8:Q:783:GLN:HA     | 1.80                     | 0.63              |
| 10:U:956:ALA:HB1   | 10:U:960:ARG:HH21  | 1.62                     | 0.63              |
| 1:A:366:LEU:HD13   | 1:A:371:LEU:HD21   | 1.80                     | 0.63              |
| 1:A:1196:GLU:HA    | 1:A:1199:LYS:HD3   | 1.80                     | 0.63              |
| 2:B:582:THR:HG22   | 2:B:583:SER:N      | 2.13                     | 0.63              |
| 3:C:41:PHE:CE2     | 3:C:45:LEU:HD11    | 2.33                     | 0.63              |
| 2:O:82:VAL:HG13    | 2:O:83:SER:H       | 1.64                     | 0.63              |
| 10:U:117:ARG:HH22  | 10:U:163:THR:HG22  | 1.64                     | 0.63              |
| 7:L:307:CYS:CB     | 7:L:310:CYS:SG     | 2.87                     | 0.63              |
| 11:V:526:PRO:HD2   | 11:V:848:LEU:HD13  | 1.81                     | 0.63              |
| 11:V:752:ILE:O     | 11:V:755:LEU:N     | 2.23                     | 0.63              |
| 1:A:737:ALA:HB1    | 1:A:738:PRO:HD2    | 1.79                     | 0.63              |
| 1:A:1366:GLN:HA    | 1:A:1369:VAL:HG12  | 1.80                     | 0.63              |
| 11:V:623:GLN:OE1   | 11:V:623:GLN:N     | 2.28                     | 0.63              |
| 10:U:803:SER:OG    | 10:U:849:LYS:NZ    | 2.26                     | 0.63              |
| 1:S:494:LEU:HD11   | 1:S:518:LEU:HD21   | 1.79                     | 0.63              |
| 10:U:446:ASN:HD21  | 11:V:355:ARG:HE    | 1.46                     | 0.63              |
| 5:F:115:LEU:HD23   | 5:F:129:LEU:HD21   | 1.80                     | 0.63              |
| 2:O:266:ILE:HG12   | 2:O:276:VAL:HG22   | 1.80                     | 0.63              |
| 8:Q:767:ILE:HG13   | 8:Q:788:GLN:HB3    | 1.81                     | 0.63              |
| 10:U:105:LEU:HB3   | 10:U:133:ILE:HG23  | 1.81                     | 0.63              |
| 7:L:307:CYS:HB2    | 7:L:334:HIS:CE1    | 2.34                     | 0.62              |
| 2:O:475:VAL:HG21   | 2:O:617:CYS:SG     | 2.38                     | 0.62              |
| 1:S:866:LYS:HD3    | 1:S:925:VAL:HA     | 1.81                     | 0.62              |
| 1:S:1193:LEU:HD21  | 1:S:1197:LEU:HB2   | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:U:387:PHE:CE2  | 10:U:443:GLN:HB3  | 2.35                     | 0.62              |
| 11:V:372:ALA:HA   | 11:V:406:LYS:HZ3  | 1.65                     | 0.62              |
| 8:P:448:THR:O     | 8:P:451:ALA:N     | 2.24                     | 0.62              |
| 10:U:117:ARG:O    | 10:U:168:ARG:NH2  | 2.32                     | 0.62              |
| 10:U:442:GLU:OE1  | 10:U:446:ASN:ND2  | 2.33                     | 0.62              |
| 6:H:461:GLN:HE21  | 6:H:465:GLN:HE21  | 1.47                     | 0.62              |
| 11:V:645:ASP:O    | 11:V:649:LEU:HG   | 1.99                     | 0.62              |
| 1:A:1161:THR:O    | 1:A:1321:ARG:NH2  | 2.31                     | 0.62              |
| 3:C:213:GLU:HA    | 3:C:213:GLU:OE2   | 1.99                     | 0.62              |
| 10:U:1218:ASN:OD1 | 10:U:1219:LYS:N   | 2.33                     | 0.62              |
| 6:H:598:SER:HA    | 6:H:601:ARG:HD3   | 1.81                     | 0.62              |
| 7:M:216:PRO:HG2   | 7:M:226:ARG:HD3   | 1.82                     | 0.62              |
| 7:M:249:PRO:HG2   | 7:M:251:CYS:SG    | 2.40                     | 0.62              |
| 11:V:51:LEU:HD23  | 11:V:54:ILE:HD11  | 1.82                     | 0.62              |
| 4:E:318:GLU:HA    | 7:M:76:HIS:CE1    | 2.30                     | 0.62              |
| 6:H:206:VAL:HG13  | 6:H:325:VAL:HG22  | 1.80                     | 0.62              |
| 1:S:1292:LEU:HD12 | 1:S:1338:LEU:HG   | 1.82                     | 0.62              |
| 10:U:343:LEU:O    | 10:U:347:SER:OG   | 2.14                     | 0.62              |
| 3:C:213:GLU:OE1   | 3:C:220:PHE:CE2   | 2.52                     | 0.62              |
| 8:Q:506:ILE:HD13  | 8:Q:531:ASN:HD22  | 1.65                     | 0.62              |
| 4:E:523:LEU:HD22  | 11:V:158:PRO:HG3  | 1.82                     | 0.62              |
| 7:L:354:ILE:HG12  | 7:L:369:LYS:HG2   | 1.81                     | 0.62              |
| 8:Q:710:VAL:HG22  | 8:Q:880:LEU:HB2   | 1.81                     | 0.62              |
| 1:S:946:LEU:HB3   | 1:S:950:GLU:HG2   | 1.82                     | 0.62              |
| 1:A:372:VAL:HG21  | 1:A:406:LEU:HD13  | 1.81                     | 0.61              |
| 1:A:1072:GLN:O    | 1:A:1076:LEU:HD23 | 2.00                     | 0.61              |
| 1:A:1416:SER:HG   | 1:A:1417:HIS:CE1  | 2.18                     | 0.61              |
| 2:B:43:LEU:HD13   | 2:B:96:ILE:HD11   | 1.81                     | 0.61              |
| 2:B:718:ILE:HD11  | 8:P:556:LEU:HD22  | 1.82                     | 0.61              |
| 6:H:62:ALA:HB2    | 6:H:102:ARG:HD2   | 1.81                     | 0.61              |
| 1:A:428:VAL:HG22  | 1:A:476:PHE:CE1   | 2.35                     | 0.61              |
| 7:L:16:LEU:HD11   | 8:P:483:LEU:HD22  | 1.82                     | 0.61              |
| 2:O:68:LYS:O      | 2:O:69:GLU:HG3    | 2.01                     | 0.61              |
| 2:O:106:GLU:N     | 2:O:106:GLU:OE1   | 2.32                     | 0.61              |
| 5:F:19:SER:HB3    | 5:F:96:ARG:HD2    | 1.82                     | 0.61              |
| 6:H:178:LEU:HD13  | 6:H:211:PHE:HD2   | 1.65                     | 0.61              |
| 2:O:484:ASP:CG    | 2:O:485:ASP:H     | 2.02                     | 0.61              |
| 8:P:250:LEU:HD23  | 8:P:276:HIS:O     | 1.99                     | 0.61              |
| 8:P:398:SER:OG    | 8:P:422:ALA:HB1   | 1.99                     | 0.61              |
| 8:Q:589:ASN:ND2   | 8:Q:675:PRO:HD3   | 2.14                     | 0.61              |
| 1:A:100:ASP:O     | 1:A:103:SER:OG    | 2.11                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:313:THR:HG22   | 1:A:317:LYS:HG3    | 1.82                     | 0.61              |
| 3:C:126:ARG:HH12   | 5:F:140:ARG:HD3    | 1.63                     | 0.61              |
| 6:H:370:LEU:HA     | 6:H:373:LEU:HG     | 1.82                     | 0.61              |
| 6:G:555:LEU:HD21   | 6:G:570:LEU:HB2    | 1.82                     | 0.61              |
| 6:H:119:ARG:HH22   | 6:H:161:LEU:HB3    | 1.64                     | 0.61              |
| 7:M:107:PRO:N      | 7:M:108:PRO:HD2    | 2.16                     | 0.61              |
| 8:P:537:LEU:HD23   | 8:P:572:LEU:HD23   | 1.82                     | 0.61              |
| 11:V:766:GLU:OE2   | 11:V:770:LYS:NZ    | 2.25                     | 0.61              |
| 1:A:1250:ASP:O     | 1:A:1298:ARG:NH1   | 2.33                     | 0.61              |
| 3:C:387:CYS:SG     | 3:C:393:SER:OG     | 2.57                     | 0.61              |
| 10:U:261:SER:O     | 10:U:265:ARG:CG    | 2.44                     | 0.61              |
| 3:C:123:SER:HA     | 5:F:140:ARG:NH2    | 2.16                     | 0.61              |
| 6:G:249:TYR:HA     | 6:G:252:LEU:HD12   | 1.82                     | 0.61              |
| 1:S:555:ILE:HD13   | 1:S:603:PHE:HB2    | 1.83                     | 0.61              |
| 10:U:272:ILE:HG23  | 10:U:312:LEU:HD12  | 1.82                     | 0.61              |
| 2:B:283:ASP:HB3    | 2:B:304:ILE:HD12   | 1.82                     | 0.61              |
| 3:C:449:VAL:O      | 3:C:453:LEU:HD23   | 2.01                     | 0.61              |
| 7:M:207:ILE:O      | 7:M:211:THR:OG1    | 2.18                     | 0.61              |
| 7:M:215:GLU:HG2    | 7:M:319:ILE:CG1    | 2.30                     | 0.61              |
| 2:O:669:LEU:O      | 2:O:709:GLN:NE2    | 2.34                     | 0.61              |
| 8:P:579:GLU:OE2    | 8:Q:516:ARG:NH2    | 2.33                     | 0.61              |
| 10:U:493:LEU:HD23  | 10:U:493:LEU:H     | 1.65                     | 0.61              |
| 6:G:369:ASP:OD1    | 1:S:29:ARG:HD2     | 2.01                     | 0.60              |
| 8:P:324:ILE:HA     | 8:P:337:GLU:O      | 2.01                     | 0.60              |
| 11:V:1299:ARG:HH11 | 11:V:1359:LEU:HD12 | 1.64                     | 0.60              |
| 6:H:499:CYS:SG     | 6:H:500:GLU:N      | 2.73                     | 0.60              |
| 8:P:424:SER:O      | 8:P:427:GLY:N      | 2.32                     | 0.60              |
| 1:S:1358:VAL:HG11  | 1:S:1418:VAL:HG13  | 1.83                     | 0.60              |
| 10:U:751:GLU:OE2   | 10:U:841:TYR:OH    | 2.14                     | 0.60              |
| 2:B:79:CYS:HA      | 2:B:93:TYR:CE1     | 2.36                     | 0.60              |
| 2:B:176:ILE:HD12   | 2:B:182:VAL:HG11   | 1.82                     | 0.60              |
| 11:V:938:CYS:HG    | 11:V:960:LEU:N     | 1.99                     | 0.60              |
| 2:B:423:TYR:CZ     | 8:P:606:LEU:HB3    | 2.36                     | 0.60              |
| 3:C:132:ALA:O      | 3:C:136:GLN:NE2    | 2.34                     | 0.60              |
| 1:S:455:SER:O      | 1:S:460:ARG:N      | 2.30                     | 0.60              |
| 1:S:1252:GLU:HB3   | 1:S:1256:LEU:HD22  | 1.83                     | 0.60              |
| 4:E:403:LEU:HB3    | 4:E:440:GLN:NE2    | 2.15                     | 0.60              |
| 2:O:247:ILE:HG23   | 2:O:249:LYS:O      | 2.01                     | 0.60              |
| 5:F:202:LEU:HA     | 5:F:205:ILE:HD12   | 1.82                     | 0.60              |
| 8:Q:674:ASP:HB3    | 8:Q:677:ALA:H      | 1.66                     | 0.60              |
| 10:U:366:GLU:HA    | 10:U:369:LYS:HD2   | 1.84                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:V:638:LEU:C    | 11:V:638:LEU:HD23  | 2.21                     | 0.60              |
| 1:A:918:GLU:HA    | 1:A:921:LYS:HE3    | 1.84                     | 0.60              |
| 1:A:1079:LYS:HD2  | 1:A:1127:THR:HG21  | 1.84                     | 0.60              |
| 2:B:504:VAL:HG21  | 2:B:578:ILE:HD13   | 1.82                     | 0.60              |
| 3:C:267:ASN:O     | 3:C:555:ARG:NH2    | 2.34                     | 0.60              |
| 7:M:23:THR:HG23   | 7:M:24:VAL:HG23    | 1.83                     | 0.60              |
| 10:U:507:LEU:O    | 10:U:514:ARG:NH1   | 2.35                     | 0.60              |
| 6:H:555:LEU:HD23  | 6:H:558:LEU:HD21   | 1.84                     | 0.60              |
| 10:U:508:LYS:HG2  | 10:U:547:PHE:HE1   | 1.67                     | 0.60              |
| 1:A:795:ARG:NH1   | 1:A:858:SER:O      | 2.34                     | 0.60              |
| 1:A:1106:GLU:OE1  | 1:A:1106:GLU:N     | 2.28                     | 0.60              |
| 11:V:451:ILE:HG22 | 11:V:491:THR:HG21  | 1.84                     | 0.60              |
| 11:V:1360:LEU:O   | 11:V:1364:LEU:HD13 | 2.01                     | 0.60              |
| 8:P:47:TYR:CE1    | 8:P:54:LEU:HB3     | 2.37                     | 0.60              |
| 8:P:776:LEU:HD13  | 8:P:879:ILE:HD12   | 1.83                     | 0.60              |
| 2:O:504:VAL:HG12  | 2:O:601:ILE:HG12   | 1.82                     | 0.59              |
| 11:V:1123:GLN:O   | 11:V:1165:ARG:NH2  | 2.35                     | 0.59              |
| 11:V:1167:TRP:O   | 11:V:1174:LYS:NZ   | 2.27                     | 0.59              |
| 8:Q:726:VAL:HG22  | 8:Q:727:PRO:HD2    | 1.85                     | 0.59              |
| 10:U:9:ALA:HA     | 10:U:17:LEU:HD11   | 1.84                     | 0.59              |
| 3:C:191:ILE:HG23  | 3:C:232:ILE:HD12   | 1.84                     | 0.59              |
| 7:L:16:LEU:HD11   | 8:P:483:LEU:CD2    | 2.32                     | 0.59              |
| 1:S:171:TRP:NE1   | 1:S:196:LEU:O      | 2.32                     | 0.59              |
| 1:S:761:VAL:O     | 1:S:765:LEU:HG     | 2.02                     | 0.59              |
| 1:A:992:HIS:O     | 1:A:1073:ARG:NH2   | 2.36                     | 0.59              |
| 6:H:213:TYR:HD2   | 6:H:329:LEU:HD22   | 1.68                     | 0.59              |
| 8:P:234:THR:O     | 8:P:237:GLN:NE2    | 2.30                     | 0.59              |
| 8:Q:719:LEU:HD11  | 8:Q:732:THR:HA     | 1.84                     | 0.59              |
| 10:U:1068:LYS:HB3 | 10:U:1071:HIS:HD2  | 1.67                     | 0.59              |
| 1:A:1171:LEU:HD22 | 1:A:1229:ALA:HB2   | 1.85                     | 0.59              |
| 7:M:47:GLN:HE22   | 7:M:50:ASN:HB2     | 1.67                     | 0.59              |
| 11:V:60:LYS:HZ3   | 11:V:63:GLU:HB3    | 1.66                     | 0.59              |
| 2:B:266:ILE:HD12  | 2:B:268:PHE:CE2    | 2.38                     | 0.59              |
| 4:E:102:LEU:HD22  | 4:E:109:LEU:HD11   | 1.83                     | 0.59              |
| 7:L:4:THR:HG23    | 7:L:8:LEU:HB2      | 1.85                     | 0.59              |
| 7:M:16:LEU:HD11   | 2:O:422:SER:OG     | 2.03                     | 0.59              |
| 2:O:102:ASN:HB3   | 2:O:104:VAL:HG22   | 1.85                     | 0.59              |
| 8:Q:536:SER:HB3   | 8:Q:574:PRO:HD3    | 1.85                     | 0.59              |
| 1:S:730:LEU:HD12  | 1:S:733:ALA:HB3    | 1.84                     | 0.59              |
| 10:U:5:ILE:HG12   | 10:U:20:PHE:HE2    | 1.67                     | 0.59              |
| 10:U:438:GLN:HB2  | 10:U:477:CYS:SG    | 2.42                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:826:THR:HG23   | 1:S:829:SER:H      | 1.68                     | 0.59              |
| 1:A:1364:LEU:HD11  | 1:A:1395:LEU:HD13  | 1.83                     | 0.59              |
| 5:F:160:ASP:OD1    | 5:F:161:SER:N      | 2.34                     | 0.59              |
| 8:Q:48:ASP:O       | 8:Q:50:GLU:N       | 2.35                     | 0.59              |
| 10:U:396:LYS:HG3   | 10:U:397:LYS:HD3   | 1.85                     | 0.59              |
| 10:U:658:ILE:HD11  | 10:U:738:LYS:HE3   | 1.85                     | 0.59              |
| 11:V:637:ASN:O     | 11:V:641:HIS:CE1   | 2.55                     | 0.59              |
| 11:V:1295:LEU:HD22 | 11:V:1353:LEU:HD22 | 1.85                     | 0.59              |
| 8:Q:373:ARG:HH11   | 8:Q:385:GLU:HA     | 1.67                     | 0.59              |
| 11:V:94:GLU:OE1    | 11:V:94:GLU:N      | 2.27                     | 0.59              |
| 11:V:738:ARG:HD2   | 11:V:799:ALA:HA    | 1.85                     | 0.59              |
| 1:A:827:ARG:HD3    | 1:A:945:ALA:HA     | 1.85                     | 0.59              |
| 1:A:1155:ILE:HD13  | 1:A:1158:LYS:HZ1   | 1.67                     | 0.59              |
| 8:P:581:THR:O      | 8:Q:518:GLN:HA     | 2.03                     | 0.59              |
| 8:Q:652:CYS:HB3    | 8:Q:759:PRO:HB3    | 1.82                     | 0.59              |
| 1:S:1308:LEU:HB3   | 1:S:1320:LEU:HD21  | 1.84                     | 0.59              |
| 1:A:717:MET:O      | 1:A:721:LEU:HG     | 2.03                     | 0.58              |
| 1:A:955:HIS:HB3    | 1:A:1020:ARG:HD2   | 1.85                     | 0.58              |
| 3:C:227:ILE:CD1    | 3:C:239:VAL:HG12   | 2.33                     | 0.58              |
| 10:U:413:MET:SD    | 10:U:417:HIS:HD2   | 2.26                     | 0.58              |
| 10:U:593:ARG:HD3   | 11:V:182:TRP:HZ3   | 1.68                     | 0.58              |
| 1:A:827:ARG:HH21   | 1:A:944:ASP:H      | 1.50                     | 0.58              |
| 2:B:711:THR:O      | 2:B:713:PHE:N      | 2.37                     | 0.58              |
| 5:F:18:SER:O       | 5:F:100:ASN:ND2    | 2.36                     | 0.58              |
| 8:P:607:ARG:NH2    | 8:P:636:GLU:O      | 2.35                     | 0.58              |
| 1:S:117:VAL:HG13   | 1:S:148:LEU:HD21   | 1.84                     | 0.58              |
| 1:S:366:LEU:HD13   | 1:S:371:LEU:HD21   | 1.83                     | 0.58              |
| 1:A:845:LEU:HD11   | 1:A:913:HIS:CD2    | 2.39                     | 0.58              |
| 2:B:521:LEU:O      | 2:B:521:LEU:HD23   | 2.02                     | 0.58              |
| 7:L:228:ILE:O      | 7:L:235:SER:OG     | 2.15                     | 0.58              |
| 8:Q:36:PHE:CD2     | 8:Q:76:LEU:HD11    | 2.37                     | 0.58              |
| 1:A:117:VAL:HG23   | 1:A:148:LEU:HD21   | 1.84                     | 0.58              |
| 1:A:1422:LEU:HD23  | 1:A:1437:GLN:HE21  | 1.67                     | 0.58              |
| 2:O:301:VAL:HB     | 2:O:309:CYS:SG     | 2.44                     | 0.58              |
| 8:P:77:TYR:CD2     | 8:P:135:LEU:HD11   | 2.38                     | 0.58              |
| 8:P:133:PHE:C      | 8:P:133:PHE:CD2    | 2.73                     | 0.58              |
| 10:U:237:PHE:CZ    | 10:U:271:ILE:HG13  | 2.38                     | 0.58              |
| 10:U:263:GLU:N     | 10:U:263:GLU:OE1   | 2.36                     | 0.58              |
| 10:U:1068:LYS:HB3  | 10:U:1071:HIS:CD2  | 2.37                     | 0.58              |
| 11:V:349:VAL:O     | 11:V:352:SER:OG    | 2.19                     | 0.58              |
| 11:V:793:PHE:HA    | 11:V:796:ILE:HD12  | 1.85                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:G:100:LEU:HD22  | 6:G:125:VAL:HG21   | 1.86                     | 0.58              |
| 2:O:46:ARG:NH2    | 2:O:48:MET:SD      | 2.75                     | 0.58              |
| 8:P:84:GLY:O      | 8:P:130:LEU:HD21   | 2.04                     | 0.58              |
| 11:V:1325:LEU:O   | 11:V:1329:GLU:HG2  | 2.03                     | 0.58              |
| 10:U:295:VAL:HG23 | 10:U:301:SER:HA    | 1.85                     | 0.58              |
| 10:U:379:THR:HA   | 10:U:382:LEU:HD12  | 1.85                     | 0.58              |
| 2:B:781:GLU:HG2   | 2:B:830:VAL:HG22   | 1.85                     | 0.58              |
| 4:E:429:LEU:HB3   | 4:E:460:ARG:HH12   | 1.67                     | 0.58              |
| 8:P:479:ARG:HH21  | 8:P:479:ARG:HG3    | 1.69                     | 0.58              |
| 8:P:715:LEU:O     | 8:P:719:LEU:N      | 2.36                     | 0.58              |
| 3:C:448:ALA:O     | 3:C:452:HIS:ND1    | 2.35                     | 0.58              |
| 8:Q:362:THR:HG23  | 8:Q:365:ASP:H      | 1.69                     | 0.58              |
| 1:S:650:LEU:HA    | 1:S:653:LEU:HD12   | 1.85                     | 0.58              |
| 11:V:1236:ARG:HG3 | 11:V:1293:VAL:HG21 | 1.86                     | 0.58              |
| 1:A:1243:ARG:HA   | 1:A:1243:ARG:NE    | 2.19                     | 0.58              |
| 4:E:280:LEU:O     | 4:E:285:GLN:NE2    | 2.32                     | 0.58              |
| 6:G:79:ILE:HD11   | 6:G:198:GLN:HE21   | 1.67                     | 0.58              |
| 8:Q:720:LYS:HD3   | 8:Q:725:GLY:HA3    | 1.85                     | 0.58              |
| 1:S:731:MET:O     | 1:S:735:SER:OG     | 2.21                     | 0.58              |
| 10:U:835:SER:HB3  | 10:U:838:PHE:HB3   | 1.85                     | 0.58              |
| 1:A:287:GLU:OE1   | 1:A:287:GLU:N      | 2.37                     | 0.58              |
| 2:B:749:SER:O     | 2:B:755:LEU:HD11   | 2.04                     | 0.58              |
| 4:E:291:LEU:O     | 4:E:295:LEU:HD13   | 2.04                     | 0.58              |
| 2:O:139:GLY:O     | 2:O:141:LEU:N      | 2.36                     | 0.58              |
| 8:P:525:ALA:HB2   | 8:P:584:LEU:HD11   | 1.86                     | 0.58              |
| 1:S:723:LEU:HD11  | 9:W:90:PHE:HE1     | 1.69                     | 0.58              |
| 11:V:153:LEU:HG   | 11:V:176:ILE:HD11  | 1.86                     | 0.58              |
| 11:V:568:PHE:HD2  | 11:V:851:THR:HG21  | 1.69                     | 0.58              |
| 1:A:417:GLN:OE1   | 1:A:423:GLN:NE2    | 2.37                     | 0.57              |
| 2:B:690:GLU:OE2   | 2:B:690:GLU:N      | 2.35                     | 0.57              |
| 5:F:69:GLU:HA     | 5:F:74:ARG:NH2     | 2.18                     | 0.57              |
| 5:F:151:TYR:CZ    | 5:F:162:LEU:HD23   | 2.39                     | 0.57              |
| 6:G:140:HIS:HB2   | 6:G:187:PRO:HG3    | 1.86                     | 0.57              |
| 6:H:538:LEU:HD12  | 6:H:539:LEU:N      | 2.19                     | 0.57              |
| 7:L:23:THR:HG23   | 7:L:24:VAL:HG23    | 1.85                     | 0.57              |
| 1:S:313:THR:HG23  | 1:S:316:LEU:HD23   | 1.86                     | 0.57              |
| 1:S:899:PRO:O     | 1:S:905:ARG:NH2    | 2.37                     | 0.57              |
| 1:S:929:TYR:HB2   | 1:S:972:GLY:HA2    | 1.86                     | 0.57              |
| 11:V:306:ASP:O    | 11:V:308:GLN:NE2   | 2.37                     | 0.57              |
| 11:V:630:LEU:HD13 | 11:V:843:PHE:HB3   | 1.84                     | 0.57              |
| 11:V:637:ASN:HB3  | 11:V:641:HIS:CE1   | 2.33                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:955:HIS:NE2    | 1:A:1016:ASP:OD2   | 2.34                     | 0.57              |
| 1:A:1087:SER:OG    | 1:A:1133:HIS:O     | 2.15                     | 0.57              |
| 6:G:267:LEU:HB3    | 1:S:93:PHE:HE2     | 1.68                     | 0.57              |
| 2:O:611:LYS:HD3    | 2:O:613:ARG:HE     | 1.69                     | 0.57              |
| 10:U:440:ILE:O     | 10:U:444:VAL:HG23  | 2.02                     | 0.57              |
| 11:V:413:GLN:OE1   | 11:V:413:GLN:N     | 2.37                     | 0.57              |
| 1:A:35:TYR:CD1     | 1:A:39:ARG:HG2     | 2.40                     | 0.57              |
| 3:C:186:VAL:O      | 3:C:186:VAL:HG12   | 2.03                     | 0.57              |
| 4:E:293:GLN:O      | 4:E:297:THR:HG23   | 2.03                     | 0.57              |
| 10:U:434:GLU:OE1   | 10:U:434:GLU:N     | 2.36                     | 0.57              |
| 1:A:124:ILE:HD11   | 1:A:141:GLN:O      | 2.04                     | 0.57              |
| 1:A:1121:SER:O     | 1:A:1122:HIS:ND1   | 2.38                     | 0.57              |
| 1:S:652:GLN:O      | 1:S:683:ARG:NH2    | 2.38                     | 0.57              |
| 1:A:1053:ARG:HG3   | 1:A:1057:GLN:HE21  | 1.70                     | 0.57              |
| 3:C:247:LEU:HB2    | 4:E:132:TRP:CE2    | 2.39                     | 0.57              |
| 10:U:480:LYS:HA    | 10:U:483:GLU:OE2   | 2.05                     | 0.57              |
| 10:U:1180:TYR:HA   | 10:U:1183:VAL:HG12 | 1.86                     | 0.57              |
| 2:B:150:PHE:CE1    | 2:B:170:ILE:HB     | 2.39                     | 0.57              |
| 2:B:829:LYS:HB3    | 8:P:824:ASP:HB3    | 1.85                     | 0.57              |
| 2:O:486:SER:HA     | 2:O:582:THR:O      | 2.05                     | 0.57              |
| 1:S:750:VAL:HG21   | 1:S:790:HIS:HB3    | 1.87                     | 0.57              |
| 1:S:1332:PRO:HG2   | 1:S:1367:LEU:HD11  | 1.86                     | 0.57              |
| 2:O:170:ILE:HD11   | 2:O:183:LEU:HB3    | 1.87                     | 0.57              |
| 8:Q:311:CYS:SG     | 8:Q:312:LEU:N      | 2.78                     | 0.57              |
| 10:U:4:LYS:HE2     | 10:U:20:PHE:CZ     | 2.40                     | 0.57              |
| 11:V:1078:PHE:O    | 11:V:1084:GLN:NE2  | 2.37                     | 0.57              |
| 1:A:1392:PRO:HA    | 1:A:1395:LEU:HG    | 1.87                     | 0.57              |
| 2:B:582:THR:CG2    | 2:B:583:SER:N      | 2.68                     | 0.57              |
| 10:U:852:GLN:HG2   | 10:U:859:VAL:HA    | 1.87                     | 0.57              |
| 2:B:170:ILE:HD11   | 2:B:183:LEU:HD13   | 1.87                     | 0.57              |
| 6:H:530:ASP:O      | 6:H:534:LEU:HG     | 2.04                     | 0.57              |
| 8:Q:39:THR:HG1     | 8:Q:41:SER:HG      | 1.48                     | 0.57              |
| 8:Q:279:GLU:OE1    | 8:Q:279:GLU:N      | 2.37                     | 0.57              |
| 8:Q:508:CYS:SG     | 8:Q:527:CYS:SG     | 3.03                     | 0.57              |
| 8:Q:570:ASP:OD1    | 8:Q:578:ARG:NH2    | 2.35                     | 0.57              |
| 1:S:918:GLU:HA     | 1:S:921:LYS:HD2    | 1.87                     | 0.57              |
| 1:S:1312:ASP:HB2   | 1:S:1316:GLY:HA3   | 1.85                     | 0.57              |
| 10:U:593:ARG:HD3   | 11:V:182:TRP:CZ3   | 2.40                     | 0.57              |
| 11:V:1265:LEU:HD22 | 11:V:1323:ASP:HB3  | 1.86                     | 0.57              |
| 1:A:310:VAL:HG13   | 1:A:311:ILE:HG13   | 1.86                     | 0.57              |
| 6:G:474:SER:O      | 6:G:477:SER:OG     | 2.18                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:O:750:GLY:HA2   | 8:Q:556:LEU:HD12   | 1.86                     | 0.57              |
| 6:H:70:GLU:O      | 6:H:74:THR:HG22    | 2.04                     | 0.56              |
| 7:M:84:MET:HB3    | 7:M:88:LYS:NZ      | 2.19                     | 0.56              |
| 2:O:181:MET:HB3   | 2:O:217:LEU:HD23   | 1.85                     | 0.56              |
| 8:Q:549:THR:HA    | 8:Q:596:VAL:HG12   | 1.86                     | 0.56              |
| 10:U:202:PHE:CE1  | 10:U:210:ILE:HG23  | 2.40                     | 0.56              |
| 10:U:1248:LYS:HG3 | 10:U:1252:ASN:HD21 | 1.70                     | 0.56              |
| 1:A:335:LYS:HE2   | 1:A:383:GLU:HB2    | 1.87                     | 0.56              |
| 7:M:104:LEU:HD12  | 7:M:105:PRO:HD2    | 1.86                     | 0.56              |
| 8:P:850:ARG:HH11  | 8:P:856:GLU:HB2    | 1.70                     | 0.56              |
| 8:Q:464:ASN:O     | 8:Q:467:GLU:HG3    | 2.05                     | 0.56              |
| 1:S:141:GLN:O     | 1:S:145:LEU:HG     | 2.06                     | 0.56              |
| 1:A:198:GLU:OE2   | 1:A:262:MET:N      | 2.39                     | 0.56              |
| 1:A:981:CYS:HA    | 1:A:984:LEU:HD12   | 1.86                     | 0.56              |
| 2:B:777:ILE:HD12  | 2:B:830:VAL:HG11   | 1.86                     | 0.56              |
| 4:E:388:THR:O     | 4:E:426:MET:HE3    | 2.05                     | 0.56              |
| 6:H:606:ASP:HA    | 6:H:609:LEU:HG     | 1.87                     | 0.56              |
| 8:Q:21:LEU:HB2    | 8:Q:399:LEU:HD21   | 1.88                     | 0.56              |
| 8:Q:28:VAL:CG2    | 8:Q:37:LEU:HD13    | 2.36                     | 0.56              |
| 8:Q:143:LEU:HD12  | 8:Q:197:LEU:HD21   | 1.87                     | 0.56              |
| 1:S:346:TRP:CZ2   | 1:S:387:GLN:HG2    | 2.39                     | 0.56              |
| 1:S:1257:LEU:HD12 | 1:S:1260:LEU:HD11  | 1.87                     | 0.56              |
| 1:S:1302:TRP:CH2  | 1:S:1348:ILE:HD13  | 2.40                     | 0.56              |
| 10:U:735:ILE:O    | 10:U:739:ASN:ND2   | 2.33                     | 0.56              |
| 8:P:424:SER:O     | 8:P:424:SER:OG     | 2.23                     | 0.56              |
| 8:Q:529:LEU:HD22  | 8:Q:572:LEU:HD11   | 1.87                     | 0.56              |
| 1:S:603:PHE:O     | 1:S:607:LEU:HG     | 2.05                     | 0.56              |
| 1:S:1045:GLU:HA   | 1:S:1104:ARG:HG2   | 1.86                     | 0.56              |
| 10:U:494:GLN:OE1  | 10:U:498:ARG:NH2   | 2.32                     | 0.56              |
| 1:A:1155:ILE:HA   | 1:A:1158:LYS:HZ3   | 1.69                     | 0.56              |
| 1:A:1268:LEU:HA   | 1:A:1284:ALA:HB1   | 1.87                     | 0.56              |
| 2:B:279:LEU:HD23  | 2:B:303:PHE:CZ     | 2.40                     | 0.56              |
| 3:C:157:LEU:CD1   | 5:F:146:LEU:HD12   | 2.35                     | 0.56              |
| 6:G:19:LYS:HE2    | 6:G:23:LEU:HD11    | 1.87                     | 0.56              |
| 6:G:257:ARG:NE    | 6:G:285:GLU:OE2    | 2.31                     | 0.56              |
| 8:Q:758:ALA:HB3   | 8:Q:761:GLY:H      | 1.71                     | 0.56              |
| 1:S:288:GLU:HG3   | 1:S:292:HIS:CG     | 2.41                     | 0.56              |
| 10:U:635:TYR:OH   | 10:U:712:ARG:NH1   | 2.39                     | 0.56              |
| 1:A:285:VAL:HG23  | 1:A:287:GLU:OE1    | 2.06                     | 0.56              |
| 2:B:231:PRO:O     | 2:B:234:SER:OG     | 2.24                     | 0.56              |
| 2:B:814:LYS:O     | 2:B:818:ARG:HD2    | 2.05                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:126:ARG:O     | 5:F:147:ARG:NH2   | 2.39                     | 0.56              |
| 7:M:271:ILE:HG12  | 10:U:472:LEU:HD21 | 1.87                     | 0.56              |
| 2:O:601:ILE:HG22  | 2:O:611:LYS:NZ    | 2.20                     | 0.56              |
| 8:Q:479:ARG:HE    | 8:Q:610:VAL:HG11  | 1.71                     | 0.56              |
| 10:U:82:GLN:H     | 10:U:85:ILE:HD11  | 1.70                     | 0.56              |
| 11:V:265:LEU:O    | 11:V:269:LYS:NZ   | 2.31                     | 0.56              |
| 11:V:832:VAL:HG12 | 11:V:833:THR:HG23 | 1.86                     | 0.56              |
| 3:C:501:GLY:O     | 3:C:502:HIS:ND1   | 2.39                     | 0.56              |
| 6:H:46:ALA:O      | 6:H:50:LEU:HG     | 2.05                     | 0.56              |
| 7:L:342:LEU:HD22  | 7:L:357:GLY:HA3   | 1.87                     | 0.56              |
| 2:O:509:LEU:HB2   | 2:O:596:THR:OG1   | 2.05                     | 0.56              |
| 8:P:875:HIS:HB3   | 8:P:876:PRO:HD3   | 1.88                     | 0.56              |
| 11:V:745:HIS:HB3  | 11:V:748:ASN:HB2  | 1.88                     | 0.56              |
| 11:V:1092:HIS:HE1 | 11:V:1103:HIS:HA  | 1.71                     | 0.56              |
| 5:F:156:ASN:HB3   | 5:F:158:GLN:NE2   | 2.20                     | 0.56              |
| 2:O:338:THR:O     | 2:O:340:GLN:NE2   | 2.38                     | 0.56              |
| 8:Q:253:VAL:HB    | 8:Q:272:VAL:HG23  | 1.87                     | 0.56              |
| 8:Q:673:ARG:O     | 8:Q:674:ASP:HB2   | 2.05                     | 0.56              |
| 1:S:1239:GLU:HA   | 1:S:1242:ILE:HD12 | 1.87                     | 0.56              |
| 10:U:506:LEU:HB3  | 10:U:513:MET:CE   | 2.36                     | 0.56              |
| 6:G:198:GLN:HE22  | 6:G:203:LEU:HD11  | 1.69                     | 0.56              |
| 2:O:228:ILE:HG22  | 2:O:229:ILE:H     | 1.71                     | 0.56              |
| 2:O:323:GLU:OE1   | 2:O:323:GLU:N     | 2.39                     | 0.56              |
| 10:U:543:LEU:HB3  | 10:U:550:LEU:HD21 | 1.88                     | 0.56              |
| 10:U:642:LEU:HG   | 10:U:716:SER:HA   | 1.87                     | 0.56              |
| 1:A:60:LEU:HG     | 6:H:263:GLN:HB3   | 1.88                     | 0.56              |
| 1:A:877:SER:O     | 1:A:881:GLN:HG2   | 2.06                     | 0.56              |
| 1:A:1292:LEU:HD11 | 1:A:1342:PHE:HB2  | 1.88                     | 0.56              |
| 6:G:219:GLU:HG2   | 6:G:224:ASN:HB2   | 1.87                     | 0.56              |
| 8:P:84:GLY:HA3    | 8:P:126:PRO:HA    | 1.88                     | 0.56              |
| 8:P:510:THR:HA    | 8:P:526:THR:O     | 2.06                     | 0.56              |
| 1:S:656:ALA:HB1   | 1:S:680:ILE:HG12  | 1.88                     | 0.56              |
| 1:A:792:GLY:HA2   | 1:A:814:VAL:HG21  | 1.89                     | 0.55              |
| 6:H:90:GLU:CD     | 6:H:90:GLU:H      | 2.08                     | 0.55              |
| 8:P:173:VAL:HG12  | 8:P:174:GLU:H     | 1.71                     | 0.55              |
| 10:U:826:GLN:HE22 | 10:U:833:ARG:HH12 | 1.54                     | 0.55              |
| 11:V:542:SER:HB2  | 11:V:545:ASN:ND2  | 2.21                     | 0.55              |
| 1:A:361:ARG:O     | 1:A:365:MET:HG2   | 2.05                     | 0.55              |
| 2:B:523:CYS:SG    | 2:B:582:THR:OG1   | 2.40                     | 0.55              |
| 8:P:50:GLU:OE1    | 8:P:50:GLU:N      | 2.39                     | 0.55              |
| 8:P:734:GLN:HE22  | 8:P:747:ARG:HB2   | 1.71                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:688:LEU:HD21  | 1:A:757:VAL:HG22   | 1.88                     | 0.55              |
| 2:B:284:PRO:HA    | 2:B:303:PHE:HD1    | 1.70                     | 0.55              |
| 7:M:206:GLU:HG2   | 7:M:281:LEU:HD12   | 1.88                     | 0.55              |
| 11:V:1251:PRO:HA  | 11:V:1312:LEU:HD21 | 1.88                     | 0.55              |
| 1:A:244:LEU:HD23  | 1:A:248:GLN:HE22   | 1.70                     | 0.55              |
| 1:A:403:ALA:HB1   | 1:A:406:LEU:HD11   | 1.89                     | 0.55              |
| 1:S:393:VAL:HG12  | 1:S:396:LEU:HD12   | 1.89                     | 0.55              |
| 1:S:481:VAL:HB    | 1:S:517:ARG:HD3    | 1.88                     | 0.55              |
| 1:A:491:VAL:HA    | 1:A:494:LEU:HD12   | 1.87                     | 0.55              |
| 3:C:281:LEU:N     | 3:C:282:PRO:HD2    | 2.22                     | 0.55              |
| 6:G:479:CYS:O     | 6:G:483:LEU:HD13   | 2.07                     | 0.55              |
| 2:O:691:VAL:HG12  | 2:O:706:THR:HG22   | 1.88                     | 0.55              |
| 8:P:390:LEU:N     | 8:P:390:LEU:HD23   | 2.22                     | 0.55              |
| 8:P:728:LEU:HB2   | 8:P:770:GLU:OE2    | 2.06                     | 0.55              |
| 8:P:735:TRP:O     | 8:P:807:ARG:NH2    | 2.39                     | 0.55              |
| 8:Q:715:LEU:O     | 8:Q:719:LEU:HB2    | 2.06                     | 0.55              |
| 1:S:1186:ARG:O    | 1:S:1190:GLN:NE2   | 2.34                     | 0.55              |
| 1:S:1363:LYS:O    | 1:S:1367:LEU:HG    | 2.07                     | 0.55              |
| 11:V:565:SER:O    | 11:V:571:LYS:NZ    | 2.34                     | 0.55              |
| 11:V:1261:HIS:HA  | 11:V:1264:LYS:HE2  | 1.88                     | 0.55              |
| 2:O:526:ARG:HD3   | 8:Q:559:ALA:HA     | 1.89                     | 0.55              |
| 10:U:595:LEU:O    | 10:U:602:ARG:NE    | 2.39                     | 0.55              |
| 10:U:1052:ASP:HB3 | 10:U:1075:VAL:HG11 | 1.88                     | 0.55              |
| 1:A:666:ASP:HB3   | 1:A:669:GLN:HE21   | 1.70                     | 0.55              |
| 1:A:795:ARG:HH12  | 1:A:858:SER:C      | 2.09                     | 0.55              |
| 1:A:946:LEU:HD13  | 1:A:950:GLU:HB3    | 1.88                     | 0.55              |
| 6:G:151:LEU:HD11  | 6:G:211:PHE:HB2    | 1.88                     | 0.55              |
| 7:L:44:GLU:OE1    | 7:L:44:GLU:N       | 2.39                     | 0.55              |
| 8:Q:35:VAL:HG22   | 8:Q:47:TYR:O       | 2.06                     | 0.55              |
| 10:U:823:GLN:HA   | 10:U:826:GLN:HB2   | 1.89                     | 0.55              |
| 11:V:526:PRO:HB2  | 11:V:848:LEU:HD22  | 1.87                     | 0.55              |
| 11:V:1307:LYS:HG3 | 11:V:1308:GLN:HG2  | 1.88                     | 0.55              |
| 2:B:132:ASP:O     | 2:B:134:LEU:N      | 2.40                     | 0.55              |
| 6:H:555:LEU:HD21  | 6:H:570:LEU:HB2    | 1.89                     | 0.55              |
| 8:P:781:PRO:HG2   | 8:P:783:GLN:H      | 1.72                     | 0.55              |
| 8:Q:733:LEU:HD11  | 8:Q:754:ILE:HG12   | 1.89                     | 0.55              |
| 10:U:84:GLU:O     | 10:U:87:SER:OG     | 2.23                     | 0.55              |
| 10:U:98:HIS:O     | 10:U:140:LYS:NZ    | 2.37                     | 0.55              |
| 10:U:298:GLN:HG2  | 10:U:299:GLY:N     | 2.22                     | 0.55              |
| 2:B:139:GLY:O     | 2:B:141:LEU:HB2    | 2.06                     | 0.55              |
| 2:B:690:GLU:HG2   | 2:B:691:VAL:HG23   | 1.89                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:G:195:LEU:HD12   | 6:G:196:THR:H     | 1.71                     | 0.55              |
| 8:Q:74:ARG:HG3     | 8:Q:90:LEU:HB2    | 1.89                     | 0.55              |
| 1:S:184:HIS:HA     | 1:S:187:VAL:HG22  | 1.88                     | 0.55              |
| 1:S:284:GLY:O      | 1:S:286:GLN:NE2   | 2.39                     | 0.55              |
| 1:S:514:ALA:HA     | 1:S:517:ARG:HD2   | 1.89                     | 0.55              |
| 1:S:931:ASP:O      | 1:S:935:LEU:HG    | 2.06                     | 0.55              |
| 1:S:1080:ARG:NH2   | 1:S:1080:ARG:HA   | 2.21                     | 0.55              |
| 1:S:1360:MET:HA    | 1:S:1363:LYS:HE2  | 1.89                     | 0.55              |
| 11:V:1092:HIS:CE1  | 11:V:1103:HIS:HA  | 2.42                     | 0.55              |
| 1:A:126:THR:HG23   | 1:A:176:SER:OG    | 2.07                     | 0.55              |
| 3:C:213:GLU:OE1    | 3:C:220:PHE:CZ    | 2.60                     | 0.55              |
| 6:G:256:HIS:HA     | 6:G:259:MET:HG2   | 1.89                     | 0.55              |
| 6:G:374:LEU:HD13   | 6:G:393:MET:CE    | 2.37                     | 0.55              |
| 6:H:548:ARG:HH21   | 6:H:609:LEU:HD21  | 1.71                     | 0.55              |
| 7:M:107:PRO:HG2    | 7:M:108:PRO:CD    | 2.31                     | 0.55              |
| 8:P:28:VAL:HG23    | 8:P:400:ASN:HD21  | 1.72                     | 0.55              |
| 1:S:335:LYS:HE2    | 1:S:383:GLU:HB3   | 1.88                     | 0.55              |
| 1:S:673:ILE:O      | 1:S:677:VAL:HG23  | 2.07                     | 0.55              |
| 1:S:1052:PHE:O     | 1:S:1056:LEU:HG   | 2.06                     | 0.55              |
| 1:S:1151:MET:O     | 1:S:1155:ILE:HG12 | 2.07                     | 0.55              |
| 10:U:537:VAL:HG21  | 10:U:601:VAL:HG13 | 1.89                     | 0.55              |
| 6:G:406:GLN:HG2    | 6:G:599:TRP:CE3   | 2.42                     | 0.54              |
| 7:L:216:PRO:HG2    | 7:L:226:ARG:HD3   | 1.87                     | 0.54              |
| 2:O:140:PRO:HG2    | 2:O:155:SER:HB3   | 1.90                     | 0.54              |
| 2:O:520:LEU:HG     | 2:O:521:LEU:H     | 1.73                     | 0.54              |
| 2:O:854:GLN:O      | 2:O:858:ASN:ND2   | 2.40                     | 0.54              |
| 8:P:767:ILE:CG1    | 8:P:788:GLN:HB3   | 2.36                     | 0.54              |
| 1:S:752:THR:OG1    | 1:S:753:MET:SD    | 2.65                     | 0.54              |
| 1:S:1094:SER:HA    | 1:S:1145:SER:HB3  | 1.89                     | 0.54              |
| 10:U:234:ILE:HD13  | 10:U:293:LEU:HD21 | 1.89                     | 0.54              |
| 6:G:79:ILE:HG13    | 6:G:145:LEU:HD21  | 1.89                     | 0.54              |
| 2:O:73:HIS:HB3     | 2:O:99:ASN:HB3    | 1.89                     | 0.54              |
| 11:V:101:GLU:HA    | 11:V:104:ILE:HG12 | 1.88                     | 0.54              |
| 11:V:186:VAL:O     | 11:V:186:VAL:HG23 | 2.07                     | 0.54              |
| 11:V:514:VAL:O     | 11:V:517:ILE:HG22 | 2.07                     | 0.54              |
| 11:V:1025:ASN:HD22 | 11:V:1097:ARG:HD3 | 1.72                     | 0.54              |
| 1:A:1261:PHE:O     | 1:A:1265:LEU:HG   | 2.06                     | 0.54              |
| 5:F:129:LEU:O      | 5:F:132:SER:OG    | 2.24                     | 0.54              |
| 7:M:212:TRP:NE1    | 7:M:298:LEU:HB2   | 2.22                     | 0.54              |
| 1:S:155:LEU:HA     | 1:S:160:MET:HE2   | 1.89                     | 0.54              |
| 1:S:504:ARG:HE     | 1:S:507:LEU:HD12  | 1.71                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:1018:ILE:HG12  | 1:S:1084:ARG:HD2   | 1.89                     | 0.54              |
| 10:U:1029:MET:HG3  | 10:U:1087:LEU:HD22 | 1.88                     | 0.54              |
| 10:U:1167:CYS:O    | 10:U:1171:THR:HG23 | 2.07                     | 0.54              |
| 11:V:173:PRO:HA    | 11:V:176:ILE:HG22  | 1.89                     | 0.54              |
| 11:V:1115:VAL:HG21 | 11:V:1142:LEU:HG   | 1.90                     | 0.54              |
| 11:V:1306:LEU:HD21 | 11:V:1367:LEU:HB3  | 1.89                     | 0.54              |
| 2:B:619:ARG:HH12   | 8:P:635:GLN:HB3    | 1.72                     | 0.54              |
| 3:C:127:PHE:HE1    | 5:F:147:ARG:HD3    | 1.72                     | 0.54              |
| 7:L:351:SER:OG     | 7:L:354:ILE:HB     | 2.07                     | 0.54              |
| 2:O:186:LEU:HB3    | 2:O:212:PHE:CD1    | 2.43                     | 0.54              |
| 2:O:765:LYS:HZ1    | 2:O:848:LYS:HB2    | 1.72                     | 0.54              |
| 8:P:41:SER:OG      | 8:P:42:GLU:N       | 2.41                     | 0.54              |
| 8:Q:807:ARG:O      | 8:Q:810:THR:OG1    | 2.24                     | 0.54              |
| 10:U:85:ILE:O      | 10:U:89:ILE:HG12   | 2.08                     | 0.54              |
| 11:V:278:LEU:HA    | 11:V:281:ILE:HD12  | 1.90                     | 0.54              |
| 1:A:179:LEU:HD23   | 1:A:217:LEU:HD11   | 1.90                     | 0.54              |
| 2:B:122:LEU:HD21   | 2:B:155:SER:HA     | 1.90                     | 0.54              |
| 2:B:426:LEU:O      | 2:B:429:LEU:HG     | 2.07                     | 0.54              |
| 3:C:137:GLY:O      | 5:F:195:ARG:NH2    | 2.40                     | 0.54              |
| 7:L:320:PRO:HA     | 7:L:333:PHE:O      | 2.07                     | 0.54              |
| 10:U:134:LEU:HB3   | 10:U:157:LYS:HG3   | 1.89                     | 0.54              |
| 11:V:383:VAL:HG21  | 11:V:424:HIS:CD2   | 2.43                     | 0.54              |
| 2:B:423:TYR:CE1    | 8:P:606:LEU:HB3    | 2.41                     | 0.54              |
| 4:E:290:ARG:NH2    | 4:E:312:GLU:OE2    | 2.41                     | 0.54              |
| 8:P:177:SER:OG     | 8:P:249:GLN:NE2    | 2.41                     | 0.54              |
| 8:P:815:GLN:O      | 8:P:818:GLN:NE2    | 2.40                     | 0.54              |
| 1:S:1415:PHE:HB3   | 1:S:1440:GLN:HG2   | 1.89                     | 0.54              |
| 11:V:273:ILE:HG22  | 11:V:274:ARG:O     | 2.07                     | 0.54              |
| 11:V:371:THR:O     | 11:V:377:HIS:HE1   | 1.91                     | 0.54              |
| 11:V:1111:LEU:HD11 | 11:V:1144:LYS:HE2  | 1.88                     | 0.54              |
| 1:A:779:PRO:HA     | 1:A:782:LEU:HG     | 1.90                     | 0.54              |
| 1:A:932:TRP:CZ3    | 1:A:936:GLU:HG2    | 2.42                     | 0.54              |
| 8:Q:585:GLY:O      | 8:Q:587:GLY:N      | 2.41                     | 0.54              |
| 1:S:934:HIS:HA     | 1:S:937:LEU:HD12   | 1.87                     | 0.54              |
| 1:A:653:LEU:HD11   | 1:A:687:VAL:HG11   | 1.89                     | 0.54              |
| 4:E:438:LEU:HD11   | 4:E:462:VAL:HG11   | 1.88                     | 0.54              |
| 6:H:63:ALA:O       | 6:H:66:VAL:HG12    | 2.07                     | 0.54              |
| 2:O:855:LYS:HA     | 2:O:858:ASN:HD21   | 1.73                     | 0.54              |
| 3:C:408:ALA:HB3    | 3:C:493:ASN:HD22   | 1.73                     | 0.54              |
| 2:O:767:LEU:HD13   | 8:Q:841:LEU:HA     | 1.90                     | 0.54              |
| 11:V:59:LEU:HD13   | 11:V:66:ASN:HD21   | 1.73                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:Q:76:LEU:HG      | 8:Q:90:LEU:HD21   | 1.88                     | 0.54              |
| 8:Q:767:ILE:CG1    | 8:Q:788:GLN:HB3   | 2.36                     | 0.54              |
| 1:S:764:ARG:HH21   | 1:S:768:LEU:HD23  | 1.73                     | 0.54              |
| 11:V:243:VAL:HG13  | 11:V:244:PRO:HD3  | 1.89                     | 0.54              |
| 1:A:31:LYS:NZ      | 6:H:377:SER:OG    | 2.34                     | 0.53              |
| 1:A:1112:VAL:HA    | 1:A:1116:MET:HG2  | 1.88                     | 0.53              |
| 1:A:1178:GLU:CG    | 1:A:1179:PRO:HD3  | 2.38                     | 0.53              |
| 6:G:62:ALA:HB2     | 6:G:102:ARG:HD2   | 1.90                     | 0.53              |
| 2:O:585:SER:OG     | 2:O:586:PRO:HD3   | 2.08                     | 0.53              |
| 8:P:366:LEU:HD23   | 8:P:366:LEU:C     | 2.28                     | 0.53              |
| 8:P:526:THR:HG22   | 8:P:581:THR:HG22  | 1.90                     | 0.53              |
| 1:S:171:TRP:CE3    | 1:S:200:HIS:HD2   | 2.26                     | 0.53              |
| 1:S:555:ILE:HG21   | 1:S:1007:VAL:HG11 | 1.89                     | 0.53              |
| 1:S:739:PRO:HD3    | 1:S:898:LEU:HD11  | 1.90                     | 0.53              |
| 1:S:769:LEU:HG     | 1:S:821:LEU:HD11  | 1.90                     | 0.53              |
| 11:V:282:ILE:HA    | 11:V:285:ILE:HD12 | 1.89                     | 0.53              |
| 11:V:752:ILE:HG13  | 11:V:755:LEU:HB2  | 1.90                     | 0.53              |
| 1:A:1165:LEU:HD11  | 1:A:1321:ARG:O    | 2.07                     | 0.53              |
| 5:F:246:GLU:N      | 5:F:246:GLU:OE1   | 2.40                     | 0.53              |
| 8:P:51:GLY:O       | 8:P:53:LEU:N      | 2.38                     | 0.53              |
| 1:S:171:TRP:HZ2    | 1:S:197:LEU:HA    | 1.74                     | 0.53              |
| 10:U:1036:HIS:CE1  | 10:U:1042:PRO:HA  | 2.43                     | 0.53              |
| 10:U:1277:GLN:HE22 | 10:U:1278:HIS:CD2 | 2.26                     | 0.53              |
| 11:V:532:LEU:HD23  | 11:V:536:LEU:HD13 | 1.89                     | 0.53              |
| 1:A:191:VAL:HG12   | 1:A:192:SER:H     | 1.72                     | 0.53              |
| 1:A:232:ARG:HA     | 1:A:235:LEU:HG    | 1.91                     | 0.53              |
| 1:A:288:GLU:OE2    | 1:A:288:GLU:N     | 2.38                     | 0.53              |
| 2:B:143:LEU:HD11   | 2:B:183:LEU:HD21  | 1.89                     | 0.53              |
| 3:C:430:TYR:O      | 4:E:176:ARG:HG3   | 2.09                     | 0.53              |
| 5:F:35:LEU:HD23    | 5:F:90:ASP:OD1    | 2.09                     | 0.53              |
| 6:G:89:THR:HG21    | 8:P:147:PRO:HB3   | 1.91                     | 0.53              |
| 10:U:708:SER:HG    | 10:U:712:ARG:HH11 | 1.54                     | 0.53              |
| 2:B:635:THR:O      | 2:B:639:LYS:HB2   | 2.08                     | 0.53              |
| 3:C:66:THR:HG22    | 3:C:69:GLN:HB2    | 1.89                     | 0.53              |
| 2:O:762:THR:HB     | 2:O:849:SER:HA    | 1.91                     | 0.53              |
| 8:P:529:LEU:HD12   | 8:P:543:LEU:HD22  | 1.90                     | 0.53              |
| 8:Q:806:GLY:O      | 8:Q:810:THR:HG23  | 2.08                     | 0.53              |
| 10:U:785:LEU:HB3   | 10:U:799:LYS:HD3  | 1.89                     | 0.53              |
| 10:U:827:GLU:OE1   | 10:U:827:GLU:N    | 2.42                     | 0.53              |
| 2:B:90:ASN:O       | 2:B:91:LEU:HG     | 2.09                     | 0.53              |
| 4:E:156:LEU:HB3    | 4:E:160:CYS:SG    | 2.48                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S:57:LEU:HD11   | 1:S:101:GLN:HG3    | 1.91                     | 0.53              |
| 11:V:624:SER:HB3  | 11:V:627:ALA:HB3   | 1.91                     | 0.53              |
| 1:A:1422:LEU:HD21 | 1:A:1433:SER:HB3   | 1.89                     | 0.53              |
| 3:C:64:PHE:N      | 3:C:65:PRO:HD2     | 2.24                     | 0.53              |
| 4:E:487:MET:N     | 4:E:487:MET:SD     | 2.82                     | 0.53              |
| 6:G:267:LEU:HB3   | 1:S:93:PHE:CE2     | 2.44                     | 0.53              |
| 6:H:176:ASP:OD1   | 6:H:178:LEU:N      | 2.42                     | 0.53              |
| 7:M:151:THR:HB    | 7:M:166:PHE:HB2    | 1.90                     | 0.53              |
| 8:P:328:TRP:HA    | 8:P:333:LYS:O      | 2.08                     | 0.53              |
| 11:V:255:ASP:OD1  | 11:V:255:ASP:N     | 2.41                     | 0.53              |
| 1:A:399:CYS:SG    | 1:A:400:PHE:N      | 2.81                     | 0.53              |
| 3:C:245:ARG:HA    | 4:E:96:ARG:NH1     | 2.24                     | 0.53              |
| 4:E:360:ALA:O     | 4:E:364:THR:HG23   | 2.09                     | 0.53              |
| 5:F:9:ASP:OD1     | 5:F:10:ARG:N       | 2.41                     | 0.53              |
| 5:F:111:LEU:HG    | 5:F:115:LEU:HD11   | 1.91                     | 0.53              |
| 7:M:214:LEU:HD12  | 7:M:229:ALA:HB2    | 1.90                     | 0.53              |
| 8:Q:227:LEU:HD13  | 8:Q:334:LEU:HB3    | 1.90                     | 0.53              |
| 1:S:1311:SER:HA   | 1:S:1317:ARG:HD2   | 1.90                     | 0.53              |
| 10:U:549:VAL:HG23 | 10:U:580:ASN:ND2   | 2.23                     | 0.53              |
| 10:U:602:ARG:NH1  | 10:U:662:GLU:HB2   | 2.23                     | 0.53              |
| 1:A:460:ARG:NH2   | 1:A:497:PRO:O      | 2.42                     | 0.53              |
| 2:B:54:THR:OG1    | 2:B:56:VAL:HG22    | 2.08                     | 0.53              |
| 2:B:65:PHE:CD1    | 2:B:118:PHE:HB2    | 2.44                     | 0.53              |
| 3:C:364:TRP:HH2   | 3:C:538:ILE:HG13   | 1.72                     | 0.53              |
| 6:H:461:GLN:NE2   | 6:H:465:GLN:HE21   | 2.06                     | 0.53              |
| 8:P:459:LEU:HA    | 8:P:462:ILE:HD12   | 1.91                     | 0.53              |
| 8:Q:360:HIS:CE1   | 8:Q:367:CYS:HB2    | 2.44                     | 0.53              |
| 1:S:607:LEU:HB3   | 1:S:613:ILE:HD11   | 1.90                     | 0.53              |
| 10:U:298:GLN:HG2  | 10:U:299:GLY:H     | 1.73                     | 0.53              |
| 10:U:832:LEU:HB3  | 10:U:838:PHE:HE2   | 1.72                     | 0.53              |
| 10:U:931:LEU:HD23 | 10:U:934:LEU:HD12  | 1.91                     | 0.53              |
| 11:V:976:LEU:HD21 | 11:V:1016:VAL:HG11 | 1.89                     | 0.53              |
| 1:A:657:LEU:HD22  | 1:A:725:SER:HB2    | 1.91                     | 0.53              |
| 1:A:1126:LEU:HD11 | 1:A:1165:LEU:HB3   | 1.91                     | 0.53              |
| 6:H:102:ARG:O     | 6:H:105:GLU:HG2    | 2.09                     | 0.53              |
| 1:S:727:CYS:SG    | 9:W:87:TRP:NE1     | 2.76                     | 0.53              |
| 1:S:788:ALA:HB1   | 1:S:818:PHE:HE1    | 1.73                     | 0.53              |
| 4:E:298:LEU:HD21  | 4:E:347:TRP:CH2    | 2.43                     | 0.53              |
| 2:O:89:ILE:O      | 2:O:91:LEU:HD12    | 2.09                     | 0.53              |
| 8:P:227:LEU:HB2   | 8:P:334:LEU:HD21   | 1.91                     | 0.53              |
| 8:Q:328:TRP:HA    | 8:Q:333:LYS:O      | 2.09                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:S:915:THR:O    | 1:S:919:VAL:HG23  | 2.09                     | 0.53              |
| 1:S:1087:SER:OG  | 1:S:1133:HIS:O    | 2.18                     | 0.53              |
| 10:U:447:ARG:HG2 | 10:U:451:ARG:HH21 | 1.73                     | 0.53              |
| 3:C:339:THR:HG22 | 3:C:339:THR:O     | 2.09                     | 0.52              |
| 2:O:603:GLU:HG3  | 2:O:611:LYS:HE2   | 1.90                     | 0.52              |
| 2:O:675:TRP:CZ3  | 2:O:734:LEU:HD12  | 2.43                     | 0.52              |
| 8:Q:796:ASP:OD1  | 8:Q:799:ARG:NH1   | 2.42                     | 0.52              |
| 1:S:278:LEU:HD11 | 1:S:327:ILE:HA    | 1.90                     | 0.52              |
| 2:B:357:PHE:CD1  | 2:B:357:PHE:C     | 2.82                     | 0.52              |
| 4:E:22:LEU:O     | 4:E:27:ARG:NH2    | 2.42                     | 0.52              |
| 4:E:156:LEU:HB3  | 4:E:160:CYS:HG    | 1.74                     | 0.52              |
| 7:L:307:CYS:HB3  | 7:L:310:CYS:SG    | 2.48                     | 0.52              |
| 7:M:123:TRP:HB3  | 2:O:386:ASN:HB3   | 1.91                     | 0.52              |
| 2:O:385:GLU:O    | 2:O:389:LEU:HB2   | 2.09                     | 0.52              |
| 1:S:801:VAL:HG22 | 9:W:6:UNK:HA      | 1.91                     | 0.52              |
| 10:U:889:PRO:HG2 | 10:U:892:VAL:HG13 | 1.90                     | 0.52              |
| 10:U:1028:LEU:O  | 10:U:1032:LEU:HG  | 2.09                     | 0.52              |
| 1:A:1053:ARG:O   | 1:A:1057:GLN:HG3  | 2.09                     | 0.52              |
| 2:B:31:ASN:O     | 2:B:39:LYS:N      | 2.37                     | 0.52              |
| 6:G:89:THR:HG22  | 6:G:90:GLU:H      | 1.73                     | 0.52              |
| 6:H:117:GLY:O    | 6:H:121:LEU:HD23  | 2.09                     | 0.52              |
| 6:H:242:ARG:O    | 6:H:246:VAL:HG23  | 2.09                     | 0.52              |
| 7:M:201:TRP:CH2  | 7:M:221:ARG:HB3   | 2.43                     | 0.52              |
| 8:P:77:TYR:HE1   | 8:P:87:CYS:HG     | 1.57                     | 0.52              |
| 1:S:372:VAL:HA   | 1:S:375:LEU:HD12  | 1.91                     | 0.52              |
| 1:S:1003:ASN:OD1 | 9:W:1:UNK:N       | 2.39                     | 0.52              |
| 1:A:404:GLN:O    | 1:A:407:LEU:HG    | 2.09                     | 0.52              |
| 2:B:777:ILE:HD12 | 2:B:830:VAL:CG1   | 2.39                     | 0.52              |
| 7:M:104:LEU:CD1  | 7:M:105:PRO:HD2   | 2.40                     | 0.52              |
| 7:M:170:PRO:HD2  | 7:M:197:LEU:HD21  | 1.92                     | 0.52              |
| 8:P:202:PRO:HB3  | 8:P:225:PHE:CE2   | 2.44                     | 0.52              |
| 1:S:91:SER:OG    | 1:S:92:SER:N      | 2.42                     | 0.52              |
| 1:S:928:THR:HB   | 1:S:971:GLY:HA3   | 1.92                     | 0.52              |
| 1:A:1415:PHE:CZ  | 1:A:1439:ARG:HG2  | 2.44                     | 0.52              |
| 6:G:58:GLN:HE22  | 6:G:98:ARG:HG2    | 1.75                     | 0.52              |
| 6:H:337:PRO:HG2  | 6:H:338:LEU:HD22  | 1.91                     | 0.52              |
| 7:M:349:ARG:NH1  | 10:U:374:SER:O    | 2.42                     | 0.52              |
| 1:S:288:GLU:OE1  | 1:S:288:GLU:N     | 2.40                     | 0.52              |
| 1:S:787:LEU:O    | 1:S:791:LEU:HG    | 2.10                     | 0.52              |
| 1:A:831:PHE:O    | 1:A:834:LEU:HG    | 2.10                     | 0.52              |
| 1:A:985:VAL:O    | 1:A:989:MET:HG2   | 2.10                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:423:TYR:CD1    | 8:P:606:LEU:HD13   | 2.44                     | 0.52              |
| 4:E:359:ASN:HD21   | 7:M:73:ARG:HH12    | 1.57                     | 0.52              |
| 8:P:150:TRP:HZ3    | 8:P:195:PRO:HG3    | 1.73                     | 0.52              |
| 1:S:746:ALA:O      | 1:S:750:VAL:HG23   | 2.08                     | 0.52              |
| 10:U:757:ASN:HA    | 10:U:760:ILE:HD12  | 1.90                     | 0.52              |
| 11:V:933:PHE:CE2   | 11:V:972:LEU:HD13  | 2.45                     | 0.52              |
| 4:E:310:PRO:HB2    | 4:E:312:GLU:OE1    | 2.10                     | 0.52              |
| 2:O:78:CYS:HB2     | 2:O:95:VAL:HB      | 1.92                     | 0.52              |
| 1:S:314:ASP:HB2    | 1:S:315:PRO:HD3    | 1.91                     | 0.52              |
| 11:V:1350:ASP:HB3  | 11:V:1353:LEU:HB2  | 1.90                     | 0.52              |
| 1:A:649:PRO:HB2    | 1:A:687:VAL:HG12   | 1.92                     | 0.52              |
| 1:A:656:ALA:HA     | 1:A:659:GLU:HB3    | 1.92                     | 0.52              |
| 1:A:956:GLN:OE1    | 1:A:1020:ARG:NH1   | 2.43                     | 0.52              |
| 1:A:1080:ARG:NH2   | 1:S:952:GLN:HB2    | 2.24                     | 0.52              |
| 1:A:1178:GLU:HG3   | 1:A:1179:PRO:HD3   | 1.91                     | 0.52              |
| 6:G:327:LEU:HD12   | 6:G:327:LEU:H      | 1.75                     | 0.52              |
| 8:P:165:ARG:HG3    | 8:P:166:PRO:HD2    | 1.91                     | 0.52              |
| 1:S:399:CYS:O      | 1:S:670:ARG:NH1    | 2.42                     | 0.52              |
| 10:U:671:ILE:HG23  | 10:U:702:LEU:HD11  | 1.92                     | 0.52              |
| 11:V:243:VAL:CG1   | 11:V:244:PRO:HD3   | 2.40                     | 0.52              |
| 11:V:268:ASP:O     | 11:V:304:LYS:NZ    | 2.42                     | 0.52              |
| 11:V:830:LEU:HD12  | 11:V:916:LEU:HB3   | 1.92                     | 0.52              |
| 11:V:1082:GLU:OE2  | 11:V:1082:GLU:N    | 2.39                     | 0.52              |
| 11:V:1135:ILE:HD11 | 11:V:1155:ILE:HG23 | 1.92                     | 0.52              |
| 1:A:64:VAL:HG23    | 1:A:65:GLU:H       | 1.75                     | 0.52              |
| 2:B:40:THR:OG1     | 2:B:41:PRO:HD2     | 2.10                     | 0.52              |
| 2:O:520:LEU:HD12   | 8:Q:567:ILE:CG1    | 2.38                     | 0.52              |
| 8:P:712:ALA:H      | 8:P:782:ILE:HG21   | 1.74                     | 0.52              |
| 8:Q:729:CYS:HB3    | 8:Q:752:SER:OG     | 2.10                     | 0.52              |
| 11:V:372:ALA:HA    | 11:V:406:LYS:NZ    | 2.24                     | 0.52              |
| 11:V:613:LEU:O     | 11:V:617:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:1231:HIS:O     | 1:A:1235:GLN:HG3   | 2.09                     | 0.52              |
| 2:B:25:PHE:CD2     | 2:B:94:ILE:HD11    | 2.44                     | 0.52              |
| 3:C:127:PHE:CZ     | 5:F:162:LEU:HD11   | 2.45                     | 0.52              |
| 4:E:160:CYS:SG     | 4:E:161:GLN:N      | 2.83                     | 0.52              |
| 6:G:453:SER:OG     | 6:G:454:ALA:N      | 2.42                     | 0.52              |
| 7:M:277:GLU:OE1    | 7:M:277:GLU:N      | 2.41                     | 0.52              |
| 2:O:111:ILE:HD12   | 2:O:121:ARG:HG3    | 1.92                     | 0.52              |
| 8:P:545:ILE:HD11   | 8:P:565:TYR:HB2    | 1.92                     | 0.52              |
| 1:S:1019:SER:O     | 1:S:1022:GLN:HB2   | 2.10                     | 0.52              |
| 10:U:66:ARG:NH2    | 10:U:111:GLU:OE2   | 2.41                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:414:LEU:O     | 1:A:417:GLN:HG3    | 2.10                     | 0.51              |
| 1:A:1412:LYS:HD2  | 1:A:1443:ALA:HB2   | 1.90                     | 0.51              |
| 2:B:195:GLU:O     | 2:B:195:GLU:HG2    | 2.09                     | 0.51              |
| 2:B:423:TYR:CD1   | 8:P:606:LEU:HD22   | 2.45                     | 0.51              |
| 4:E:333:LEU:HA    | 4:E:336:LEU:HD23   | 1.92                     | 0.51              |
| 2:O:707:TRP:CH2   | 2:O:715:GLY:HA3    | 2.44                     | 0.51              |
| 2:O:774:SER:OG    | 8:Q:834:HIS:HB2    | 2.11                     | 0.51              |
| 8:P:165:ARG:HE    | 8:P:166:PRO:HD2    | 1.71                     | 0.51              |
| 8:P:173:VAL:HG12  | 8:P:174:GLU:N      | 2.25                     | 0.51              |
| 8:Q:31:HIS:O      | 8:Q:33:ALA:N       | 2.37                     | 0.51              |
| 8:Q:526:THR:HG22  | 8:Q:581:THR:HG22   | 1.92                     | 0.51              |
| 10:U:840:ARG:O    | 10:U:844:ASN:ND2   | 2.39                     | 0.51              |
| 10:U:1173:LEU:HA  | 10:U:1176:LEU:HD12 | 1.92                     | 0.51              |
| 1:A:102:ALA:HB2   | 1:A:112:LEU:HD12   | 1.93                     | 0.51              |
| 1:A:827:ARG:HH21  | 1:A:944:ASP:N      | 2.08                     | 0.51              |
| 3:C:241:CYS:SG    | 4:E:37:PRO:HD2     | 2.48                     | 0.51              |
| 8:Q:739:GLU:N     | 8:Q:739:GLU:OE1    | 2.40                     | 0.51              |
| 10:U:332:THR:O    | 10:U:336:LYS:HG2   | 2.10                     | 0.51              |
| 11:V:154:PHE:CZ   | 11:V:196:ILE:HG22  | 2.46                     | 0.51              |
| 1:A:1134:PHE:CE2  | 1:A:1138:LEU:HD11  | 2.45                     | 0.51              |
| 3:C:457:SER:HB3   | 3:C:494:PHE:HE1    | 1.76                     | 0.51              |
| 6:H:565:ASP:OD1   | 6:H:565:ASP:N      | 2.43                     | 0.51              |
| 7:M:215:GLU:CD    | 7:M:319:ILE:HD11   | 2.31                     | 0.51              |
| 1:S:1148:PRO:O    | 1:S:1152:VAL:HG23  | 2.10                     | 0.51              |
| 10:U:1076:ASN:HB2 | 10:U:1079:THR:HG23 | 1.92                     | 0.51              |
| 11:V:78:LYS:HD2   | 11:V:81:GLN:HE21   | 1.75                     | 0.51              |
| 11:V:456:LEU:HD12 | 11:V:460:TYR:CE2   | 2.45                     | 0.51              |
| 11:V:1370:ARG:O   | 11:V:1374:MET:HG2  | 2.10                     | 0.51              |
| 1:A:1193:LEU:O    | 1:A:1198:GLN:NE2   | 2.43                     | 0.51              |
| 2:B:347:ASP:OD1   | 2:B:347:ASP:N      | 2.43                     | 0.51              |
| 4:E:408:GLN:HE21  | 4:E:444:LEU:HD22   | 1.76                     | 0.51              |
| 6:G:241:PRO:O     | 6:G:244:VAL:HG12   | 2.10                     | 0.51              |
| 7:M:107:PRO:CD    | 7:M:108:PRO:HD2    | 2.40                     | 0.51              |
| 2:O:711:THR:O     | 2:O:713:PHE:N      | 2.44                     | 0.51              |
| 8:P:801:HIS:O     | 8:P:805:VAL:HG22   | 2.09                     | 0.51              |
| 1:S:512:SER:O     | 1:S:516:THR:HG23   | 2.10                     | 0.51              |
| 10:U:1:MET:HA     | 10:U:4:LYS:NZ      | 2.26                     | 0.51              |
| 11:V:362:GLU:O    | 11:V:366:LYS:HG3   | 2.10                     | 0.51              |
| 11:V:620:CYS:O    | 11:V:623:GLN:OE1   | 2.28                     | 0.51              |
| 2:B:187:LYS:HG2   | 2:B:229:ILE:HD11   | 1.91                     | 0.51              |
| 3:C:19:LEU:HD12   | 3:C:70:LEU:HD12    | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:C:361:ARG:HD2    | 3:C:538:ILE:HD12   | 1.92                     | 0.51              |
| 6:G:270:VAL:HG23   | 1:S:48:VAL:HG23    | 1.91                     | 0.51              |
| 8:P:505:PRO:HA     | 8:P:533:SER:HB2    | 1.93                     | 0.51              |
| 8:P:866:LEU:HA     | 8:P:869:VAL:HG22   | 1.93                     | 0.51              |
| 1:S:291:THR:HA     | 1:S:294:ILE:HD12   | 1.91                     | 0.51              |
| 1:S:717:MET:O      | 1:S:721:LEU:HG     | 2.10                     | 0.51              |
| 1:S:984:LEU:HD22   | 1:S:1021:LEU:HD13  | 1.91                     | 0.51              |
| 10:U:642:LEU:HD11  | 10:U:715:LYS:HG3   | 1.93                     | 0.51              |
| 10:U:987:THR:O     | 10:U:990:THR:OG1   | 2.24                     | 0.51              |
| 11:V:582:ALA:HB1   | 11:V:610:VAL:HG23  | 1.93                     | 0.51              |
| 11:V:843:PHE:CD2   | 11:V:847:THR:HG21  | 2.46                     | 0.51              |
| 11:V:1111:LEU:HD21 | 11:V:1144:LYS:HB2  | 1.93                     | 0.51              |
| 2:B:506:LEU:H      | 2:B:525:ASN:ND2    | 2.05                     | 0.51              |
| 3:C:123:SER:O      | 3:C:123:SER:OG     | 2.28                     | 0.51              |
| 2:O:18:TYR:OH      | 2:O:90:ASN:O       | 2.15                     | 0.51              |
| 8:P:125:LEU:HD23   | 8:P:166:PRO:HB3    | 1.93                     | 0.51              |
| 8:Q:33:ALA:HB1     | 8:Q:50:GLU:OE2     | 2.10                     | 0.51              |
| 1:S:152:ALA:HA     | 1:S:155:LEU:HD12   | 1.91                     | 0.51              |
| 1:S:1143:LEU:HB3   | 1:S:1188:HIS:CD2   | 2.45                     | 0.51              |
| 10:U:54:SER:O      | 10:U:65:ARG:NH2    | 2.42                     | 0.51              |
| 10:U:72:CYS:HA     | 10:U:75:LEU:HG     | 1.91                     | 0.51              |
| 10:U:591:LEU:HD22  | 10:U:605:LEU:HD11  | 1.92                     | 0.51              |
| 5:F:199:ASN:OD1    | 5:F:203:LYS:NZ     | 2.44                     | 0.51              |
| 6:H:501:GLN:HA     | 6:H:504:LYS:HD3    | 1.91                     | 0.51              |
| 2:O:636:PHE:HZ     | 2:O:651:LEU:HD21   | 1.74                     | 0.51              |
| 1:S:759:PRO:O      | 1:S:763:THR:HG23   | 2.10                     | 0.51              |
| 10:U:1006:MET:O    | 10:U:1010:THR:HG23 | 2.11                     | 0.51              |
| 2:B:385:GLU:N      | 7:L:123:TRP:HB2    | 2.26                     | 0.51              |
| 2:B:835:TYR:O      | 2:B:839:THR:HG23   | 2.10                     | 0.51              |
| 3:C:87:GLN:HG2     | 3:C:88:LYS:N       | 2.26                     | 0.51              |
| 3:C:213:GLU:OE1    | 3:C:220:PHE:HE2    | 1.93                     | 0.51              |
| 3:C:213:GLU:HG3    | 3:C:215:LEU:O      | 2.10                     | 0.51              |
| 4:E:400:SER:HA     | 4:E:440:GLN:NE2    | 2.25                     | 0.51              |
| 2:O:83:SER:HA      | 2:O:89:ILE:O       | 2.11                     | 0.51              |
| 8:P:249:GLN:HB3    | 8:P:277:HIS:HD2    | 1.76                     | 0.51              |
| 8:Q:14:PHE:N       | 8:Q:427:GLY:O      | 2.31                     | 0.51              |
| 10:U:648:GLU:OE1   | 10:U:648:GLU:N     | 2.39                     | 0.51              |
| 11:V:442:LEU:HD22  | 11:V:450:ILE:HG23  | 1.93                     | 0.51              |
| 1:A:22:TRP:HH2     | 6:H:375:LEU:HD13   | 1.76                     | 0.51              |
| 2:O:141:LEU:HD11   | 2:O:152:PHE:HB2    | 1.91                     | 0.51              |
| 8:Q:570:ASP:OD1    | 8:Q:578:ARG:NH1    | 2.42                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:424:LEU:O      | 1:S:428:VAL:HG23   | 2.11                     | 0.51              |
| 10:U:368:VAL:O     | 10:U:371:SER:HB2   | 2.11                     | 0.51              |
| 11:V:48:PHE:HA     | 11:V:96:PHE:CE1    | 2.46                     | 0.51              |
| 1:A:713:PRO:O      | 1:A:717:MET:HG2    | 2.11                     | 0.51              |
| 4:E:516:LEU:HD13   | 4:E:527:LEU:HB3    | 1.93                     | 0.51              |
| 7:M:274:TRP:HE3    | 7:M:287:VAL:HG21   | 1.75                     | 0.51              |
| 10:U:1135:ILE:HG13 | 10:U:1197:LEU:HD22 | 1.92                     | 0.51              |
| 1:A:1310:GLU:O     | 1:A:1317:ARG:NH1   | 2.43                     | 0.50              |
| 2:B:281:PHE:HB2    | 2:B:303:PHE:CE2    | 2.47                     | 0.50              |
| 3:C:87:GLN:O       | 3:C:91:ILE:HG13    | 2.11                     | 0.50              |
| 3:C:124:ALA:O      | 5:F:140:ARG:NH1    | 2.45                     | 0.50              |
| 3:C:265:GLU:HG3    | 3:C:268:CYS:HB3    | 1.93                     | 0.50              |
| 8:P:31:HIS:O       | 8:P:32:GLU:C       | 2.49                     | 0.50              |
| 8:P:729:CYS:SG     | 8:P:752:SER:OG     | 2.56                     | 0.50              |
| 8:P:733:LEU:HD22   | 8:P:746:VAL:HG11   | 1.92                     | 0.50              |
| 1:S:572:SER:OG     | 1:S:612:LYS:NZ     | 2.44                     | 0.50              |
| 11:V:364:TRP:HZ2   | 11:V:380:PHE:CE1   | 2.28                     | 0.50              |
| 3:C:174:ARG:NE     | 3:C:209:ARG:NH1    | 2.60                     | 0.50              |
| 7:M:107:PRO:CB     | 2:O:401:CYS:SG     | 2.99                     | 0.50              |
| 1:S:650:LEU:O      | 1:S:654:THR:HG23   | 2.11                     | 0.50              |
| 1:S:936:GLU:O      | 1:S:1014:ASN:ND2   | 2.39                     | 0.50              |
| 1:S:1112:VAL:HA    | 1:S:1116:MET:HG2   | 1.93                     | 0.50              |
| 10:U:50:ILE:O      | 10:U:54:SER:OG     | 2.26                     | 0.50              |
| 10:U:465:ASN:O     | 10:U:468:MET:HG3   | 2.11                     | 0.50              |
| 11:V:76:GLN:NE2    | 11:V:138:LEU:O     | 2.44                     | 0.50              |
| 11:V:84:ARG:HA     | 11:V:89:TYR:HE1    | 1.75                     | 0.50              |
| 11:V:1208:VAL:HG13 | 11:V:1209:PRO:HD3  | 1.94                     | 0.50              |
| 1:A:179:LEU:HD23   | 1:A:217:LEU:CD1    | 2.42                     | 0.50              |
| 1:A:1139:LEU:HD22  | 1:A:1184:ARG:HD3   | 1.92                     | 0.50              |
| 1:A:1169:SER:O     | 1:A:1172:VAL:HG22  | 2.11                     | 0.50              |
| 2:B:242:ILE:HG12   | 2:B:256:LEU:HD12   | 1.92                     | 0.50              |
| 5:F:252:CYS:HB3    | 5:F:274:TYR:CE1    | 2.47                     | 0.50              |
| 6:G:31:GLN:HE22    | 6:G:322:LEU:HB2    | 1.77                     | 0.50              |
| 8:P:806:GLY:O      | 8:P:810:THR:HG23   | 2.12                     | 0.50              |
| 1:S:377:GLU:O      | 1:S:381:THR:OG1    | 2.20                     | 0.50              |
| 1:S:1108:PHE:O     | 1:S:1112:VAL:HG23  | 2.12                     | 0.50              |
| 11:V:696:ALA:HA    | 11:V:758:CYS:SG    | 2.51                     | 0.50              |
| 1:A:1025:VAL:O     | 1:A:1029:GLU:HG2   | 2.11                     | 0.50              |
| 2:B:196:CYS:O      | 2:B:197:THR:OG1    | 2.25                     | 0.50              |
| 3:C:212:GLN:HE21   | 3:C:212:GLN:CA     | 2.16                     | 0.50              |
| 3:C:324:GLU:O      | 3:C:328:LYS:HB2    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:E:455:GLN:HE21  | 4:E:495:THR:HG21  | 1.76                     | 0.50              |
| 8:P:340:GLU:N     | 8:P:340:GLU:OE2   | 2.45                     | 0.50              |
| 8:P:773:MET:O     | 8:P:781:PRO:HB3   | 2.11                     | 0.50              |
| 1:S:460:ARG:HA    | 1:S:463:HIS:CD2   | 2.46                     | 0.50              |
| 1:S:1080:ARG:NH2  | 1:S:1083:LEU:HD12 | 2.26                     | 0.50              |
| 10:U:51:PHE:O     | 10:U:65:ARG:NH2   | 2.44                     | 0.50              |
| 10:U:497:GLN:HG2  | 10:U:538:ALA:HB1  | 1.94                     | 0.50              |
| 6:H:29:VAL:O      | 6:H:33:SER:OG     | 2.27                     | 0.50              |
| 8:Q:538:ASP:CG    | 8:Q:539:GLN:H     | 2.15                     | 0.50              |
| 1:S:904:GLN:OE1   | 1:S:904:GLN:N     | 2.43                     | 0.50              |
| 10:U:546:ASN:O    | 10:U:615:ARG:NH2  | 2.43                     | 0.50              |
| 11:V:580:THR:O    | 11:V:584:ILE:HG12 | 2.12                     | 0.50              |
| 1:A:23:ALA:HA     | 1:A:26:LEU:CD1    | 2.39                     | 0.50              |
| 1:A:1019:SER:O    | 1:A:1023:GLU:HG3  | 2.12                     | 0.50              |
| 1:A:1402:PHE:O    | 1:A:1406:LEU:HD23 | 2.12                     | 0.50              |
| 8:Q:31:HIS:HB2    | 8:Q:69:LEU:HD11   | 1.93                     | 0.50              |
| 8:Q:655:PHE:CZ    | 8:Q:754:ILE:HD12  | 2.46                     | 0.50              |
| 10:U:488:LEU:HD12 | 10:U:491:LEU:HD12 | 1.94                     | 0.50              |
| 11:V:394:GLN:N    | 11:V:394:GLN:OE1  | 2.42                     | 0.50              |
| 1:A:417:GLN:NE2   | 1:A:426:SER:OG    | 2.45                     | 0.50              |
| 2:B:693:PHE:HD2   | 2:B:704:LEU:HD21  | 1.76                     | 0.50              |
| 3:C:127:PHE:HZ    | 5:F:162:LEU:HD11  | 1.76                     | 0.50              |
| 5:F:15:LEU:O      | 5:F:18:SER:OG     | 2.21                     | 0.50              |
| 6:G:367:TYR:OH    | 6:G:399:GLU:OE2   | 2.29                     | 0.50              |
| 6:G:416:LEU:HD12  | 1:S:22:TRP:CZ3    | 2.41                     | 0.50              |
| 2:O:74:LEU:HD21   | 2:O:98:LYS:HD3    | 1.93                     | 0.50              |
| 2:O:661:GLN:HB2   | 2:O:747:LEU:HD11  | 1.93                     | 0.50              |
| 8:Q:709:LYS:HB2   | 8:Q:879:ILE:HD12  | 1.92                     | 0.50              |
| 1:S:932:TRP:HE3   | 1:S:933:LEU:HD23  | 1.77                     | 0.50              |
| 10:U:470:ALA:O    | 10:U:473:VAL:HG12 | 2.12                     | 0.50              |
| 11:V:165:LYS:NZ   | 11:V:169:GLU:OE1  | 2.33                     | 0.50              |
| 1:A:1420:GLU:OE1  | 1:A:1420:GLU:N    | 2.43                     | 0.50              |
| 7:M:89:MET:O      | 7:M:93:VAL:HG23   | 2.12                     | 0.50              |
| 2:O:218:GLU:HB3   | 2:O:220:GLN:HE22  | 1.75                     | 0.50              |
| 8:P:344:PRO:HD2   | 8:P:390:LEU:HD11  | 1.93                     | 0.50              |
| 8:Q:47:TYR:CZ     | 8:Q:54:LEU:HB3    | 2.46                     | 0.50              |
| 1:S:485:SER:O     | 1:S:490:GLN:NE2   | 2.45                     | 0.50              |
| 11:V:1109:GLU:OE2 | 11:V:1113:GLN:NE2 | 2.44                     | 0.50              |
| 11:V:1210:GLU:OE1 | 11:V:1210:GLU:N   | 2.44                     | 0.50              |
| 1:A:664:MET:HE1   | 1:A:733:ALA:HB2   | 1.94                     | 0.50              |
| 1:A:1329:ARG:HB3  | 1:A:1330:LEU:HD12 | 1.94                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:150:PHE:CZ    | 2:B:170:ILE:HB     | 2.46                     | 0.50              |
| 6:G:23:LEU:HD23   | 6:G:50:LEU:HD12    | 1.93                     | 0.50              |
| 7:L:267:LEU:O     | 7:L:271:ILE:HG23   | 2.12                     | 0.50              |
| 2:O:635:THR:HG22  | 2:O:639:LYS:HE3    | 1.94                     | 0.50              |
| 8:P:361:SER:CB    | 8:P:398:SER:O      | 2.59                     | 0.50              |
| 1:S:764:ARG:O     | 1:S:768:LEU:HG     | 2.11                     | 0.50              |
| 1:S:1113:ASN:O    | 1:S:1117:ARG:NE    | 2.40                     | 0.50              |
| 11:V:234:LEU:HD22 | 11:V:245:ILE:HD11  | 1.92                     | 0.50              |
| 11:V:526:PRO:HA   | 11:V:529:ILE:HD12  | 1.93                     | 0.50              |
| 1:A:121:VAL:HA    | 1:A:124:ILE:HG22   | 1.93                     | 0.49              |
| 2:B:479:TRP:HZ2   | 2:B:577:ILE:HD12   | 1.77                     | 0.49              |
| 3:C:126:ARG:HH22  | 5:F:140:ARG:HG2    | 1.76                     | 0.49              |
| 6:H:596:TYR:O     | 6:H:600:ILE:HD12   | 2.12                     | 0.49              |
| 7:L:83:PHE:C      | 7:L:83:PHE:CD1     | 2.85                     | 0.49              |
| 7:M:326:ASN:HD22  | 7:M:364:LYS:HG3    | 1.77                     | 0.49              |
| 2:O:216:SER:CB    | 2:O:220:GLN:HB2    | 2.42                     | 0.49              |
| 2:O:529:LYS:HG2   | 2:O:576:GLN:HG3    | 1.92                     | 0.49              |
| 8:P:150:TRP:CE2   | 8:P:178:TYR:HE2    | 2.29                     | 0.49              |
| 1:S:34:LYS:HB3    | 1:S:39:ARG:HH21    | 1.76                     | 0.49              |
| 1:S:313:THR:HG23  | 1:S:316:LEU:HB3    | 1.92                     | 0.49              |
| 1:S:788:ALA:HB1   | 1:S:818:PHE:CE1    | 2.46                     | 0.49              |
| 10:U:654:GLN:O    | 10:U:657:LYS:NZ    | 2.44                     | 0.49              |
| 10:U:1029:MET:HA  | 10:U:1032:LEU:HD12 | 1.94                     | 0.49              |
| 11:V:1009:ALA:O   | 11:V:1013:VAL:HG23 | 2.11                     | 0.49              |
| 11:V:1122:HIS:HB3 | 11:V:1158:LEU:HD11 | 1.94                     | 0.49              |
| 2:B:281:PHE:HB2   | 2:B:303:PHE:CD2    | 2.48                     | 0.49              |
| 5:F:111:LEU:O     | 5:F:115:LEU:HD12   | 2.11                     | 0.49              |
| 6:G:541:VAL:HG21  | 6:G:554:LEU:HD22   | 1.94                     | 0.49              |
| 6:H:558:LEU:O     | 6:H:562:ASP:N      | 2.41                     | 0.49              |
| 8:P:200:VAL:O     | 8:P:200:VAL:CG1    | 2.61                     | 0.49              |
| 8:P:864:GLN:OE1   | 8:P:871:ARG:NH2    | 2.45                     | 0.49              |
| 8:Q:598:VAL:HG13  | 8:Q:645:HIS:HB3    | 1.94                     | 0.49              |
| 1:S:307:LEU:O     | 1:S:311:ILE:HG22   | 2.12                     | 0.49              |
| 9:W:77:VAL:HB     | 9:W:85:PHE:HD2     | 1.76                     | 0.49              |
| 10:U:364:ILE:O    | 10:U:367:VAL:HB    | 2.13                     | 0.49              |
| 10:U:579:ALA:HA   | 10:U:582:THR:HG22  | 1.94                     | 0.49              |
| 11:V:928:LEU:O    | 11:V:975:LYS:NZ    | 2.40                     | 0.49              |
| 2:B:526:ARG:NH2   | 2:B:655:PHE:O      | 2.40                     | 0.49              |
| 3:C:23:ASP:OD2    | 3:C:24:GLN:HG3     | 2.12                     | 0.49              |
| 3:C:142:PRO:HA    | 3:C:145:TYR:HE2    | 1.72                     | 0.49              |
| 4:E:24:ALA:HA     | 4:E:27:ARG:NH2     | 2.27                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:E:408:GLN:NE2   | 4:E:444:LEU:HD22   | 2.27                     | 0.49              |
| 6:G:186:PRO:HD3   | 6:G:204:LYS:HD2    | 1.94                     | 0.49              |
| 6:G:553:HIS:O     | 6:G:557:THR:HG23   | 2.12                     | 0.49              |
| 7:L:54:LEU:HG     | 7:L:55:CYS:H       | 1.77                     | 0.49              |
| 8:P:35:VAL:CG1    | 8:P:47:TYR:HB2     | 2.42                     | 0.49              |
| 8:Q:393:MET:HG3   | 8:Q:395:CYS:SG     | 2.52                     | 0.49              |
| 1:S:169:GLU:HA    | 1:S:172:LYS:HD2    | 1.95                     | 0.49              |
| 1:S:1335:PHE:HD2  | 1:S:1360:MET:HG2   | 1.76                     | 0.49              |
| 10:U:90:ILE:HD11  | 10:U:128:GLU:HB2   | 1.94                     | 0.49              |
| 10:U:435:MET:N    | 10:U:435:MET:HE2   | 2.27                     | 0.49              |
| 11:V:163:GLU:N    | 11:V:163:GLU:OE2   | 2.46                     | 0.49              |
| 11:V:665:VAL:HG13 | 11:V:695:ILE:HG23  | 1.92                     | 0.49              |
| 1:A:393:VAL:HA    | 1:A:396:LEU:HD12   | 1.94                     | 0.49              |
| 1:A:751:ARG:HA    | 1:A:754:CYS:SG     | 2.52                     | 0.49              |
| 6:H:158:ASP:OD1   | 6:H:159:LEU:N      | 2.45                     | 0.49              |
| 7:M:41:VAL:HB     | 7:M:52:ARG:HB2     | 1.94                     | 0.49              |
| 2:O:738:LEU:HD13  | 2:O:742:CYS:SG     | 2.53                     | 0.49              |
| 10:U:206:ASN:O    | 10:U:209:GLU:HG2   | 2.12                     | 0.49              |
| 10:U:306:SER:N    | 10:U:309:SER:HB3   | 2.27                     | 0.49              |
| 10:U:1041:SER:CB  | 10:U:1137:GLN:HE22 | 2.25                     | 0.49              |
| 11:V:383:VAL:HG21 | 11:V:424:HIS:HD2   | 1.77                     | 0.49              |
| 11:V:477:LEU:O    | 11:V:481:ILE:HG13  | 2.11                     | 0.49              |
| 1:A:1056:LEU:HD13 | 1:A:1115:GLU:HG3   | 1.95                     | 0.49              |
| 2:B:239:TYR:HB3   | 2:B:259:LEU:HD21   | 1.95                     | 0.49              |
| 2:B:287:VAL:HG12  | 2:B:301:VAL:HG22   | 1.94                     | 0.49              |
| 2:B:524:GLN:O     | 2:B:580:ALA:HA     | 2.12                     | 0.49              |
| 3:C:434:ASP:OD2   | 4:E:177:ARG:NH1    | 2.45                     | 0.49              |
| 5:F:283:GLN:HG2   | 5:F:347:TRP:HZ2    | 1.78                     | 0.49              |
| 6:G:334:LEU:H     | 6:G:334:LEU:HD23   | 1.77                     | 0.49              |
| 6:H:156:LEU:HB3   | 6:H:177:LEU:HD11   | 1.95                     | 0.49              |
| 8:P:25:LYS:N      | 8:P:26:PRO:CD      | 2.75                     | 0.49              |
| 8:P:606:LEU:O     | 8:P:609:VAL:HG22   | 2.13                     | 0.49              |
| 8:P:850:ARG:NH1   | 8:P:856:GLU:HB2    | 2.26                     | 0.49              |
| 8:Q:361:SER:OG    | 8:Q:366:LEU:HG     | 2.13                     | 0.49              |
| 10:U:504:GLN:HG2  | 10:U:505:PRO:HD3   | 1.95                     | 0.49              |
| 11:V:72:GLN:HE21  | 11:V:138:LEU:HD21  | 1.76                     | 0.49              |
| 1:A:1099:GLN:CD   | 1:A:1099:GLN:H     | 2.15                     | 0.49              |
| 2:B:259:LEU:HD11  | 2:B:284:PRO:HB2    | 1.95                     | 0.49              |
| 3:C:245:ARG:NH2   | 4:E:92:ARG:HH21    | 2.10                     | 0.49              |
| 4:E:352:SER:O     | 4:E:353:PRO:O      | 2.31                     | 0.49              |
| 6:H:115:GLU:N     | 6:H:121:LEU:HD21   | 2.27                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:249:PRO:HD3   | 7:L:274:TRP:CZ2   | 2.48                     | 0.49              |
| 8:Q:178:TYR:CE2   | 8:Q:246:PRO:HD2   | 2.48                     | 0.49              |
| 10:U:540:PHE:HA   | 10:U:543:LEU:HD12 | 1.93                     | 0.49              |
| 11:V:84:ARG:HA    | 11:V:89:TYR:CE1   | 2.47                     | 0.49              |
| 11:V:210:ASP:O    | 11:V:213:THR:HG22 | 2.13                     | 0.49              |
| 11:V:412:ILE:HG23 | 11:V:416:LEU:HD23 | 1.95                     | 0.49              |
| 1:A:136:LEU:HD11  | 1:A:231:ALA:HB2   | 1.95                     | 0.49              |
| 1:A:929:TYR:HB2   | 1:A:972:GLY:HA2   | 1.93                     | 0.49              |
| 7:M:275:ASP:O     | 7:M:283:ASN:ND2   | 2.44                     | 0.49              |
| 1:S:57:LEU:HA     | 1:S:60:LEU:HB3    | 1.94                     | 0.49              |
| 1:S:166:PHE:O     | 1:S:170:LEU:HG    | 2.13                     | 0.49              |
| 1:S:341:GLN:HG3   | 1:S:484:GLU:HB3   | 1.95                     | 0.49              |
| 1:S:567:THR:HG22  | 1:S:1065:VAL:HG13 | 1.95                     | 0.49              |
| 1:S:1090:LEU:HD13 | 1:S:1134:PHE:CD1  | 2.47                     | 0.49              |
| 10:U:665:ASP:OD1  | 10:U:665:ASP:N    | 2.44                     | 0.49              |
| 10:U:1022:ALA:O   | 10:U:1026:LYS:HG2 | 2.13                     | 0.49              |
| 11:V:134:SER:OG   | 11:V:137:LYS:HG3  | 2.12                     | 0.49              |
| 11:V:146:GLN:HE22 | 11:V:186:VAL:HA   | 1.78                     | 0.49              |
| 11:V:920:ASN:OD1  | 11:V:921:SER:N    | 2.45                     | 0.49              |
| 1:A:287:GLU:O     | 1:A:289:SER:N     | 2.46                     | 0.49              |
| 1:A:822:LEU:HD11  | 1:A:833:CYS:HB2   | 1.94                     | 0.49              |
| 6:G:198:GLN:OE1   | 6:G:203:LEU:HG    | 2.12                     | 0.49              |
| 8:P:74:ARG:HD3    | 8:P:91:ASP:OD1    | 2.13                     | 0.49              |
| 8:P:220:LEU:HD13  | 8:P:224:LEU:HD22  | 1.93                     | 0.49              |
| 8:Q:28:VAL:HG22   | 8:Q:37:LEU:HD13   | 1.94                     | 0.49              |
| 8:Q:364:SER:OG    | 8:Q:365:ASP:N     | 2.45                     | 0.49              |
| 10:U:418:ALA:O    | 10:U:421:LEU:HB3  | 2.12                     | 0.49              |
| 6:G:67:LEU:HD21   | 6:G:103:VAL:HG22  | 1.95                     | 0.49              |
| 6:G:257:ARG:HG3   | 6:G:289:LEU:HD13  | 1.95                     | 0.49              |
| 6:H:265:ALA:O     | 6:H:269:LEU:HG    | 2.13                     | 0.49              |
| 2:O:72:SER:OG     | 2:O:101:LYS:HE3   | 2.13                     | 0.49              |
| 2:O:675:TRP:O     | 2:O:679:HIS:HB2   | 2.13                     | 0.49              |
| 8:Q:538:ASP:OD1   | 8:Q:539:GLN:N     | 2.45                     | 0.49              |
| 1:S:186:HIS:CD2   | 1:S:193:LEU:H     | 2.26                     | 0.49              |
| 1:S:583:PHE:HZ    | 1:S:613:ILE:HG23  | 1.78                     | 0.49              |
| 1:S:1393:VAL:O    | 1:S:1397:THR:HG23 | 2.13                     | 0.49              |
| 10:U:600:ASP:N    | 10:U:600:ASP:OD1  | 2.45                     | 0.49              |
| 10:U:664:LEU:HD13 | 10:U:667:LEU:HD22 | 1.95                     | 0.49              |
| 11:V:369:GLU:OE1  | 11:V:398:TYR:OH   | 2.28                     | 0.49              |
| 1:A:677:VAL:HG11  | 1:A:748:LEU:HB3   | 1.95                     | 0.49              |
| 2:B:39:LYS:HG3    | 2:B:40:THR:O      | 2.13                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:E:514:MET:HA    | 4:E:517:GLU:HG2    | 1.94                     | 0.49              |
| 6:H:31:GLN:O      | 6:H:39:ARG:NH1     | 2.45                     | 0.49              |
| 7:M:21:SER:O      | 7:M:23:THR:N       | 2.45                     | 0.49              |
| 7:M:121:LEU:HG    | 7:M:125:LYS:HG3    | 1.95                     | 0.49              |
| 8:Q:219:THR:HG21  | 8:Q:306:ASP:HB3    | 1.94                     | 0.49              |
| 1:S:321:SER:O     | 1:S:325:THR:HG23   | 2.12                     | 0.49              |
| 1:S:1188:HIS:ND1  | 1:S:1189:CYS:SG    | 2.81                     | 0.49              |
| 10:U:747:MET:HG2  | 10:U:778:TYR:CD1   | 2.48                     | 0.49              |
| 10:U:1033:PHE:O   | 10:U:1037:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:346:TRP:CZ2   | 1:A:387:GLN:HG2    | 2.47                     | 0.48              |
| 1:A:1168:THR:O    | 1:A:1171:LEU:HB2   | 2.12                     | 0.48              |
| 1:A:1315:LEU:HB3  | 1:A:1319:LEU:HD22  | 1.95                     | 0.48              |
| 3:C:60:VAL:HG23   | 3:C:64:PHE:CE1     | 2.48                     | 0.48              |
| 5:F:83:PHE:HA     | 5:F:86:LEU:HD13    | 1.94                     | 0.48              |
| 7:M:16:LEU:HD23   | 7:M:26:GLU:O       | 2.12                     | 0.48              |
| 8:Q:791:SER:HB3   | 8:Q:797:ILE:HD11   | 1.94                     | 0.48              |
| 10:U:284:GLU:OE1  | 10:U:284:GLU:N     | 2.45                     | 0.48              |
| 10:U:817:LEU:HD21 | 10:U:839:MET:HG2   | 1.95                     | 0.48              |
| 10:U:1079:THR:O   | 10:U:1083:THR:OG1  | 2.22                     | 0.48              |
| 11:V:113:CYS:SG   | 11:V:135:LEU:HD22  | 2.53                     | 0.48              |
| 11:V:278:LEU:N    | 11:V:279:PRO:HD2   | 2.28                     | 0.48              |
| 11:V:1343:GLY:O   | 11:V:1347:ILE:HG13 | 2.13                     | 0.48              |
| 3:C:58:ASN:ND2    | 3:C:99:ASN:HB2     | 2.28                     | 0.48              |
| 3:C:241:CYS:SG    | 4:E:37:PRO:HD3     | 2.49                     | 0.48              |
| 1:S:286:GLN:N     | 1:S:287:GLU:OE1    | 2.44                     | 0.48              |
| 11:V:347:PHE:HA   | 11:V:350:ILE:HD12  | 1.95                     | 0.48              |
| 11:V:643:LYS:O    | 11:V:643:LYS:HG2   | 2.12                     | 0.48              |
| 11:V:786:ILE:HG21 | 11:V:826:LEU:HB2   | 1.94                     | 0.48              |
| 5:F:252:CYS:HB3   | 5:F:274:TYR:HE1    | 1.78                     | 0.48              |
| 6:G:150:TRP:CE2   | 6:G:155:ARG:HD2    | 2.47                     | 0.48              |
| 8:P:733:LEU:HD21  | 8:P:754:ILE:HD13   | 1.95                     | 0.48              |
| 8:Q:366:LEU:HD11  | 8:Q:401:ILE:HD12   | 1.96                     | 0.48              |
| 1:S:764:ARG:HH12  | 9:W:95:TRP:HZ3     | 1.61                     | 0.48              |
| 1:A:822:LEU:HD22  | 1:A:867:LYS:HD3    | 1.95                     | 0.48              |
| 1:A:946:LEU:HD22  | 1:A:950:GLU:HB3    | 1.95                     | 0.48              |
| 1:A:1257:LEU:HA   | 1:A:1260:LEU:HG    | 1.95                     | 0.48              |
| 2:B:329:LEU:HD12  | 2:B:342:LEU:HD23   | 1.95                     | 0.48              |
| 2:O:342:LEU:HD11  | 2:O:357:PHE:HB2    | 1.95                     | 0.48              |
| 2:O:854:GLN:HB3   | 8:Q:798:CYS:HB2    | 1.95                     | 0.48              |
| 10:U:117:ARG:HE   | 10:U:167:GLY:HA3   | 1.78                     | 0.48              |
| 11:V:59:LEU:HD13  | 11:V:66:ASN:ND2    | 2.28                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:660:PHE:CZ    | 2:B:731:LEU:HD11   | 2.49                     | 0.48              |
| 10:U:4:LYS:HE2    | 10:U:20:PHE:HZ     | 1.78                     | 0.48              |
| 10:U:237:PHE:CD1  | 10:U:240:LEU:HD12  | 2.48                     | 0.48              |
| 10:U:654:GLN:OE1  | 10:U:654:GLN:N     | 2.46                     | 0.48              |
| 10:U:724:ASP:OD2  | 10:U:725:LYS:NZ    | 2.40                     | 0.48              |
| 10:U:1043:VAL:HA  | 10:U:1046:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:113:SER:HB2   | 1:A:155:LEU:HD13   | 1.93                     | 0.48              |
| 1:A:740:GLU:OE1   | 1:A:849:SER:HB2    | 2.13                     | 0.48              |
| 2:B:25:PHE:HA     | 2:B:44:HIS:O       | 2.13                     | 0.48              |
| 3:C:186:VAL:O     | 3:C:186:VAL:CG1    | 2.61                     | 0.48              |
| 6:H:548:ARG:NH2   | 6:H:606:ASP:OD2    | 2.46                     | 0.48              |
| 7:L:268:SER:O     | 7:L:271:ILE:HG12   | 2.12                     | 0.48              |
| 7:M:42:LEU:HD21   | 7:M:80:LEU:HD12    | 1.94                     | 0.48              |
| 2:O:761:PHE:O     | 2:O:765:LYS:HG2    | 2.14                     | 0.48              |
| 8:P:325:LYS:HG2   | 8:P:326:ALA:H      | 1.78                     | 0.48              |
| 8:Q:531:ASN:OD1   | 8:Q:574:PRO:HA     | 2.13                     | 0.48              |
| 1:S:1261:PHE:O    | 1:S:1265:LEU:HG    | 2.13                     | 0.48              |
| 10:U:341:LEU:HD13 | 10:U:359:TYR:CE2   | 2.48                     | 0.48              |
| 10:U:723:LEU:O    | 10:U:725:LYS:HG2   | 2.13                     | 0.48              |
| 11:V:107:GLU:OE1  | 11:V:111:ARG:NE    | 2.44                     | 0.48              |
| 11:V:429:LYS:HG3  | 11:V:430:ASP:H     | 1.78                     | 0.48              |
| 11:V:656:ILE:HG23 | 11:V:733:TYR:CE1   | 2.48                     | 0.48              |
| 4:E:358:SER:O     | 4:E:361:THR:OG1    | 2.27                     | 0.48              |
| 7:L:64:SER:HA     | 7:L:67:HIS:NE2     | 2.28                     | 0.48              |
| 8:P:504:ARG:N     | 8:P:505:PRO:CD     | 2.77                     | 0.48              |
| 1:S:1302:TRP:O    | 1:S:1305:LEU:HG    | 2.12                     | 0.48              |
| 10:U:776:MET:O    | 10:U:780:LYS:HG3   | 2.14                     | 0.48              |
| 11:V:777:LYS:O    | 11:V:781:PHE:CD1   | 2.66                     | 0.48              |
| 1:A:1222:PRO:HG2  | 1:A:1225:LEU:HD13  | 1.96                     | 0.48              |
| 2:B:673:LYS:NZ    | 2:B:709:GLN:OE1    | 2.47                     | 0.48              |
| 3:C:457:SER:HB3   | 3:C:494:PHE:CE1    | 2.48                     | 0.48              |
| 4:E:64:LEU:HD11   | 4:E:109:LEU:HD22   | 1.94                     | 0.48              |
| 5:F:345:SER:HB2   | 5:F:348:THR:HG23   | 1.96                     | 0.48              |
| 6:G:266:LEU:HD21  | 1:S:51:LEU:O       | 2.12                     | 0.48              |
| 2:O:10:ASN:HD21   | 2:O:74:LEU:H       | 1.62                     | 0.48              |
| 2:O:323:GLU:O     | 2:O:324:LYS:HG2    | 2.13                     | 0.48              |
| 8:P:253:VAL:HB    | 8:P:272:VAL:HG22   | 1.94                     | 0.48              |
| 8:Q:337:GLU:OE1   | 8:Q:383:PRO:HG2    | 2.13                     | 0.48              |
| 1:S:1343:HIS:CE1  | 1:S:1348:ILE:HB    | 2.48                     | 0.48              |
| 9:W:79:THR:HG22   | 9:W:80:VAL:H       | 1.79                     | 0.48              |
| 10:U:184:VAL:HG13 | 10:U:186:LEU:HG    | 1.95                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:U:450:THR:HG21 | 11:V:356:TYR:HA  | 1.95                     | 0.48              |
| 1:A:221:MET:HG3   | 1:A:222:GLU:OE1  | 2.14                     | 0.48              |
| 1:A:1343:HIS:CE1  | 1:A:1348:ILE:HB  | 2.49                     | 0.48              |
| 4:E:492:LEU:O     | 4:E:495:THR:OG1  | 2.28                     | 0.48              |
| 6:G:54:LEU:O      | 6:G:58:GLN:HG3   | 2.14                     | 0.48              |
| 7:L:37:HIS:CD2    | 7:L:38:LEU:H     | 2.32                     | 0.48              |
| 8:P:145:GLN:HG3   | 8:P:150:TRP:NE1  | 2.28                     | 0.48              |
| 9:W:76:GLU:HG3    | 9:W:84:THR:HB    | 1.96                     | 0.48              |
| 10:U:417:HIS:ND1  | 10:U:420:LYS:HD3 | 2.29                     | 0.48              |
| 10:U:430:PHE:O    | 10:U:437:ARG:NH2 | 2.43                     | 0.48              |
| 1:A:235:LEU:HD12  | 1:A:236:SER:N    | 2.29                     | 0.48              |
| 1:A:712:GLU:HG2   | 1:A:713:PRO:HD2  | 1.96                     | 0.48              |
| 1:A:828:ASP:OD1   | 1:A:828:ASP:N    | 2.47                     | 0.48              |
| 1:A:1193:LEU:HD23 | 1:A:1198:GLN:HG3 | 1.95                     | 0.48              |
| 1:A:1367:LEU:HD11 | 1:A:1372:ASP:HB3 | 1.95                     | 0.48              |
| 2:B:582:THR:HG22  | 2:B:583:SER:O    | 2.14                     | 0.48              |
| 2:B:747:LEU:HD22  | 2:B:750:GLY:O    | 2.14                     | 0.48              |
| 6:H:354:CYS:SG    | 6:H:359:ARG:HB2  | 2.53                     | 0.48              |
| 2:O:312:TRP:CD1   | 2:O:319:ALA:HB2  | 2.49                     | 0.48              |
| 2:O:328:VAL:HG23  | 2:O:343:LEU:HD23 | 1.96                     | 0.48              |
| 2:O:679:HIS:O     | 2:O:681:LYS:NZ   | 2.46                     | 0.48              |
| 8:P:36:PHE:CD2    | 8:P:46:VAL:HG22  | 2.48                     | 0.48              |
| 8:P:312:LEU:O     | 8:P:323:ALA:HA   | 2.14                     | 0.48              |
| 8:P:655:PHE:CE2   | 8:P:754:ILE:HD12 | 2.49                     | 0.48              |
| 8:Q:730:CYS:O     | 8:Q:734:GLN:HG2  | 2.14                     | 0.48              |
| 1:S:328:LEU:HD11  | 1:S:384:VAL:HG13 | 1.96                     | 0.48              |
| 1:S:1296:GLU:O    | 1:S:1299:LYS:NZ  | 2.43                     | 0.48              |
| 1:A:650:LEU:HD21  | 1:A:714:ARG:NH2  | 2.24                     | 0.47              |
| 1:A:739:PRO:HA    | 1:A:742:GLN:HB2  | 1.96                     | 0.47              |
| 2:B:240:VAL:HG12  | 2:B:241:HIS:N    | 2.28                     | 0.47              |
| 2:B:315:SER:O     | 2:B:317:GLN:N    | 2.47                     | 0.47              |
| 2:B:323:GLU:C     | 2:B:324:LYS:HD3  | 2.34                     | 0.47              |
| 4:E:465:THR:OG1   | 4:E:468:LYS:HE2  | 2.14                     | 0.47              |
| 4:E:493:MET:O     | 4:E:497:MET:HG3  | 2.14                     | 0.47              |
| 6:H:141:ARG:NH1   | 6:H:196:THR:HG21 | 2.29                     | 0.47              |
| 7:L:54:LEU:HG     | 7:L:55:CYS:N     | 2.27                     | 0.47              |
| 7:M:272:HIS:CE1   | 7:M:273:LEU:HG   | 2.49                     | 0.47              |
| 2:O:390:VAL:C     | 2:O:393:PRO:HD2  | 2.35                     | 0.47              |
| 8:P:28:VAL:HG23   | 8:P:400:ASN:ND2  | 2.29                     | 0.47              |
| 8:P:870:TYR:CZ    | 8:P:874:ARG:HG3  | 2.49                     | 0.47              |
| 1:S:424:LEU:HD21  | 1:S:472:PHE:HB3  | 1.96                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:U:324:ASP:N     | 10:U:324:ASP:OD1   | 2.46                     | 0.47              |
| 10:U:331:LYS:O     | 10:U:335:VAL:HG23  | 2.13                     | 0.47              |
| 10:U:835:SER:HB2   | 10:U:838:PHE:HB3   | 1.91                     | 0.47              |
| 10:U:858:HIS:HB2   | 10:U:864:GLY:O     | 2.13                     | 0.47              |
| 10:U:1010:THR:HB   | 10:U:1032:LEU:HD23 | 1.96                     | 0.47              |
| 11:V:382:LEU:HD13  | 11:V:417:LEU:HD12  | 1.96                     | 0.47              |
| 1:A:264:GLN:HA     | 1:A:267:VAL:HG12   | 1.95                     | 0.47              |
| 1:A:1335:PHE:HD2   | 1:A:1360:MET:HG2   | 1.79                     | 0.47              |
| 2:B:846:GLN:HE22   | 8:P:877:SER:CB     | 2.22                     | 0.47              |
| 3:C:87:GLN:CD      | 3:C:87:GLN:H       | 2.17                     | 0.47              |
| 3:C:140:TYR:CD2    | 5:F:169:LEU:HD22   | 2.50                     | 0.47              |
| 3:C:429:TYR:HE1    | 4:E:176:ARG:HH21   | 1.62                     | 0.47              |
| 6:G:57:LEU:HD22    | 6:G:66:VAL:HG23    | 1.96                     | 0.47              |
| 6:H:450:LEU:O      | 6:H:453:SER:OG     | 2.25                     | 0.47              |
| 8:Q:850:ARG:O      | 8:Q:853:THR:HG22   | 2.14                     | 0.47              |
| 1:S:767:GLN:HE22   | 1:S:1003:ASN:ND2   | 2.13                     | 0.47              |
| 1:S:815:PRO:HA     | 1:S:818:PHE:HD2    | 1.80                     | 0.47              |
| 1:S:1102:THR:OG1   | 1:S:1158:LYS:HE3   | 2.14                     | 0.47              |
| 9:W:78:PHE:HA      | 9:W:82:PRO:HB3     | 1.95                     | 0.47              |
| 10:U:1138:LEU:HD13 | 10:U:1176:LEU:HD11 | 1.96                     | 0.47              |
| 11:V:686:LEU:HB3   | 11:V:688:GLU:OE1   | 2.14                     | 0.47              |
| 11:V:845:VAL:O     | 11:V:848:LEU:HG    | 2.15                     | 0.47              |
| 1:A:171:TRP:CD2    | 1:A:200:HIS:HD2    | 2.32                     | 0.47              |
| 1:A:405:GLN:OE1    | 1:A:405:GLN:N      | 2.46                     | 0.47              |
| 1:A:1406:LEU:O     | 1:A:1409:ARG:N     | 2.46                     | 0.47              |
| 2:B:526:ARG:NH1    | 2:B:653:ALA:O      | 2.48                     | 0.47              |
| 6:G:177:LEU:HD12   | 6:G:211:PHE:CZ     | 2.49                     | 0.47              |
| 6:G:565:ASP:OD1    | 6:G:565:ASP:N      | 2.47                     | 0.47              |
| 7:L:309:ILE:HD11   | 7:L:360:PRO:HG2    | 1.97                     | 0.47              |
| 7:M:101:LEU:HD21   | 8:Q:339:ARG:HG3    | 1.95                     | 0.47              |
| 2:O:662:ILE:HG12   | 2:O:744:LEU:HD13   | 1.95                     | 0.47              |
| 2:O:724:GLN:HG2    | 2:O:727:MET:HE3    | 1.97                     | 0.47              |
| 10:U:706:LEU:O     | 10:U:710:THR:HG23  | 2.13                     | 0.47              |
| 11:V:220:GLY:N     | 11:V:223:GLN:HE22  | 2.13                     | 0.47              |
| 11:V:500:VAL:HG12  | 11:V:507:MET:HG2   | 1.96                     | 0.47              |
| 11:V:569:LYS:HD3   | 11:V:851:THR:HG22  | 1.96                     | 0.47              |
| 1:A:1165:LEU:HD11  | 1:A:1322:VAL:HA    | 1.96                     | 0.47              |
| 7:M:101:LEU:HD21   | 8:Q:339:ARG:NE     | 2.30                     | 0.47              |
| 7:M:307:CYS:HB2    | 7:M:334:HIS:CE1    | 2.50                     | 0.47              |
| 2:O:40:THR:HG21    | 2:O:67:ILE:HB      | 1.96                     | 0.47              |
| 8:P:325:LYS:HB2    | 8:P:384:GLU:OE2    | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:399:LEU:O     | 8:P:400:ASN:HB3   | 2.14                     | 0.47              |
| 8:Q:292:PRO:HG3   | 8:Q:355:GLY:HA2   | 1.97                     | 0.47              |
| 1:S:346:TRP:CE2   | 1:S:387:GLN:HG2   | 2.49                     | 0.47              |
| 1:S:474:PHE:O     | 1:S:478:SER:N     | 2.41                     | 0.47              |
| 10:U:106:VAL:O    | 10:U:110:ASN:ND2  | 2.47                     | 0.47              |
| 10:U:447:ARG:HD3  | 10:U:459:PHE:CZ   | 2.49                     | 0.47              |
| 10:U:547:PHE:HB2  | 10:U:550:LEU:HD11 | 1.97                     | 0.47              |
| 10:U:1269:LYS:HG3 | 10:U:1270:LYS:HG3 | 1.95                     | 0.47              |
| 11:V:1283:LYS:H   | 11:V:1283:LYS:HD2 | 1.78                     | 0.47              |
| 1:A:1265:LEU:HD23 | 1:A:1288:CYS:SG   | 2.55                     | 0.47              |
| 2:B:15:LEU:HD22   | 2:B:24:VAL:HG22   | 1.95                     | 0.47              |
| 2:B:79:CYS:CB     | 2:B:94:ILE:HD13   | 2.45                     | 0.47              |
| 4:E:118:LEU:HD21  | 4:E:140:LEU:HD23  | 1.96                     | 0.47              |
| 4:E:523:LEU:HD22  | 11:V:158:PRO:CG   | 2.45                     | 0.47              |
| 2:O:73:HIS:CB     | 2:O:99:ASN:HB3    | 2.45                     | 0.47              |
| 8:P:60:PHE:HZ     | 8:P:88:LEU:HD11   | 1.79                     | 0.47              |
| 1:S:587:LEU:HD12  | 1:S:617:LEU:HB3   | 1.96                     | 0.47              |
| 1:S:1210:PHE:HD2  | 1:S:1230:LEU:HD11 | 1.79                     | 0.47              |
| 11:V:417:LEU:HD13 | 11:V:453:PHE:CZ   | 2.50                     | 0.47              |
| 1:A:163:ARG:HB2   | 8:P:849:ASP:OD2   | 2.14                     | 0.47              |
| 1:A:1027:ASP:HA   | 1:A:1030:LEU:HD21 | 1.96                     | 0.47              |
| 3:C:258:PHE:CD1   | 3:C:261:LEU:HD21  | 2.49                     | 0.47              |
| 6:G:510:GLN:NE2   | 6:G:543:MET:HG3   | 2.29                     | 0.47              |
| 6:H:127:ARG:HA    | 6:H:130:CYS:SG    | 2.54                     | 0.47              |
| 6:H:164:GLU:HG3   | 6:H:171:SER:O     | 2.15                     | 0.47              |
| 2:O:215:TYR:OH    | 2:O:219:SER:HA    | 2.14                     | 0.47              |
| 1:S:675:ALA:O     | 1:S:679:VAL:HG23  | 2.14                     | 0.47              |
| 1:S:911:TRP:O     | 1:S:917:ARG:HD3   | 2.15                     | 0.47              |
| 1:S:947:SER:N     | 1:S:950:GLU:OE2   | 2.41                     | 0.47              |
| 11:V:173:PRO:O    | 11:V:176:ILE:HG22 | 2.15                     | 0.47              |
| 11:V:791:ASN:OD1  | 11:V:925:PHE:HA   | 2.15                     | 0.47              |
| 1:A:31:LYS:HD2    | 6:H:380:PRO:HG3   | 1.97                     | 0.47              |
| 1:A:393:VAL:O     | 1:A:397:VAL:HG13  | 2.15                     | 0.47              |
| 2:B:11:GLU:HG3    | 2:B:12:GLN:HG2    | 1.97                     | 0.47              |
| 2:B:272:THR:O     | 2:B:274:LYS:N     | 2.48                     | 0.47              |
| 3:C:58:ASN:OD1    | 3:C:107:GLN:HG2   | 2.14                     | 0.47              |
| 4:E:379:ALA:HB2   | 4:E:419:LEU:HD21  | 1.96                     | 0.47              |
| 6:G:31:GLN:HE21   | 6:G:321:PHE:N     | 2.13                     | 0.47              |
| 6:G:176:ASP:O     | 6:G:180:LEU:HD23  | 2.15                     | 0.47              |
| 6:G:344:SER:OG    | 6:G:383:SER:HB3   | 2.15                     | 0.47              |
| 7:L:307:CYS:HB2   | 7:L:334:HIS:ND1   | 2.30                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:M:28:PHE:CE1    | 2:O:418:ILE:HG13   | 2.49                     | 0.47              |
| 7:M:107:PRO:CG    | 7:M:108:PRO:CD     | 2.92                     | 0.47              |
| 2:O:603:GLU:HG3   | 2:O:611:LYS:CE     | 2.45                     | 0.47              |
| 8:P:60:PHE:CZ     | 8:P:88:LEU:HD11    | 2.49                     | 0.47              |
| 8:P:66:HIS:CD2    | 8:P:67:LEU:N       | 2.83                     | 0.47              |
| 8:P:835:ALA:O     | 8:P:839:THR:HG22   | 2.14                     | 0.47              |
| 1:S:36:ASN:ND2    | 1:S:39:ARG:HB2     | 2.30                     | 0.47              |
| 1:S:185:LEU:HD11  | 1:S:191:VAL:HG23   | 1.96                     | 0.47              |
| 1:S:940:GLN:HA    | 1:S:1013:GLY:HA2   | 1.97                     | 0.47              |
| 1:S:966:GLU:HA    | 1:S:974:ASP:OD1    | 2.14                     | 0.47              |
| 1:S:1303:LEU:HA   | 1:S:1306:PHE:CD2   | 2.50                     | 0.47              |
| 1:S:1336:TYR:CB   | 1:S:1395:LEU:HD11  | 2.45                     | 0.47              |
| 10:U:424:ASN:O    | 10:U:428:GLU:HG2   | 2.14                     | 0.47              |
| 10:U:832:LEU:HB3  | 10:U:838:PHE:CE2   | 2.50                     | 0.47              |
| 10:U:1081:ALA:HB3 | 10:U:1082:PRO:HD3  | 1.97                     | 0.47              |
| 11:V:60:LYS:NZ    | 11:V:63:GLU:HB3    | 2.28                     | 0.47              |
| 11:V:562:GLN:O    | 11:V:565:SER:OG    | 2.22                     | 0.47              |
| 1:A:747:ALA:O     | 1:A:750:VAL:HG22   | 2.14                     | 0.47              |
| 1:A:1299:LYS:NZ   | 1:A:1348:ILE:HD11  | 2.30                     | 0.47              |
| 1:A:1415:PHE:O    | 1:A:1418:VAL:HG22  | 2.15                     | 0.47              |
| 2:B:529:LYS:HG2   | 2:B:576:GLN:HG3    | 1.96                     | 0.47              |
| 2:B:655:PHE:CZ    | 2:B:722:ARG:HB3    | 2.50                     | 0.47              |
| 3:C:485:GLN:HG2   | 3:C:488:ARG:HH11   | 1.80                     | 0.47              |
| 4:E:149:SER:OG    | 4:E:151:GLU:OE2    | 2.33                     | 0.47              |
| 6:H:267:LEU:O     | 6:H:270:VAL:HG22   | 2.15                     | 0.47              |
| 7:L:107:PRO:N     | 7:L:108:PRO:HD2    | 2.30                     | 0.47              |
| 8:P:557:ASP:OD1   | 8:P:557:ASP:N      | 2.48                     | 0.47              |
| 11:V:175:LEU:O    | 11:V:178:SER:OG    | 2.19                     | 0.47              |
| 11:V:1038:ALA:HA  | 11:V:1041:ASN:HD21 | 1.80                     | 0.47              |
| 11:V:1054:GLU:HA  | 11:V:1057:ILE:HG12 | 1.96                     | 0.47              |
| 11:V:1105:GLN:NE2 | 11:V:1109:GLU:HG3  | 2.30                     | 0.47              |
| 1:A:963:PHE:HE1   | 1:A:980:ALA:HB2    | 1.80                     | 0.47              |
| 1:A:1085:LEU:HB3  | 1:A:1086:PRO:HD2   | 1.97                     | 0.47              |
| 1:A:1313:LEU:HA   | 1:A:1317:ARG:HG2   | 1.97                     | 0.47              |
| 2:B:146:HIS:CE1   | 2:B:151:PHE:HE2    | 2.33                     | 0.47              |
| 2:B:680:MET:HE1   | 2:B:696:ARG:HH11   | 1.80                     | 0.47              |
| 2:B:770:LEU:O     | 2:B:773:LEU:HB3    | 2.15                     | 0.47              |
| 6:G:16:TRP:CZ3    | 6:G:60:LEU:HD11    | 2.50                     | 0.47              |
| 6:G:117:GLY:O     | 6:G:121:LEU:HD23   | 2.15                     | 0.47              |
| 6:G:601:ARG:HD3   | 6:G:605:ARG:CZ     | 2.45                     | 0.47              |
| 8:P:288:LEU:HB2   | 8:P:311:CYS:HB3    | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:346:PRO:O     | 8:P:363:PRO:HD3   | 2.15                     | 0.47              |
| 8:P:712:ALA:H     | 8:P:782:ILE:CG2   | 2.28                     | 0.47              |
| 8:Q:366:LEU:O     | 8:Q:393:MET:HG2   | 2.15                     | 0.47              |
| 8:Q:569:VAL:HG11  | 8:Q:572:LEU:HD12  | 1.97                     | 0.47              |
| 8:Q:570:ASP:C     | 8:Q:572:LEU:H     | 2.18                     | 0.47              |
| 1:S:190:ILE:HG22  | 1:S:191:VAL:HG23  | 1.97                     | 0.47              |
| 1:S:337:SER:OG    | 1:S:428:VAL:HG11  | 2.15                     | 0.47              |
| 1:S:449:ALA:HB2   | 1:S:492:HIS:CE1   | 2.49                     | 0.47              |
| 1:S:929:TYR:CZ    | 1:S:933:LEU:HD21  | 2.50                     | 0.47              |
| 1:S:1083:LEU:HD11 | 1:S:1129:ASP:OD1  | 2.15                     | 0.47              |
| 1:S:1126:LEU:H    | 1:S:1169:SER:HB3  | 1.80                     | 0.47              |
| 10:U:179:SER:O    | 10:U:182:LYS:HE3  | 2.14                     | 0.47              |
| 10:U:446:ASN:ND2  | 11:V:355:ARG:HE   | 2.12                     | 0.47              |
| 1:A:61:LEU:HD12   | 1:A:77:VAL:CG2    | 2.44                     | 0.47              |
| 1:A:1142:CYS:SG   | 1:A:1143:LEU:N    | 2.88                     | 0.47              |
| 2:B:821:LYS:O     | 2:B:825:GLN:HG3   | 2.15                     | 0.47              |
| 4:E:106:ARG:NE    | 4:E:143:ASP:OD1   | 2.48                     | 0.47              |
| 6:H:12:CYS:SG     | 2:O:205:TYR:HD2   | 2.38                     | 0.47              |
| 6:H:564:ARG:HG3   | 6:H:565:ASP:H     | 1.79                     | 0.47              |
| 7:L:321:ASP:O     | 7:L:323:VAL:HG13  | 2.15                     | 0.47              |
| 8:P:148:ALA:O     | 8:P:180:PRO:HD2   | 2.15                     | 0.47              |
| 8:P:349:CYS:SG    | 8:P:401:ILE:HG22  | 2.55                     | 0.47              |
| 8:P:586:PRO:HB2   | 8:P:590:GLY:HA2   | 1.97                     | 0.47              |
| 8:P:717:ALA:HB3   | 8:P:815:GLN:HE22  | 1.79                     | 0.47              |
| 8:Q:28:VAL:HG12   | 8:Q:402:CYS:SG    | 2.55                     | 0.47              |
| 8:Q:324:ILE:HG12  | 8:Q:338:LEU:HD22  | 1.96                     | 0.47              |
| 8:Q:495:ALA:CB    | 8:Q:505:PRO:HG3   | 2.45                     | 0.47              |
| 1:S:360:ARG:O     | 1:S:364:VAL:HG23  | 2.15                     | 0.47              |
| 1:S:414:LEU:HD21  | 1:S:426:SER:HB2   | 1.96                     | 0.47              |
| 1:S:757:VAL:O     | 1:S:761:VAL:HG23  | 2.15                     | 0.47              |
| 1:S:929:TYR:O     | 1:S:933:LEU:HG    | 2.14                     | 0.47              |
| 1:S:1287:VAL:O    | 1:S:1291:ILE:HG12 | 2.15                     | 0.47              |
| 1:A:137:LEU:HB2   | 1:A:141:GLN:OE1   | 2.16                     | 0.46              |
| 1:A:469:ALA:O     | 1:A:473:LEU:HG    | 2.16                     | 0.46              |
| 1:A:875:LEU:HD11  | 1:A:945:ALA:HB1   | 1.96                     | 0.46              |
| 2:B:150:PHE:CE2   | 2:B:167:PHE:HB2   | 2.50                     | 0.46              |
| 2:B:228:ILE:HG22  | 2:B:229:ILE:H     | 1.80                     | 0.46              |
| 3:C:151:LYS:HE2   | 3:C:155:LEU:HD13  | 1.96                     | 0.46              |
| 4:E:491:LYS:NZ    | 11:V:202:ILE:O    | 2.45                     | 0.46              |
| 6:G:137:SER:HA    | 6:G:187:PRO:HG2   | 1.97                     | 0.46              |
| 6:G:398:LEU:HD22  | 6:G:458:LEU:HD12  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:G:606:ASP:HA     | 6:G:609:LEU:HB2   | 1.97                     | 0.46              |
| 2:O:592:LYS:HA     | 2:O:622:LEU:O     | 2.14                     | 0.46              |
| 2:O:734:LEU:O      | 2:O:737:ILE:HG22  | 2.14                     | 0.46              |
| 1:S:843:TYR:HA     | 1:S:846:CYS:SG    | 2.55                     | 0.46              |
| 10:U:15:ASP:OD2    | 10:U:16:LYS:NZ    | 2.42                     | 0.46              |
| 11:V:190:LYS:CD    | 11:V:190:LYS:H    | 2.27                     | 0.46              |
| 11:V:558:VAL:HG22  | 11:V:562:GLN:NE2  | 2.26                     | 0.46              |
| 1:A:494:LEU:CD1    | 1:A:518:LEU:HD12  | 2.46                     | 0.46              |
| 1:A:1030:LEU:HD22  | 1:S:1140:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:1069:LEU:HD12  | 1:A:1070:GLN:N    | 2.30                     | 0.46              |
| 2:B:231:PRO:HA     | 2:B:234:SER:HB3   | 1.95                     | 0.46              |
| 2:O:122:LEU:HD21   | 2:O:155:SER:HA    | 1.97                     | 0.46              |
| 2:O:482:VAL:HG13   | 2:O:584:LEU:HD11  | 1.96                     | 0.46              |
| 8:P:431:THR:O      | 8:P:431:THR:OG1   | 2.27                     | 0.46              |
| 8:P:479:ARG:HG3    | 8:P:479:ARG:NH2   | 2.30                     | 0.46              |
| 8:P:516:ARG:O      | 8:P:517:LEU:HD22  | 2.15                     | 0.46              |
| 1:S:218:CYS:HB3    | 1:S:294:ILE:HA    | 1.97                     | 0.46              |
| 1:S:553:LYS:O      | 1:S:557:VAL:HG12  | 2.14                     | 0.46              |
| 9:W:77:VAL:HB      | 9:W:85:PHE:CD2    | 2.50                     | 0.46              |
| 10:U:467:VAL:HG22  | 10:U:474:LEU:HD11 | 1.97                     | 0.46              |
| 11:V:1025:ASN:OD1  | 11:V:1026:HIS:N   | 2.48                     | 0.46              |
| 1:A:397:VAL:HG12   | 1:A:407:LEU:HD22  | 1.96                     | 0.46              |
| 2:B:622:LEU:HD23   | 2:B:622:LEU:HA    | 1.61                     | 0.46              |
| 3:C:162:ARG:HH12   | 3:C:166:LEU:HG    | 1.80                     | 0.46              |
| 6:G:534:LEU:HD12   | 6:G:538:LEU:HD23  | 1.96                     | 0.46              |
| 7:L:109:GLN:HE22   | 7:L:159:PRO:HG2   | 1.80                     | 0.46              |
| 7:M:57:TRP:CE2     | 8:Q:277:HIS:HB3   | 2.51                     | 0.46              |
| 8:Q:724:SER:OG     | 8:Q:725:GLY:N     | 2.48                     | 0.46              |
| 1:S:653:LEU:O      | 1:S:657:LEU:HG    | 2.15                     | 0.46              |
| 1:S:983:ILE:HA     | 1:S:986:ASN:HD22  | 1.80                     | 0.46              |
| 10:U:879:ARG:NH1   | 10:U:933:ALA:HB1  | 2.30                     | 0.46              |
| 11:V:72:GLN:NE2    | 11:V:138:LEU:HD21 | 2.30                     | 0.46              |
| 11:V:208:GLN:O     | 11:V:212:ILE:HG22 | 2.15                     | 0.46              |
| 11:V:1197:LEU:HD13 | 11:V:1270:MET:HG3 | 1.98                     | 0.46              |
| 2:B:17:CYS:O       | 2:B:17:CYS:SG     | 2.74                     | 0.46              |
| 7:M:146:ARG:HD3    | 7:M:205:ASP:OD2   | 2.15                     | 0.46              |
| 8:Q:243:CYS:SG     | 8:Q:251:CYS:HB2   | 2.56                     | 0.46              |
| 8:Q:655:PHE:HD1    | 8:Q:756:GLY:HA3   | 1.79                     | 0.46              |
| 1:S:185:LEU:HD21   | 1:S:191:VAL:HB    | 1.97                     | 0.46              |
| 1:S:1075:LEU:HD11  | 1:S:1115:GLU:HB3  | 1.97                     | 0.46              |
| 1:S:1299:LYS:HZ1   | 1:S:1348:ILE:HD11 | 1.80                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:U:871:PHE:HE2  | 10:U:929:GLN:HE21  | 1.64                     | 0.46              |
| 10:U:1054:HIS:CD2 | 10:U:1151:THR:HG22 | 2.51                     | 0.46              |
| 10:U:1056:HIS:CE1 | 10:U:1069:THR:HG22 | 2.50                     | 0.46              |
| 10:U:1086:LEU:O   | 10:U:1089:LEU:HG   | 2.15                     | 0.46              |
| 11:V:485:ASN:OD1  | 11:V:485:ASN:N     | 2.48                     | 0.46              |
| 11:V:652:VAL:O    | 11:V:656:ILE:HG12  | 2.16                     | 0.46              |
| 11:V:1021:THR:OG1 | 11:V:1022:PRO:HD3  | 2.14                     | 0.46              |
| 2:B:711:THR:O     | 2:B:711:THR:OG1    | 2.33                     | 0.46              |
| 2:B:723:ASN:OD1   | 2:B:723:ASN:N      | 2.46                     | 0.46              |
| 4:E:400:SER:HA    | 4:E:440:GLN:HE22   | 1.79                     | 0.46              |
| 5:F:42:ARG:NH2    | 5:F:127:GLU:O      | 2.49                     | 0.46              |
| 7:M:98:ARG:HG2    | 7:M:101:LEU:HD12   | 1.98                     | 0.46              |
| 8:P:150:TRP:CD2   | 8:P:178:TYR:HE2    | 2.33                     | 0.46              |
| 8:P:223:ALA:HB1   | 8:P:328:TRP:HZ3    | 1.80                     | 0.46              |
| 8:P:778:PRO:HD3   | 8:P:824:ASP:O      | 2.15                     | 0.46              |
| 1:S:174:GLN:HA    | 1:S:177:LEU:HD12   | 1.97                     | 0.46              |
| 1:S:1292:LEU:O    | 1:S:1296:GLU:HG2   | 2.16                     | 0.46              |
| 10:U:87:SER:HB2   | 11:V:560:ARG:NH2   | 2.31                     | 0.46              |
| 1:A:897:HIS:ND1   | 1:A:898:LEU:HG     | 2.30                     | 0.46              |
| 3:C:553:GLU:O     | 3:C:556:THR:OG1    | 2.26                     | 0.46              |
| 6:G:261:ASN:HB3   | 1:S:63:GLU:OE1     | 2.16                     | 0.46              |
| 6:H:13:LEU:HD23   | 6:H:14:ASP:H       | 1.81                     | 0.46              |
| 6:H:21:ASP:OD1    | 6:H:195:LEU:HD13   | 2.16                     | 0.46              |
| 6:H:558:LEU:HD11  | 6:H:567:ALA:HB2    | 1.98                     | 0.46              |
| 8:Q:92:HIS:CE1    | 8:Q:116:ILE:HD13   | 2.51                     | 0.46              |
| 1:S:584:LEU:O     | 1:S:588:LEU:HG     | 2.16                     | 0.46              |
| 1:S:600:ARG:O     | 1:S:604:ILE:HG12   | 2.16                     | 0.46              |
| 10:U:356:HIS:ND1  | 10:U:356:HIS:O     | 2.48                     | 0.46              |
| 10:U:642:LEU:O    | 10:U:644:PRO:HD3   | 2.14                     | 0.46              |
| 10:U:1036:HIS:HE1 | 10:U:1042:PRO:HA   | 1.80                     | 0.46              |
| 11:V:342:CYS:SG   | 11:V:343:ILE:N     | 2.88                     | 0.46              |
| 11:V:358:LYS:HD3  | 11:V:358:LYS:HA    | 1.61                     | 0.46              |
| 11:V:794:ARG:HG2  | 11:V:928:LEU:HD11  | 1.97                     | 0.46              |
| 7:M:118:ILE:HD11  | 7:M:126:LEU:HB2    | 1.97                     | 0.46              |
| 2:O:249:LYS:HB3   | 2:O:250:ASN:H      | 1.62                     | 0.46              |
| 1:S:517:ARG:O     | 1:S:521:LEU:HG     | 2.15                     | 0.46              |
| 1:S:937:LEU:HA    | 1:S:1014:ASN:ND2   | 2.31                     | 0.46              |
| 11:V:384:MET:HA   | 11:V:384:MET:HE2   | 1.98                     | 0.46              |
| 1:A:415:MET:CE    | 1:A:427:MET:HA     | 2.41                     | 0.46              |
| 1:A:486:PRO:HG2   | 1:A:489:LEU:HB2    | 1.98                     | 0.46              |
| 4:E:291:LEU:HD23  | 4:E:312:GLU:HB3    | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:538:LEU:HD12  | 6:H:539:LEU:HG    | 1.96                     | 0.46              |
| 7:L:169:PHE:CZ    | 7:L:173:PHE:HB2   | 2.51                     | 0.46              |
| 7:L:322:GLN:O     | 7:L:333:PHE:N     | 2.48                     | 0.46              |
| 2:O:66:THR:O      | 2:O:68:LYS:NZ     | 2.48                     | 0.46              |
| 2:O:141:LEU:HD21  | 2:O:217:LEU:HD21  | 1.97                     | 0.46              |
| 8:P:220:LEU:HD13  | 8:P:224:LEU:CD2   | 2.46                     | 0.46              |
| 8:P:448:THR:O     | 8:P:450:SER:N     | 2.48                     | 0.46              |
| 8:P:538:ASP:HA    | 8:P:571:GLN:HA    | 1.97                     | 0.46              |
| 8:P:655:PHE:N     | 8:P:655:PHE:CD1   | 2.81                     | 0.46              |
| 1:S:149:LEU:HD12  | 1:S:190:ILE:HG13  | 1.97                     | 0.46              |
| 10:U:102:GLY:HA3  | 10:U:144:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:196:LEU:HD23  | 1:A:196:LEU:HA    | 1.72                     | 0.46              |
| 1:A:818:PHE:HA    | 1:A:821:LEU:HD12  | 1.97                     | 0.46              |
| 6:H:79:ILE:CG1    | 6:H:145:LEU:HD21  | 2.46                     | 0.46              |
| 2:O:780:HIS:ND1   | 2:O:830:VAL:HG13  | 2.31                     | 0.46              |
| 8:P:28:VAL:N      | 8:P:400:ASN:HD21  | 2.14                     | 0.46              |
| 1:S:460:ARG:HA    | 1:S:463:HIS:NE2   | 2.31                     | 0.46              |
| 1:S:758:LEU:O     | 1:S:762:LEU:HG    | 2.16                     | 0.46              |
| 10:U:298:GLN:NE2  | 10:U:1104:THR:O   | 2.49                     | 0.46              |
| 10:U:1266:HIS:HA  | 10:U:1269:LYS:HE3 | 1.98                     | 0.46              |
| 11:V:83:LEU:O     | 11:V:92:ILE:HD11  | 2.16                     | 0.46              |
| 11:V:282:ILE:O    | 11:V:286:LEU:HG   | 2.15                     | 0.46              |
| 11:V:766:GLU:HG2  | 11:V:767:PRO:HD2  | 1.98                     | 0.46              |
| 1:A:474:PHE:HA    | 1:A:477:LEU:HB2   | 1.98                     | 0.46              |
| 2:B:605:GLU:HG3   | 2:B:606:SER:N     | 2.31                     | 0.46              |
| 7:M:3:VAL:CG2     | 7:M:5:GLU:HG2     | 2.46                     | 0.46              |
| 2:O:179:LEU:HD22  | 2:O:223:LEU:HD11  | 1.98                     | 0.46              |
| 8:Q:54:LEU:HD11   | 8:Q:114:PRO:HB2   | 1.97                     | 0.46              |
| 1:S:206:VAL:O     | 1:S:210:LEU:HG    | 2.16                     | 0.46              |
| 1:S:552:GLU:O     | 1:S:556:MET:HG2   | 2.16                     | 0.46              |
| 10:U:187:THR:HG22 | 10:U:190:GLU:HG3  | 1.97                     | 0.46              |
| 10:U:295:VAL:O    | 10:U:297:GLN:N    | 2.46                     | 0.46              |
| 10:U:430:PHE:O    | 10:U:437:ARG:NE   | 2.44                     | 0.46              |
| 11:V:220:GLY:H    | 11:V:223:GLN:HE22 | 1.63                     | 0.46              |
| 1:A:1335:PHE:CD2  | 1:A:1360:MET:HG2  | 2.51                     | 0.45              |
| 4:E:292:GLN:O     | 4:E:296:LYS:HG2   | 2.16                     | 0.45              |
| 4:E:489:TYR:CE2   | 4:E:493:MET:HG3   | 2.51                     | 0.45              |
| 5:F:142:ALA:O     | 5:F:146:LEU:HD23  | 2.16                     | 0.45              |
| 7:L:295:ARG:HB3   | 7:L:298:LEU:HG    | 1.98                     | 0.45              |
| 7:L:320:PRO:HB2   | 7:L:332:PRO:HB2   | 1.98                     | 0.45              |
| 2:O:10:ASN:ND2    | 2:O:74:LEU:HB2    | 2.31                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:210:THR:CG2    | 2:O:228:ILE:HB     | 2.46                     | 0.45              |
| 2:O:345:PHE:HE2    | 2:O:358:LYS:HB2    | 1.80                     | 0.45              |
| 8:P:322:LEU:HA     | 8:P:339:ARG:O      | 2.16                     | 0.45              |
| 8:Q:589:ASN:HD22   | 8:Q:675:PRO:HD3    | 1.80                     | 0.45              |
| 1:S:862:PRO:O      | 1:S:866:LYS:HG2    | 2.15                     | 0.45              |
| 1:S:877:SER:HA     | 1:S:880:ARG:HE     | 1.80                     | 0.45              |
| 11:V:686:LEU:HD12  | 11:V:757:ASP:HA    | 1.98                     | 0.45              |
| 11:V:1088:TYR:CE1  | 11:V:1107:LEU:HD13 | 2.51                     | 0.45              |
| 11:V:1313:LEU:O    | 11:V:1317:PHE:HB2  | 2.16                     | 0.45              |
| 1:A:1272:HIS:CE1   | 1:A:1333:PHE:HE2   | 2.34                     | 0.45              |
| 2:B:857:SER:OG     | 8:P:867:LEU:HD13   | 2.16                     | 0.45              |
| 4:E:338:ASP:N      | 4:E:338:ASP:OD1    | 2.46                     | 0.45              |
| 4:E:429:LEU:HB3    | 4:E:460:ARG:NH1    | 2.31                     | 0.45              |
| 4:E:506:GLU:OE2    | 4:E:509:ARG:NH2    | 2.40                     | 0.45              |
| 6:G:483:LEU:HD21   | 6:G:512:LEU:HD23   | 1.99                     | 0.45              |
| 2:O:7:MET:N        | 2:O:13:GLU:O       | 2.48                     | 0.45              |
| 8:P:767:ILE:HG12   | 8:P:788:GLN:HB3    | 1.97                     | 0.45              |
| 8:Q:125:LEU:HD23   | 8:Q:166:PRO:HB3    | 1.99                     | 0.45              |
| 10:U:66:ARG:HG3    | 10:U:104:LEU:HD22  | 1.98                     | 0.45              |
| 10:U:295:VAL:CG2   | 10:U:301:SER:HA    | 2.46                     | 0.45              |
| 11:V:71:ASP:OD1    | 11:V:72:GLN:N      | 2.48                     | 0.45              |
| 11:V:728:LEU:HD23  | 11:V:840:LEU:HD21  | 1.97                     | 0.45              |
| 11:V:1246:VAL:O    | 11:V:1249:ILE:HG22 | 2.17                     | 0.45              |
| 11:V:1375:LEU:HD12 | 11:V:1376:THR:N    | 2.32                     | 0.45              |
| 1:A:299:PHE:CD1    | 1:A:358:LEU:HD13   | 2.51                     | 0.45              |
| 1:A:477:LEU:HD23   | 1:A:480:LEU:HD12   | 1.98                     | 0.45              |
| 1:A:746:ALA:O      | 1:A:750:VAL:HG13   | 2.16                     | 0.45              |
| 1:A:1234:ILE:O     | 1:A:1237:VAL:HG12  | 2.15                     | 0.45              |
| 1:A:1326:GLN:O     | 1:A:1330:LEU:HD13  | 2.15                     | 0.45              |
| 2:B:78:CYS:SG      | 2:B:136:VAL:HG23   | 2.55                     | 0.45              |
| 2:B:764:GLU:O      | 2:B:768:VAL:HG23   | 2.15                     | 0.45              |
| 3:C:227:ILE:HD11   | 3:C:239:VAL:HG12   | 1.98                     | 0.45              |
| 5:F:341:VAL:HG13   | 5:F:342:PRO:HD2    | 1.97                     | 0.45              |
| 6:G:430:LYS:HE2    | 8:P:332:GLY:HA2    | 1.98                     | 0.45              |
| 7:M:254:LEU:HD22   | 7:M:321:ASP:HB2    | 1.98                     | 0.45              |
| 2:O:57:PHE:CG      | 2:O:354:LEU:HD21   | 2.51                     | 0.45              |
| 2:O:767:LEU:HB3    | 8:Q:841:LEU:HB2    | 1.97                     | 0.45              |
| 8:P:572:LEU:HA     | 8:P:578:ARG:NH2    | 2.32                     | 0.45              |
| 8:P:713:GLU:HB3    | 8:P:782:ILE:HD11   | 1.97                     | 0.45              |
| 8:Q:572:LEU:O      | 8:Q:572:LEU:HD23   | 2.17                     | 0.45              |
| 8:Q:848:ARG:O      | 8:Q:851:LEU:HG     | 2.16                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:U:214:VAL:O     | 10:U:218:LEU:HD23  | 2.15                     | 0.45              |
| 10:U:395:PRO:HD2   | 10:U:458:HIS:CE1   | 2.51                     | 0.45              |
| 10:U:653:THR:HG23  | 10:U:658:ILE:HB    | 1.97                     | 0.45              |
| 10:U:751:GLU:O     | 10:U:754:ILE:HB    | 2.16                     | 0.45              |
| 11:V:646:PRO:O     | 11:V:649:LEU:HB2   | 2.17                     | 0.45              |
| 1:A:171:TRP:CE3    | 1:A:200:HIS:HD2    | 2.34                     | 0.45              |
| 1:A:424:LEU:O      | 1:A:428:VAL:HG23   | 2.16                     | 0.45              |
| 1:A:856:LEU:HA     | 1:A:859:CYS:SG     | 2.56                     | 0.45              |
| 2:B:31:ASN:O       | 2:B:38:THR:N       | 2.50                     | 0.45              |
| 2:B:252:LEU:HD13   | 2:B:254:ILE:HG23   | 1.96                     | 0.45              |
| 5:F:246:GLU:O      | 5:F:249:ALA:HB3    | 2.16                     | 0.45              |
| 6:G:228:ALA:O      | 6:G:232:LEU:HD23   | 2.16                     | 0.45              |
| 6:G:266:LEU:HD23   | 1:S:55:GLN:HB2     | 1.97                     | 0.45              |
| 2:O:181:MET:CB     | 2:O:217:LEU:HD23   | 2.46                     | 0.45              |
| 2:O:217:LEU:HD12   | 2:O:217:LEU:HA     | 1.70                     | 0.45              |
| 8:P:851:LEU:HD21   | 8:P:862:THR:HG21   | 1.99                     | 0.45              |
| 10:U:706:LEU:HA    | 10:U:709:ILE:HD12  | 1.97                     | 0.45              |
| 1:A:824:CYS:SG     | 1:A:825:ARG:N      | 2.89                     | 0.45              |
| 1:A:1408:PRO:O     | 1:A:1439:ARG:NH1   | 2.50                     | 0.45              |
| 1:A:1433:SER:O     | 1:A:1436:LEU:HG    | 2.16                     | 0.45              |
| 2:B:524:GLN:OE1    | 2:B:581:VAL:HG13   | 2.16                     | 0.45              |
| 6:G:177:LEU:HB2    | 6:G:211:PHE:CE2    | 2.52                     | 0.45              |
| 8:P:287:ALA:HA     | 8:P:311:CYS:O      | 2.16                     | 0.45              |
| 8:P:305:GLU:O      | 8:P:307:VAL:HG23   | 2.17                     | 0.45              |
| 1:S:402:GLU:OE2    | 1:S:405:GLN:NE2    | 2.38                     | 0.45              |
| 10:U:533:ARG:NE    | 10:U:597:GLN:HE22  | 2.14                     | 0.45              |
| 10:U:1010:THR:HG21 | 10:U:1031:LEU:HD21 | 1.99                     | 0.45              |
| 11:V:634:GLU:OE2   | 11:V:634:GLU:HA    | 2.16                     | 0.45              |
| 11:V:933:PHE:HB2   | 11:V:1019:LEU:HD13 | 1.98                     | 0.45              |
| 1:A:680:ILE:HG12   | 1:A:683:ARG:HH22   | 1.80                     | 0.45              |
| 2:B:73:HIS:HB3     | 2:B:99:ASN:HB3     | 1.97                     | 0.45              |
| 2:B:298:PHE:HE1    | 2:B:312:TRP:CD1    | 2.35                     | 0.45              |
| 2:B:707:TRP:CH2    | 2:B:715:GLY:HA3    | 2.51                     | 0.45              |
| 3:C:227:ILE:HD13   | 3:C:239:VAL:HG12   | 1.97                     | 0.45              |
| 6:G:424:THR:O      | 6:G:428:LEU:HG     | 2.16                     | 0.45              |
| 7:M:29:ILE:HD11    | 7:M:88:LYS:HZ2     | 1.80                     | 0.45              |
| 7:M:233:ASN:ND2    | 7:M:330:GLY:O      | 2.50                     | 0.45              |
| 8:P:66:HIS:HD2     | 8:P:67:LEU:N       | 2.14                     | 0.45              |
| 8:Q:538:ASP:HA     | 8:Q:571:GLN:HA     | 1.99                     | 0.45              |
| 1:S:113:SER:O      | 1:S:117:VAL:HG23   | 2.16                     | 0.45              |
| 1:S:813:PRO:HB2    | 1:S:815:PRO:HG2    | 1.98                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:U:291:LYS:HA   | 10:U:294:LYS:HE2   | 1.98                     | 0.45              |
| 10:U:456:ILE:O    | 10:U:460:LEU:HD12  | 2.17                     | 0.45              |
| 2:B:107:TYR:OH    | 2:B:130:MET:HG3    | 2.16                     | 0.45              |
| 2:B:242:ILE:HG22  | 2:B:243:CYS:N      | 2.32                     | 0.45              |
| 2:B:266:ILE:HD12  | 2:B:268:PHE:CZ     | 2.52                     | 0.45              |
| 2:B:669:LEU:HD12  | 2:B:669:LEU:HA     | 1.66                     | 0.45              |
| 3:C:49:TYR:CZ     | 3:C:53:LYS:HD3     | 2.52                     | 0.45              |
| 3:C:122:LEU:O     | 5:F:140:ARG:CZ     | 2.65                     | 0.45              |
| 3:C:330:SER:O     | 3:C:330:SER:OG     | 2.31                     | 0.45              |
| 6:G:273:LEU:HD23  | 6:G:279:TRP:HB2    | 1.99                     | 0.45              |
| 6:H:461:GLN:HG2   | 6:H:596:TYR:HE1    | 1.81                     | 0.45              |
| 2:O:184:LEU:HD11  | 2:O:242:ILE:HD11   | 1.97                     | 0.45              |
| 2:O:508:LEU:HD12  | 2:O:523:CYS:SG     | 2.56                     | 0.45              |
| 8:Q:328:TRP:HB3   | 8:Q:334:LEU:HD13   | 1.98                     | 0.45              |
| 1:S:795:ARG:HA    | 1:S:798:LEU:HD12   | 1.99                     | 0.45              |
| 1:S:947:SER:OG    | 1:S:948:ASP:N      | 2.49                     | 0.45              |
| 10:U:306:SER:H    | 10:U:309:SER:HB3   | 1.80                     | 0.45              |
| 11:V:637:ASN:C    | 11:V:641:HIS:ND1   | 2.63                     | 0.45              |
| 1:A:651:GLY:O     | 1:A:654:THR:OG1    | 2.35                     | 0.45              |
| 1:A:1017:ILE:O    | 1:A:1021:LEU:HG    | 2.17                     | 0.45              |
| 2:B:657:LYS:HD2   | 2:B:720:TYR:CE2    | 2.52                     | 0.45              |
| 6:G:342:THR:HG22  | 6:G:343:GLN:N      | 2.32                     | 0.45              |
| 8:P:763:ASN:O     | 8:P:791:SER:HB2    | 2.16                     | 0.45              |
| 8:Q:424:SER:OG    | 8:Q:428:ARG:HB2    | 2.17                     | 0.45              |
| 1:S:151:PHE:O     | 1:S:155:LEU:HG     | 2.17                     | 0.45              |
| 1:S:358:LEU:O     | 1:S:362:LEU:HG     | 2.17                     | 0.45              |
| 1:S:616:SER:O     | 1:S:620:THR:HG23   | 2.16                     | 0.45              |
| 10:U:12:LYS:HA    | 10:U:12:LYS:HD2    | 1.81                     | 0.45              |
| 10:U:460:LEU:HD12 | 10:U:460:LEU:H     | 1.82                     | 0.45              |
| 10:U:658:ILE:HG23 | 10:U:737:ILE:HG21  | 1.99                     | 0.45              |
| 10:U:969:LEU:O    | 10:U:972:SER:OG    | 2.25                     | 0.45              |
| 11:V:1128:PHE:HB2 | 11:V:1177:ILE:HG12 | 1.99                     | 0.45              |
| 11:V:1227:THR:OG1 | 11:V:1228:ARG:N    | 2.49                     | 0.45              |
| 11:V:1291:LEU:O   | 11:V:1295:LEU:HD13 | 2.17                     | 0.45              |
| 11:V:1299:ARG:NH1 | 11:V:1359:LEU:HD12 | 2.28                     | 0.45              |
| 6:G:60:LEU:HD12   | 6:G:66:VAL:HG21    | 1.99                     | 0.45              |
| 7:L:272:HIS:CE1   | 7:L:273:LEU:HG     | 2.52                     | 0.45              |
| 7:M:239:GLU:O     | 7:M:249:PRO:HB2    | 2.16                     | 0.45              |
| 7:M:307:CYS:CB    | 7:M:310:CYS:SG     | 3.04                     | 0.45              |
| 2:O:175:GLU:HA    | 2:O:180:GLY:O      | 2.16                     | 0.45              |
| 1:S:558:PHE:HD1   | 1:S:564:ILE:H      | 1.63                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:995:SER:HA    | 1:S:998:TYR:CE2   | 2.52                     | 0.45              |
| 10:U:36:GLN:HB2   | 10:U:81:LEU:HD22  | 1.99                     | 0.45              |
| 1:A:265:VAL:O     | 1:A:269:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:1080:ARG:CZ   | 1:S:952:GLN:HB2   | 2.47                     | 0.45              |
| 1:A:1416:SER:OG   | 1:A:1417:HIS:ND1  | 2.41                     | 0.45              |
| 2:B:521:LEU:HD23  | 2:B:521:LEU:C     | 2.37                     | 0.45              |
| 2:B:522:LYS:HE2   | 8:P:563:ILE:HG21  | 1.99                     | 0.45              |
| 5:F:23:VAL:HG13   | 5:F:26:TRP:CD1    | 2.53                     | 0.45              |
| 2:O:356:SER:HA    | 2:O:369:SER:OG    | 2.17                     | 0.45              |
| 8:Q:150:TRP:HE1   | 8:Q:180:PRO:HG3   | 1.82                     | 0.45              |
| 1:S:494:LEU:HD11  | 1:S:518:LEU:HD11  | 1.99                     | 0.45              |
| 1:S:576:ARG:N     | 1:S:577:PRO:HD2   | 2.32                     | 0.45              |
| 1:S:803:VAL:HA    | 9:W:4:UNK:HA      | 1.98                     | 0.45              |
| 1:S:932:TRP:CE3   | 1:S:933:LEU:HD23  | 2.51                     | 0.45              |
| 10:U:413:MET:SD   | 10:U:417:HIS:CD2  | 3.09                     | 0.45              |
| 11:V:60:LYS:CE    | 11:V:61:THR:HG22  | 2.47                     | 0.45              |
| 11:V:546:GLU:N    | 11:V:546:GLU:OE1  | 2.50                     | 0.45              |
| 11:V:555:MET:HA   | 11:V:558:VAL:HG12 | 1.98                     | 0.45              |
| 11:V:678:PHE:HB3  | 11:V:763:THR:OG1  | 2.17                     | 0.45              |
| 1:A:191:VAL:HG12  | 1:A:192:SER:N     | 2.32                     | 0.44              |
| 2:B:520:LEU:HD21  | 8:P:565:TYR:CD2   | 2.52                     | 0.44              |
| 4:E:469:PHE:O     | 4:E:473:MET:HG2   | 2.17                     | 0.44              |
| 6:G:152:SER:OG    | 6:G:328:LEU:HD23  | 2.17                     | 0.44              |
| 6:G:392:CYS:SG    | 6:G:395:GLU:HG3   | 2.57                     | 0.44              |
| 2:O:290:MET:HE1   | 2:O:341:VAL:HB    | 1.98                     | 0.44              |
| 8:P:158:PRO:HD2   | 8:P:165:ARG:O     | 2.16                     | 0.44              |
| 8:Q:39:THR:OG1    | 8:Q:41:SER:OG     | 2.23                     | 0.44              |
| 8:Q:315:PHE:CZ    | 8:Q:321:MET:SD    | 3.11                     | 0.44              |
| 8:Q:735:TRP:CH2   | 8:Q:811:MET:HB2   | 2.52                     | 0.44              |
| 1:S:936:GLU:OE2   | 1:S:1014:ASN:ND2  | 2.50                     | 0.44              |
| 10:U:882:LEU:HD13 | 10:U:934:LEU:HD22 | 1.98                     | 0.44              |
| 11:V:364:TRP:HZ2  | 11:V:380:PHE:HE1  | 1.65                     | 0.44              |
| 11:V:414:GLU:O    | 11:V:417:LEU:N    | 2.50                     | 0.44              |
| 1:A:182:VAL:HG23  | 1:A:196:LEU:HD12  | 1.98                     | 0.44              |
| 2:B:259:LEU:N     | 2:B:259:LEU:HD23  | 2.32                     | 0.44              |
| 4:E:409:ALA:O     | 4:E:412:THR:OG1   | 2.35                     | 0.44              |
| 5:F:6:GLN:O       | 5:F:10:ARG:HB2    | 2.16                     | 0.44              |
| 7:L:116:GLU:O     | 7:L:120:THR:HG23  | 2.16                     | 0.44              |
| 7:M:170:PRO:HG3   | 7:M:200:PHE:CE2   | 2.52                     | 0.44              |
| 2:O:134:LEU:CD1   | 2:O:142:ILE:HG23  | 2.47                     | 0.44              |
| 8:P:655:PHE:CZ    | 8:P:754:ILE:HD12  | 2.53                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:P:708:ILE:O      | 8:P:786:GLU:HA    | 2.17                     | 0.44              |
| 1:S:290:SER:C      | 1:S:292:HIS:H     | 2.21                     | 0.44              |
| 1:S:1302:TRP:HH2   | 1:S:1348:ILE:HD13 | 1.80                     | 0.44              |
| 10:U:395:PRO:HG2   | 10:U:455:PRO:HB2  | 1.99                     | 0.44              |
| 11:V:676:PHE:CD2   | 11:V:680:VAL:HG21 | 2.51                     | 0.44              |
| 11:V:752:ILE:O     | 11:V:754:GLY:N    | 2.50                     | 0.44              |
| 11:V:1077:GLY:O    | 11:V:1083:ASN:ND2 | 2.46                     | 0.44              |
| 11:V:1259:GLN:HG2  | 11:V:1260:ILE:H   | 1.82                     | 0.44              |
| 1:A:769:LEU:HD21   | 1:A:784:LEU:HD22  | 1.99                     | 0.44              |
| 2:B:73:HIS:CB      | 2:B:99:ASN:HB3    | 2.47                     | 0.44              |
| 5:F:188:PHE:CZ     | 5:F:192:LEU:HD11  | 2.53                     | 0.44              |
| 7:M:271:ILE:HD12   | 7:M:271:ILE:HA    | 1.89                     | 0.44              |
| 7:M:337:CYS:O      | 7:M:340:GLU:HG3   | 2.17                     | 0.44              |
| 2:O:344:LEU:HD11   | 2:O:354:LEU:HD12  | 2.00                     | 0.44              |
| 2:O:477:LYS:HG3    | 2:O:478:ILE:H     | 1.82                     | 0.44              |
| 8:P:255:LEU:O      | 8:P:256:LYS:C     | 2.54                     | 0.44              |
| 8:P:335:VAL:HG13   | 8:P:336:PRO:HD2   | 2.00                     | 0.44              |
| 8:P:648:ASP:O      | 8:P:650:LEU:N     | 2.45                     | 0.44              |
| 1:S:981:CYS:HB3    | 1:S:1021:LEU:HD11 | 1.99                     | 0.44              |
| 1:S:1053:ARG:HH11  | 1:S:1111:LEU:HD22 | 1.81                     | 0.44              |
| 10:U:357:ARG:HH22  | 10:U:1101:TRP:HZ2 | 1.66                     | 0.44              |
| 11:V:922:HIS:CD2   | 11:V:923:ALA:HB2  | 2.53                     | 0.44              |
| 11:V:937:HIS:CD2   | 11:V:1023:MET:HG2 | 2.52                     | 0.44              |
| 1:A:332:PRO:HB2    | 1:A:335:LYS:HE3   | 1.99                     | 0.44              |
| 1:A:494:LEU:HD13   | 1:A:518:LEU:HD12  | 1.98                     | 0.44              |
| 1:A:1322:VAL:HG13  | 1:A:1323:ALA:H    | 1.82                     | 0.44              |
| 4:E:21:GLN:OE1     | 4:E:21:GLN:N      | 2.50                     | 0.44              |
| 4:E:79:GLY:CA      | 7:L:73:ARG:HH22   | 2.31                     | 0.44              |
| 5:F:112:VAL:HA     | 5:F:115:LEU:HD12  | 2.00                     | 0.44              |
| 6:G:296:THR:O      | 6:G:300:LEU:HG    | 2.17                     | 0.44              |
| 6:G:483:LEU:HD23   | 6:G:513:ARG:HA    | 1.98                     | 0.44              |
| 2:O:685:ILE:HD13   | 2:O:691:VAL:HG23  | 2.00                     | 0.44              |
| 8:Q:195:PRO:HB3    | 8:Q:246:PRO:HD3   | 1.98                     | 0.44              |
| 8:Q:511:SER:HB2    | 8:Q:526:THR:OG1   | 2.17                     | 0.44              |
| 1:S:456:PHE:CE1    | 1:S:496:PRO:HB2   | 2.52                     | 0.44              |
| 1:S:776:LEU:HD23   | 1:S:781:VAL:HG12  | 2.00                     | 0.44              |
| 1:S:780:HIS:NE2    | 9:W:88:THR:O      | 2.32                     | 0.44              |
| 10:U:71:CYS:O      | 10:U:74:GLN:HG3   | 2.18                     | 0.44              |
| 11:V:78:LYS:HD2    | 11:V:81:GLN:NE2   | 2.31                     | 0.44              |
| 11:V:1227:THR:HG23 | 11:V:1230:THR:H   | 1.83                     | 0.44              |
| 4:E:357:LEU:HD13   | 4:E:397:PRO:HG3   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:G:558:LEU:HD22  | 6:G:566:GLU:OE1    | 2.18                     | 0.44              |
| 7:M:307:CYS:SG    | 7:M:334:HIS:N      | 2.91                     | 0.44              |
| 2:O:624:LEU:HA    | 2:O:624:LEU:HD12   | 1.69                     | 0.44              |
| 8:P:543:LEU:HD23  | 8:P:567:ILE:HD11   | 2.00                     | 0.44              |
| 8:P:734:GLN:HE22  | 8:P:747:ARG:CB     | 2.30                     | 0.44              |
| 8:Q:405:VAL:HG12  | 8:Q:407:LEU:HG     | 2.00                     | 0.44              |
| 8:Q:589:ASN:ND2   | 8:Q:671:PRO:HB2    | 2.32                     | 0.44              |
| 1:S:145:LEU:O     | 1:S:149:LEU:HD23   | 2.17                     | 0.44              |
| 1:S:171:TRP:CZ2   | 1:S:196:LEU:HG     | 2.52                     | 0.44              |
| 11:V:1292:HIS:CD2 | 11:V:1352:ARG:HG2  | 2.53                     | 0.44              |
| 1:A:58:ASN:O      | 1:A:62:LEU:HG      | 2.17                     | 0.44              |
| 1:A:179:LEU:HD11  | 1:A:238:PHE:CZ     | 2.53                     | 0.44              |
| 1:A:1117:ARG:HB3  | 1:A:1165:LEU:HD21  | 1.99                     | 0.44              |
| 2:B:673:LYS:HD3   | 2:B:673:LYS:N      | 2.31                     | 0.44              |
| 3:C:246:HIS:CG    | 3:C:246:HIS:O      | 2.69                     | 0.44              |
| 6:G:175:LYS:HD3   | 6:G:175:LYS:HA     | 1.52                     | 0.44              |
| 6:G:232:LEU:HD12  | 6:G:248:VAL:HG13   | 1.99                     | 0.44              |
| 6:H:214:ARG:HG2   | 6:H:330:PRO:HD3    | 1.99                     | 0.44              |
| 7:M:15:LEU:HA     | 7:M:15:LEU:HD23    | 1.75                     | 0.44              |
| 8:Q:226:GLY:HA2   | 8:Q:234:THR:OG1    | 2.18                     | 0.44              |
| 10:U:154:GLU:OE2  | 10:U:155:GLU:HG2   | 2.18                     | 0.44              |
| 10:U:496:VAL:HG12 | 10:U:500:LEU:HD12  | 2.00                     | 0.44              |
| 10:U:505:PRO:HA   | 10:U:508:LYS:HG3   | 2.00                     | 0.44              |
| 10:U:959:ILE:HG21 | 10:U:1006:MET:SD   | 2.57                     | 0.44              |
| 10:U:1010:THR:CG2 | 10:U:1031:LEU:HD21 | 2.48                     | 0.44              |
| 11:V:211:ILE:HG13 | 11:V:212:ILE:N     | 2.33                     | 0.44              |
| 11:V:1354:THR:HA  | 11:V:1357:VAL:HG23 | 1.99                     | 0.44              |
| 1:A:1209:ASP:O    | 1:A:1212:SER:OG    | 2.36                     | 0.44              |
| 6:H:80:LEU:HD12   | 6:H:197:LEU:HD11   | 1.99                     | 0.44              |
| 6:H:567:ALA:O     | 6:H:571:TRP:HD1    | 2.01                     | 0.44              |
| 2:O:284:PRO:HA    | 2:O:303:PHE:HA     | 2.00                     | 0.44              |
| 8:Q:602:LEU:HD23  | 8:Q:602:LEU:HA     | 1.91                     | 0.44              |
| 1:S:153:GLN:O     | 1:S:156:LEU:HG     | 2.18                     | 0.44              |
| 1:S:815:PRO:HB3   | 1:S:861:SER:HB3    | 2.00                     | 0.44              |
| 1:S:853:ARG:HB3   | 1:S:855:THR:HG23   | 2.00                     | 0.44              |
| 10:U:643:PRO:HB3  | 10:U:720:ASP:HB3   | 1.99                     | 0.44              |
| 10:U:658:ILE:CD1  | 10:U:738:LYS:HE3   | 2.47                     | 0.44              |
| 10:U:1251:PRO:HA  | 10:U:1254:ILE:HG12 | 1.99                     | 0.44              |
| 1:A:284:GLY:O     | 1:A:286:GLN:NE2    | 2.51                     | 0.44              |
| 1:A:386:TRP:CH2   | 1:A:429:THR:HG22   | 2.53                     | 0.44              |
| 1:A:1079:LYS:O    | 1:A:1082:LEU:HG    | 2.18                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:1239:GLU:HA   | 1:A:1242:ILE:HD12  | 1.99                     | 0.44              |
| 2:B:677:LEU:O     | 2:B:681:LYS:HA     | 2.18                     | 0.44              |
| 4:E:290:ARG:HH12  | 4:E:312:GLU:HG3    | 1.83                     | 0.44              |
| 5:F:266:ARG:HG3   | 5:F:267:HIS:CE1    | 2.53                     | 0.44              |
| 6:H:353:ARG:O     | 6:H:357:THR:HG23   | 2.18                     | 0.44              |
| 2:O:211:LYS:HB2   | 2:O:231:PRO:HB3    | 1.99                     | 0.44              |
| 8:P:26:PRO:C      | 8:P:27:ARG:HG2     | 2.38                     | 0.44              |
| 8:Q:498:SER:O     | 8:Q:499:SER:OG     | 2.34                     | 0.44              |
| 8:Q:546:GLN:HG3   | 8:Q:599:SER:OG     | 2.18                     | 0.44              |
| 8:Q:569:VAL:CG1   | 8:Q:572:LEU:HB2    | 2.47                     | 0.44              |
| 8:Q:656:PRO:HG3   | 8:Q:757:VAL:HG23   | 2.00                     | 0.44              |
| 8:Q:664:ARG:HD2   | 8:Q:664:ARG:N      | 2.33                     | 0.44              |
| 1:S:948:ASP:O     | 1:S:951:ARG:HB2    | 2.18                     | 0.44              |
| 1:S:1076:LEU:O    | 1:S:1080:ARG:HG2   | 2.17                     | 0.44              |
| 1:S:1106:GLU:OE1  | 1:S:1106:GLU:N     | 2.49                     | 0.44              |
| 10:U:439:GLU:HA   | 10:U:442:GLU:HG3   | 2.00                     | 0.44              |
| 10:U:828:SER:O    | 10:U:831:VAL:HG22  | 2.17                     | 0.44              |
| 11:V:215:LEU:N    | 11:V:216:PRO:HD3   | 2.33                     | 0.44              |
| 11:V:343:ILE:O    | 11:V:346:LEU:HB3   | 2.17                     | 0.44              |
| 11:V:1122:HIS:CB  | 11:V:1158:LEU:HD11 | 2.48                     | 0.44              |
| 1:A:163:ARG:CZ    | 8:P:845:GLN:HE21   | 2.31                     | 0.44              |
| 1:A:1331:LEU:N    | 1:A:1332:PRO:HD2   | 2.32                     | 0.44              |
| 1:A:1339:LEU:HD11 | 1:A:1343:HIS:ND1   | 2.32                     | 0.44              |
| 2:B:344:LEU:HD11  | 2:B:354:LEU:HA     | 1.99                     | 0.44              |
| 3:C:197:ASP:N     | 3:C:198:PRO:HD2    | 2.33                     | 0.44              |
| 4:E:438:LEU:O     | 4:E:442:LEU:HG     | 2.17                     | 0.44              |
| 6:H:67:LEU:O      | 6:H:71:LEU:HD12    | 2.18                     | 0.44              |
| 8:P:31:HIS:CD2    | 8:P:32:GLU:HG2     | 2.53                     | 0.44              |
| 8:P:482:ALA:O     | 8:P:485:SER:OG     | 2.30                     | 0.44              |
| 8:Q:325:LYS:O     | 8:Q:337:GLU:HG2    | 2.18                     | 0.44              |
| 1:S:57:LEU:O      | 1:S:60:LEU:HB3     | 2.18                     | 0.44              |
| 1:S:171:TRP:O     | 1:S:174:GLN:HB2    | 2.18                     | 0.44              |
| 1:S:515:LYS:O     | 1:S:518:LEU:HB2    | 2.18                     | 0.44              |
| 1:S:818:PHE:CB    | 1:S:864:LEU:HD21   | 2.47                     | 0.44              |
| 1:S:1292:LEU:HD23 | 1:S:1295:LEU:HD12  | 2.00                     | 0.44              |
| 10:U:416:GLN:NE2  | 10:U:420:LYS:HD2   | 2.33                     | 0.44              |
| 10:U:605:LEU:HD12 | 10:U:609:PHE:CZ    | 2.53                     | 0.44              |
| 10:U:739:ASN:HA   | 10:U:742:SER:OG    | 2.18                     | 0.44              |
| 10:U:998:PRO:HA   | 10:U:1003:PHE:CG   | 2.53                     | 0.44              |
| 10:U:1210:TYR:HA  | 10:U:1213:ILE:HD12 | 1.99                     | 0.44              |
| 11:V:842:ASN:O    | 11:V:846:GLU:HB2   | 2.18                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:V:1094:LEU:HD22 | 11:V:1114:SER:HA  | 1.99                     | 0.44              |
| 1:A:656:ALA:HB3    | 1:A:683:ARG:NH2   | 2.32                     | 0.43              |
| 2:B:770:LEU:HD22   | 8:P:837:HIS:NE2   | 2.33                     | 0.43              |
| 2:B:828:LEU:O      | 8:P:826:ARG:HA    | 2.18                     | 0.43              |
| 3:C:153:MET:HA     | 5:F:161:SER:OG    | 2.18                     | 0.43              |
| 6:G:174:SER:O      | 6:G:180:LEU:HD21  | 2.17                     | 0.43              |
| 6:G:484:PHE:HB3    | 6:G:485:ARG:NH2   | 2.32                     | 0.43              |
| 6:H:557:THR:HG22   | 6:H:560:ARG:NH1   | 2.32                     | 0.43              |
| 6:H:562:ASP:N      | 6:H:562:ASP:OD1   | 2.50                     | 0.43              |
| 7:L:293:PRO:HB2    | 7:L:296:ALA:HB2   | 2.00                     | 0.43              |
| 7:M:55:CYS:HB3     | 7:M:59:LEU:HB3    | 2.00                     | 0.43              |
| 7:M:320:PRO:HA     | 7:M:333:PHE:O     | 2.18                     | 0.43              |
| 2:O:182:VAL:HA     | 2:O:215:TYR:O     | 2.17                     | 0.43              |
| 8:P:227:LEU:HB2    | 8:P:334:LEU:CD2   | 2.48                     | 0.43              |
| 8:Q:398:SER:HB2    | 8:Q:422:ALA:HB1   | 1.99                     | 0.43              |
| 8:Q:529:LEU:CD2    | 8:Q:572:LEU:HD11  | 2.47                     | 0.43              |
| 8:Q:737:LEU:HD11   | 8:Q:754:ILE:CD1   | 2.48                     | 0.43              |
| 1:S:19:ARG:HA      | 1:S:19:ARG:NH1    | 2.33                     | 0.43              |
| 1:S:163:ARG:CZ     | 1:S:191:VAL:HA    | 2.47                     | 0.43              |
| 1:S:281:LEU:HD21   | 1:S:295:VAL:HG21  | 2.00                     | 0.43              |
| 1:S:293:LYS:HA     | 1:S:296:ARG:HB2   | 2.00                     | 0.43              |
| 1:S:452:PHE:O      | 1:S:455:SER:OG    | 2.26                     | 0.43              |
| 1:S:557:VAL:HG11   | 1:S:1069:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:145:LEU:O      | 1:A:149:LEU:HD23  | 2.19                     | 0.43              |
| 1:A:167:CYS:HB2    | 1:A:196:LEU:HD23  | 2.00                     | 0.43              |
| 2:B:267:SER:OG     | 2:B:268:PHE:N     | 2.52                     | 0.43              |
| 2:B:387:ARG:O      | 2:B:390:VAL:HG12  | 2.18                     | 0.43              |
| 6:G:311:ASN:HA     | 6:G:343:GLN:OE1   | 2.18                     | 0.43              |
| 2:O:604:ARG:HG3    | 2:O:605:GLU:N     | 2.33                     | 0.43              |
| 8:P:152:MET:SD     | 8:P:253:VAL:HG11  | 2.58                     | 0.43              |
| 1:S:1022:GLN:NE2   | 1:S:1084:ARG:O    | 2.51                     | 0.43              |
| 1:S:1101:ILE:HG21  | 1:S:1154:PHE:HE2  | 1.81                     | 0.43              |
| 11:V:202:ILE:HG13  | 11:V:203:ALA:N    | 2.33                     | 0.43              |
| 11:V:338:SER:OG    | 11:V:339:GLY:N    | 2.51                     | 0.43              |
| 11:V:1052:VAL:HG13 | 11:V:1053:GLN:OE1 | 2.17                     | 0.43              |
| 1:A:1260:LEU:HD12  | 1:A:1261:PHE:N    | 2.33                     | 0.43              |
| 2:B:573:GLU:HG3    | 2:B:574:CYS:O     | 2.18                     | 0.43              |
| 2:B:710:ARG:HE     | 2:B:710:ARG:HB3   | 1.68                     | 0.43              |
| 3:C:437:GLN:OE1    | 3:C:441:GLN:NE2   | 2.51                     | 0.43              |
| 4:E:464:MET:HG3    | 4:E:468:LYS:HB2   | 2.00                     | 0.43              |
| 6:H:275:GLU:OE1    | 6:H:275:GLU:HA    | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:O:100:LYS:O     | 2:O:100:LYS:HG2    | 2.18                     | 0.43              |
| 8:P:241:VAL:O     | 8:P:252:CYS:HA     | 2.18                     | 0.43              |
| 1:S:331:SER:O     | 1:S:331:SER:OG     | 2.33                     | 0.43              |
| 1:A:1322:VAL:HG13 | 1:A:1323:ALA:N     | 2.33                     | 0.43              |
| 2:B:79:CYS:HB3    | 2:B:94:ILE:HD13    | 2.00                     | 0.43              |
| 3:C:496:LEU:O     | 3:C:543:SER:OG     | 2.26                     | 0.43              |
| 4:E:67:LEU:HD23   | 4:E:67:LEU:HA      | 1.75                     | 0.43              |
| 4:E:80:ARG:NH2    | 4:E:82:GLU:HG2     | 2.34                     | 0.43              |
| 6:H:78:ILE:HG23   | 6:H:92:GLN:HG2     | 2.00                     | 0.43              |
| 6:H:397:PHE:CB    | 6:H:420:LEU:HD22   | 2.49                     | 0.43              |
| 7:L:152:LEU:HD12  | 7:L:152:LEU:N      | 2.33                     | 0.43              |
| 8:P:169:GLN:O     | 8:P:169:GLN:HG2    | 2.17                     | 0.43              |
| 8:Q:289:LYS:HA    | 8:Q:310:ASP:H      | 1.84                     | 0.43              |
| 1:S:1313:LEU:HD13 | 1:S:1317:ARG:HG3   | 2.00                     | 0.43              |
| 10:U:1036:HIS:CE1 | 10:U:1045:LEU:HD13 | 2.53                     | 0.43              |
| 11:V:190:LYS:H    | 11:V:190:LYS:HE2   | 1.83                     | 0.43              |
| 11:V:364:TRP:NE1  | 11:V:384:MET:HG2   | 2.33                     | 0.43              |
| 11:V:1273:ARG:O   | 11:V:1277:ILE:HG12 | 2.18                     | 0.43              |
| 1:A:667:PRO:HA    | 1:A:673:ILE:HD11   | 2.00                     | 0.43              |
| 6:G:141:ARG:CG    | 6:G:200:ALA:HB2    | 2.49                     | 0.43              |
| 6:G:453:SER:HB2   | 6:G:483:LEU:CD1    | 2.48                     | 0.43              |
| 6:G:551:TYR:CD2   | 6:G:574:LEU:HD21   | 2.53                     | 0.43              |
| 6:H:149:LEU:O     | 6:H:152:SER:OG     | 2.27                     | 0.43              |
| 7:L:191:LEU:HD23  | 7:L:191:LEU:HA     | 1.79                     | 0.43              |
| 8:P:504:ARG:N     | 8:P:505:PRO:HD3    | 2.33                     | 0.43              |
| 8:P:677:ALA:O     | 8:P:680:LEU:HG     | 2.19                     | 0.43              |
| 8:Q:331:SER:OG    | 8:Q:333:LYS:HG2    | 2.18                     | 0.43              |
| 8:Q:880:LEU:O     | 8:Q:881:LEU:HD12   | 2.18                     | 0.43              |
| 1:S:93:PHE:O      | 1:S:96:SER:OG      | 2.31                     | 0.43              |
| 1:S:795:ARG:HD3   | 1:S:814:VAL:HG23   | 2.01                     | 0.43              |
| 1:S:952:GLN:HA    | 1:S:955:HIS:HB2    | 2.00                     | 0.43              |
| 1:S:1126:LEU:HB3  | 1:S:1130:ILE:HD11  | 2.00                     | 0.43              |
| 10:U:29:LEU:HD13  | 10:U:71:CYS:SG     | 2.59                     | 0.43              |
| 10:U:805:LEU:HD22 | 10:U:809:PHE:CE2   | 2.54                     | 0.43              |
| 1:A:1126:LEU:HD13 | 1:A:1169:SER:HB3   | 2.01                     | 0.43              |
| 3:C:529:THR:HA    | 3:C:532:ARG:NH2    | 2.33                     | 0.43              |
| 6:G:140:HIS:CE1   | 6:G:166:LEU:HD21   | 2.54                     | 0.43              |
| 6:G:213:TYR:CD2   | 6:G:329:LEU:HD22   | 2.54                     | 0.43              |
| 6:G:433:ARG:HG3   | 6:G:446:PRO:HG3    | 2.01                     | 0.43              |
| 6:H:203:LEU:O     | 6:H:207:LEU:HG     | 2.18                     | 0.43              |
| 7:L:250:GLU:N     | 7:L:250:GLU:OE1    | 2.48                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:M:37:HIS:CD2     | 7:M:38:LEU:H      | 2.37                     | 0.43              |
| 7:M:107:PRO:N      | 7:M:108:PRO:CD    | 2.81                     | 0.43              |
| 2:O:601:ILE:HG22   | 2:O:611:LYS:HZ2   | 1.83                     | 0.43              |
| 8:Q:60:PHE:CE1     | 8:Q:118:VAL:HG21  | 2.53                     | 0.43              |
| 1:S:171:TRP:CE2    | 1:S:200:HIS:HB2   | 2.54                     | 0.43              |
| 1:S:324:LEU:HD21   | 1:S:362:LEU:HD22  | 2.00                     | 0.43              |
| 10:U:365:LEU:HB3   | 10:U:369:LYS:HZ1  | 1.83                     | 0.43              |
| 10:U:998:PRO:HA    | 10:U:1003:PHE:CD2 | 2.53                     | 0.43              |
| 11:V:92:ILE:O      | 11:V:96:PHE:HB2   | 2.19                     | 0.43              |
| 11:V:258:PHE:O     | 11:V:262:VAL:HG23 | 2.18                     | 0.43              |
| 11:V:659:ASP:HB3   | 11:V:733:TYR:OH   | 2.19                     | 0.43              |
| 11:V:1186:LEU:HD11 | 11:V:1234:PHE:CE1 | 2.54                     | 0.43              |
| 2:B:112:LEU:HD12   | 2:B:118:PHE:CZ    | 2.54                     | 0.43              |
| 3:C:187:CYS:HG     | 3:C:219:PHE:HE1   | 1.63                     | 0.43              |
| 3:C:224:ASN:ND2    | 3:C:249:SER:OG    | 2.51                     | 0.43              |
| 4:E:298:LEU:HD11   | 4:E:347:TRP:CZ3   | 2.53                     | 0.43              |
| 6:H:351:ALA:HB1    | 6:H:367:TYR:CD2   | 2.54                     | 0.43              |
| 8:P:147:PRO:O      | 8:P:149:ARG:N     | 2.52                     | 0.43              |
| 8:P:760:ASP:OD1    | 8:P:760:ASP:N     | 2.45                     | 0.43              |
| 1:S:346:TRP:CE3    | 1:S:387:GLN:HA    | 2.54                     | 0.43              |
| 1:S:763:THR:HB     | 9:W:101:UNK:HA    | 1.99                     | 0.43              |
| 1:S:842:SER:O      | 1:S:845:LEU:HG    | 2.19                     | 0.43              |
| 1:S:1118:ASN:O     | 1:S:1326:GLN:NE2  | 2.51                     | 0.43              |
| 10:U:501:LYS:HB3   | 10:U:501:LYS:HE2  | 1.72                     | 0.43              |
| 10:U:852:GLN:OE1   | 10:U:860:SER:HB3  | 2.18                     | 0.43              |
| 10:U:860:SER:OG    | 10:U:861:GLY:N    | 2.51                     | 0.43              |
| 11:V:754:GLY:HA2   | 11:V:757:ASP:OD2  | 2.18                     | 0.43              |
| 11:V:1357:VAL:O    | 11:V:1361:LYS:HG2 | 2.19                     | 0.43              |
| 1:A:455:SER:O      | 1:A:460:ARG:N     | 2.38                     | 0.43              |
| 1:A:468:LYS:HA     | 1:A:471:VAL:CG2   | 2.46                     | 0.43              |
| 3:C:306:ASP:O      | 4:E:176:ARG:HB2   | 2.19                     | 0.43              |
| 5:F:43:HIS:HE1     | 5:F:47:ARG:HH21   | 1.67                     | 0.43              |
| 6:G:597:LEU:HB3    | 6:G:601:ARG:HH21  | 1.83                     | 0.43              |
| 6:H:555:LEU:O      | 6:H:559:LYS:HG2   | 2.19                     | 0.43              |
| 6:H:569:ALA:O      | 6:H:573:ARG:HG2   | 2.19                     | 0.43              |
| 7:L:228:ILE:HD12   | 7:L:238:ILE:HD12  | 1.99                     | 0.43              |
| 2:O:260:THR:OG1    | 2:O:264:GLN:HB2   | 2.18                     | 0.43              |
| 8:P:133:PHE:O      | 8:P:133:PHE:CG    | 2.65                     | 0.43              |
| 8:P:195:PRO:HB3    | 8:P:246:PRO:HD3   | 2.00                     | 0.43              |
| 8:P:875:HIS:HB3    | 8:P:876:PRO:CD    | 2.48                     | 0.43              |
| 8:Q:289:LYS:HD3    | 8:Q:308:HIS:O     | 2.19                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Q:604:TYR:HB3    | 8:Q:638:VAL:CG1    | 2.49                     | 0.43              |
| 1:S:795:ARG:HD2    | 1:S:813:PRO:HB3    | 1.99                     | 0.43              |
| 10:U:288:GLU:OE1   | 10:U:288:GLU:HA    | 2.19                     | 0.43              |
| 10:U:595:LEU:HD11  | 10:U:626:THR:HG22  | 1.99                     | 0.43              |
| 10:U:1059:ASP:OD1  | 10:U:1060:ILE:N    | 2.51                     | 0.43              |
| 11:V:359:THR:HA    | 11:V:362:GLU:OE1   | 2.19                     | 0.43              |
| 11:V:364:TRP:CZ2   | 11:V:380:PHE:HE1   | 2.36                     | 0.43              |
| 11:V:647:LYS:HA    | 11:V:650:GLU:HG3   | 2.01                     | 0.43              |
| 11:V:668:SER:OG    | 11:V:693:ASP:O     | 2.27                     | 0.43              |
| 1:A:825:ARG:HB3    | 1:A:940:GLN:HG3    | 1.99                     | 0.43              |
| 2:B:619:ARG:HH22   | 8:P:635:GLN:HG2    | 1.84                     | 0.43              |
| 3:C:115:GLN:CD     | 5:F:108:ARG:HD2    | 2.38                     | 0.43              |
| 3:C:162:ARG:NH1    | 3:C:162:ARG:O      | 2.51                     | 0.43              |
| 3:C:339:THR:O      | 3:C:339:THR:CG2    | 2.67                     | 0.43              |
| 4:E:415:ALA:O      | 4:E:419:LEU:HD23   | 2.19                     | 0.43              |
| 6:G:256:HIS:NE2    | 6:G:268:TYR:HE2    | 2.17                     | 0.43              |
| 7:M:132:CYS:SG     | 7:M:134:SER:HB3    | 2.59                     | 0.43              |
| 2:O:723:ASN:OD1    | 2:O:726:VAL:HG23   | 2.19                     | 0.43              |
| 8:P:283:ILE:O      | 8:P:283:ILE:HG22   | 2.16                     | 0.43              |
| 8:Q:286:GLY:O      | 8:Q:312:LEU:HD12   | 2.18                     | 0.43              |
| 1:S:732:ALA:HB1    | 9:W:79:THR:HG21    | 2.01                     | 0.43              |
| 1:S:992:HIS:O      | 1:S:1073:ARG:NH2   | 2.52                     | 0.43              |
| 1:S:1020:ARG:O     | 1:S:1024:MET:HG2   | 2.19                     | 0.43              |
| 1:S:1292:LEU:HD23  | 1:S:1292:LEU:HA    | 1.82                     | 0.43              |
| 10:U:1029:MET:HE3  | 10:U:1084:VAL:HG13 | 2.01                     | 0.43              |
| 11:V:190:LYS:N     | 11:V:190:LYS:HD3   | 2.34                     | 0.43              |
| 11:V:527:GLN:HA    | 11:V:530:ARG:HH12  | 1.83                     | 0.43              |
| 11:V:656:ILE:HG21  | 11:V:736:LEU:HD22  | 1.99                     | 0.43              |
| 11:V:969:LEU:HD13  | 11:V:1065:LEU:HG   | 2.01                     | 0.43              |
| 11:V:972:LEU:HD12  | 11:V:976:LEU:HD13  | 2.01                     | 0.43              |
| 11:V:1115:VAL:HG21 | 11:V:1142:LEU:CG   | 2.48                     | 0.43              |
| 1:A:426:SER:O      | 1:A:429:THR:OG1    | 2.37                     | 0.43              |
| 1:A:1135:PHE:HA    | 1:A:1138:LEU:HD12  | 2.01                     | 0.43              |
| 4:E:101:LEU:O      | 4:E:105:VAL:HG22   | 2.19                     | 0.43              |
| 6:G:447:TYR:HA     | 6:G:487:THR:O      | 2.19                     | 0.43              |
| 6:H:373:LEU:HD12   | 6:H:374:LEU:HG     | 2.01                     | 0.43              |
| 6:H:545:PRO:HB2    | 6:H:577:GLN:OE1    | 2.19                     | 0.43              |
| 7:M:210:LYS:O      | 7:M:210:LYS:HD3    | 2.19                     | 0.43              |
| 2:O:83:SER:HB2     | 2:O:90:ASN:HA      | 2.01                     | 0.43              |
| 2:O:250:ASN:OD1    | 2:O:251:GLN:HG3    | 2.19                     | 0.43              |
| 2:O:485:ASP:O      | 2:O:583:SER:HA     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Q:258:LEU:O     | 8:Q:258:LEU:HD23  | 2.19                     | 0.43              |
| 8:Q:655:PHE:HA    | 8:Q:756:GLY:CA    | 2.49                     | 0.43              |
| 8:Q:709:LYS:HG2   | 8:Q:786:GLU:HB3   | 2.00                     | 0.43              |
| 10:U:707:GLU:O    | 10:U:710:THR:OG1  | 2.32                     | 0.43              |
| 10:U:757:ASN:ND2  | 10:U:767:ARG:O    | 2.52                     | 0.43              |
| 11:V:787:PHE:CZ   | 11:V:924:PHE:HB3  | 2.54                     | 0.43              |
| 1:A:1115:GLU:HB2  | 1:A:1116:MET:HE1  | 2.00                     | 0.42              |
| 4:E:53:ARG:NH2    | 7:L:361:TYR:O     | 2.52                     | 0.42              |
| 4:E:420:LEU:HD23  | 4:E:423:LEU:HD12  | 2.00                     | 0.42              |
| 6:G:191:LEU:O     | 6:G:193:ALA:N     | 2.52                     | 0.42              |
| 6:H:155:ARG:O     | 6:H:158:ASP:OD1   | 2.37                     | 0.42              |
| 2:O:425:ALA:O     | 2:O:429:LEU:HG    | 2.18                     | 0.42              |
| 2:O:781:GLU:HG2   | 8:Q:826:ARG:HG2   | 2.00                     | 0.42              |
| 8:P:142:THR:OG1   | 8:P:143:LEU:N     | 2.52                     | 0.42              |
| 8:P:325:LYS:HG2   | 8:P:326:ALA:N     | 2.34                     | 0.42              |
| 8:Q:655:PHE:CD1   | 8:Q:756:GLY:HA3   | 2.54                     | 0.42              |
| 1:S:21:ALA:HA     | 1:S:24:GLU:HB2    | 2.01                     | 0.42              |
| 10:U:747:MET:HG2  | 10:U:778:TYR:HD1  | 1.83                     | 0.42              |
| 11:V:190:LYS:H    | 11:V:190:LYS:HD3  | 1.83                     | 0.42              |
| 11:V:306:ASP:CG   | 11:V:307:LEU:N    | 2.72                     | 0.42              |
| 11:V:1331:PHE:HA  | 11:V:1334:ASP:OD2 | 2.19                     | 0.42              |
| 1:A:34:LYS:HE3    | 6:H:313:PRO:HD3   | 2.02                     | 0.42              |
| 1:A:346:TRP:CE2   | 1:A:387:GLN:HA    | 2.55                     | 0.42              |
| 1:A:369:GLU:HA    | 1:A:372:VAL:HG22  | 2.00                     | 0.42              |
| 3:C:302:LEU:HD12  | 3:C:302:LEU:HA    | 1.82                     | 0.42              |
| 3:C:379:VAL:HG21  | 3:C:428:PHE:CZ    | 2.54                     | 0.42              |
| 7:M:29:ILE:HD12   | 7:M:30:SER:H      | 1.84                     | 0.42              |
| 2:O:297:LEU:HD13  | 2:O:313:LYS:HD3   | 2.01                     | 0.42              |
| 2:O:507:SER:OG    | 8:Q:564:THR:HG21  | 2.19                     | 0.42              |
| 8:P:744:ASP:OD1   | 8:P:744:ASP:N     | 2.51                     | 0.42              |
| 8:Q:60:PHE:HE2    | 8:Q:78:ALA:CB     | 2.32                     | 0.42              |
| 1:S:45:GLU:O      | 1:S:48:VAL:HG12   | 2.18                     | 0.42              |
| 1:S:1135:PHE:CD2  | 1:S:1177:LEU:HD13 | 2.54                     | 0.42              |
| 10:U:364:ILE:O    | 10:U:368:VAL:HG23 | 2.19                     | 0.42              |
| 10:U:541:LEU:HD22 | 10:U:608:GLY:HA3  | 2.00                     | 0.42              |
| 11:V:391:THR:OG1  | 11:V:392:ASN:N    | 2.51                     | 0.42              |
| 1:A:43:LEU:HD23   | 1:A:44:LYS:N      | 2.34                     | 0.42              |
| 1:A:288:GLU:HG3   | 1:A:292:HIS:CD2   | 2.54                     | 0.42              |
| 2:B:281:PHE:N     | 2:B:281:PHE:CD1   | 2.87                     | 0.42              |
| 5:F:339:PHE:CG    | 5:F:344:LEU:HD22  | 2.54                     | 0.42              |
| 6:H:600:ILE:O     | 6:H:600:ILE:HG22  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:O:501:LEU:O      | 2:O:604:ARG:HG2   | 2.18                     | 0.42              |
| 2:O:656:HIS:CD2    | 2:O:657:LYS:N     | 2.87                     | 0.42              |
| 8:P:545:ILE:CD1    | 8:P:565:TYR:HB2   | 2.48                     | 0.42              |
| 8:Q:21:LEU:HB2     | 8:Q:399:LEU:CD2   | 2.47                     | 0.42              |
| 11:V:83:LEU:HG     | 11:V:92:ILE:HD12  | 2.01                     | 0.42              |
| 11:V:140:LEU:HD23  | 11:V:146:GLN:HA   | 2.00                     | 0.42              |
| 1:A:1289:ALA:O     | 1:A:1292:LEU:HG   | 2.19                     | 0.42              |
| 2:B:99:ASN:ND2     | 2:B:101:LYS:H     | 2.17                     | 0.42              |
| 2:B:280:PRO:HB2    | 2:B:281:PHE:CD1   | 2.54                     | 0.42              |
| 7:L:336:ILE:H      | 7:L:336:ILE:HD12  | 1.84                     | 0.42              |
| 8:P:859:SER:OG     | 8:P:860:CYS:N     | 2.53                     | 0.42              |
| 1:S:229:ASP:O      | 1:S:232:ARG:HG2   | 2.19                     | 0.42              |
| 1:S:814:VAL:N      | 1:S:815:PRO:HD2   | 2.34                     | 0.42              |
| 10:U:613:LEU:HD21  | 10:U:620:ALA:HA   | 2.01                     | 0.42              |
| 10:U:721:PHE:HB2   | 10:U:723:LEU:HG   | 2.01                     | 0.42              |
| 10:U:1135:ILE:HD11 | 10:U:1194:MET:HA  | 2.00                     | 0.42              |
| 11:V:51:LEU:HD13   | 11:V:83:LEU:HD11  | 2.02                     | 0.42              |
| 1:A:332:PRO:HB3    | 1:A:383:GLU:OE1   | 2.19                     | 0.42              |
| 1:A:415:MET:CE     | 1:A:415:MET:HA    | 2.49                     | 0.42              |
| 1:A:456:PHE:CE2    | 1:A:496:PRO:HB2   | 2.55                     | 0.42              |
| 1:A:1193:LEU:HD12  | 1:A:1194:PRO:HD2  | 2.01                     | 0.42              |
| 2:B:506:LEU:N      | 2:B:525:ASN:HD21  | 2.09                     | 0.42              |
| 3:C:291:PHE:CE2    | 3:C:340:TYR:HB3   | 2.55                     | 0.42              |
| 4:E:113:GLY:O      | 4:E:116:SER:OG    | 2.31                     | 0.42              |
| 4:E:129:PRO:HG3    | 4:E:134:ARG:HH12  | 1.84                     | 0.42              |
| 6:G:559:LYS:HA     | 6:G:563:ARG:HG2   | 2.02                     | 0.42              |
| 6:H:455:THR:O      | 6:H:458:LEU:HG    | 2.19                     | 0.42              |
| 1:S:1336:TYR:OH    | 1:S:1361:TYR:N    | 2.53                     | 0.42              |
| 10:U:131:PRO:HD3   | 10:U:180:MET:HG3  | 2.01                     | 0.42              |
| 10:U:488:LEU:HD21  | 10:U:500:LEU:HD11 | 2.00                     | 0.42              |
| 11:V:337:SER:N     | 11:V:340:GLN:OE1  | 2.53                     | 0.42              |
| 11:V:783:CYS:SG    | 11:V:784:SER:N    | 2.92                     | 0.42              |
| 1:A:1028:LEU:HD13  | 1:A:1047:PHE:CE2  | 2.55                     | 0.42              |
| 2:B:766:GLU:O      | 2:B:769:THR:OG1   | 2.34                     | 0.42              |
| 6:G:89:THR:HG21    | 8:P:147:PRO:CB    | 2.49                     | 0.42              |
| 6:G:598:SER:HA     | 6:G:601:ARG:CZ    | 2.49                     | 0.42              |
| 6:H:461:GLN:HG2    | 6:H:596:TYR:CE1   | 2.54                     | 0.42              |
| 7:L:55:CYS:HB3     | 7:L:59:LEU:HB3    | 2.02                     | 0.42              |
| 2:O:630:GLY:O      | 2:O:631:LYS:HB3   | 2.19                     | 0.42              |
| 8:P:395:CYS:HB3    | 8:P:396:PRO:CD    | 2.49                     | 0.42              |
| 8:P:508:CYS:SG     | 8:P:642:LEU:HD13  | 2.60                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:Q:239:PRO:HG2   | 8:Q:255:LEU:HD12   | 2.00                     | 0.42              |
| 8:Q:505:PRO:CB    | 8:Q:533:SER:HB3    | 2.50                     | 0.42              |
| 8:Q:720:LYS:C     | 8:Q:722:GLY:N      | 2.70                     | 0.42              |
| 1:S:266:THR:O     | 1:S:270:LEU:HG     | 2.20                     | 0.42              |
| 1:S:303:SER:O     | 1:S:305:HIS:ND1    | 2.52                     | 0.42              |
| 1:S:822:LEU:HG    | 1:S:833:CYS:SG     | 2.60                     | 0.42              |
| 1:S:1090:LEU:HD12 | 1:S:1091:CYS:N     | 2.35                     | 0.42              |
| 10:U:770:ASP:O    | 10:U:773:SER:OG    | 2.32                     | 0.42              |
| 10:U:868:GLU:OE1  | 10:U:926:LYS:NZ    | 2.53                     | 0.42              |
| 10:U:979:SER:O    | 10:U:983:LEU:HG    | 2.19                     | 0.42              |
| 10:U:1096:LEU:HA  | 10:U:1099:VAL:HG22 | 2.02                     | 0.42              |
| 10:U:1137:GLN:O   | 10:U:1141:LEU:HD12 | 2.20                     | 0.42              |
| 11:V:299:SER:O    | 11:V:303:GLU:HG2   | 2.20                     | 0.42              |
| 11:V:922:HIS:CG   | 11:V:923:ALA:N     | 2.88                     | 0.42              |
| 1:A:657:LEU:HD23  | 1:A:657:LEU:HA     | 1.89                     | 0.42              |
| 1:A:988:LEU:HD11  | 1:A:1081:ILE:HD11  | 2.02                     | 0.42              |
| 2:B:65:PHE:HE2    | 2:B:67:ILE:HD13    | 1.84                     | 0.42              |
| 2:B:391:VAL:O     | 2:B:394:LEU:N      | 2.52                     | 0.42              |
| 2:B:394:LEU:HD11  | 7:L:115:ILE:HD11   | 2.02                     | 0.42              |
| 3:C:25:ALA:HA     | 3:C:30:THR:OG1     | 2.20                     | 0.42              |
| 3:C:31:GLN:OE1    | 3:C:185:ARG:NE     | 2.46                     | 0.42              |
| 3:C:166:LEU:HA    | 3:C:166:LEU:HD23   | 1.79                     | 0.42              |
| 3:C:359:ILE:HD12  | 3:C:403:TRP:HH2    | 1.84                     | 0.42              |
| 5:F:282:GLY:HA3   | 5:F:347:TRP:CH2    | 2.55                     | 0.42              |
| 2:O:842:VAL:HG12  | 8:Q:878:LEU:HD21   | 2.01                     | 0.42              |
| 8:P:23:ALA:HA     | 8:P:399:LEU:HD12   | 2.01                     | 0.42              |
| 8:Q:76:LEU:HD23   | 8:Q:76:LEU:HA      | 1.87                     | 0.42              |
| 1:S:108:PRO:HG2   | 1:S:111:ILE:HD12   | 2.02                     | 0.42              |
| 1:S:605:GLU:HA    | 1:S:608:LYS:HG2    | 2.01                     | 0.42              |
| 1:S:874:ARG:HG3   | 1:S:946:LEU:HD11   | 2.00                     | 0.42              |
| 10:U:593:ARG:CD   | 11:V:182:TRP:HZ3   | 2.33                     | 0.42              |
| 10:U:672:GLN:HG3  | 10:U:756:TYR:HB2   | 2.02                     | 0.42              |
| 10:U:768:PHE:HE2  | 10:U:828:SER:HG    | 1.65                     | 0.42              |
| 11:V:215:LEU:N    | 11:V:216:PRO:CD    | 2.83                     | 0.42              |
| 11:V:607:CYS:HA   | 11:V:610:VAL:HG12  | 2.01                     | 0.42              |
| 11:V:1008:SER:O   | 11:V:1012:ILE:HG12 | 2.20                     | 0.42              |
| 1:A:822:LEU:CD2   | 1:A:867:LYS:HD3    | 2.49                     | 0.42              |
| 3:C:251:GLU:O     | 3:C:255:LEU:HG     | 2.20                     | 0.42              |
| 4:E:399:CYS:SG    | 4:E:400:SER:N      | 2.92                     | 0.42              |
| 5:F:115:LEU:HD23  | 5:F:129:LEU:CD2    | 2.46                     | 0.42              |
| 6:G:273:LEU:CD2   | 6:G:279:TRP:HB2    | 2.50                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:H:168:GLY:HA3   | 6:H:170:GLN:NE2    | 2.34                     | 0.42              |
| 6:H:539:LEU:O     | 6:H:543:MET:HG2    | 2.20                     | 0.42              |
| 7:M:248:LEU:HD21  | 10:U:472:LEU:HD11  | 2.00                     | 0.42              |
| 7:M:326:ASN:ND2   | 7:M:364:LYS:HG3    | 2.35                     | 0.42              |
| 8:Q:524:MET:SD    | 8:Q:583:PRO:HB3    | 2.59                     | 0.42              |
| 1:S:149:LEU:CD1   | 1:S:190:ILE:HG13   | 2.49                     | 0.42              |
| 1:S:393:VAL:HA    | 1:S:396:LEU:HB2    | 2.01                     | 0.42              |
| 1:S:814:VAL:HG12  | 1:S:818:PHE:CE2    | 2.54                     | 0.42              |
| 10:U:298:GLN:HE22 | 10:U:1108:GLY:HA3  | 1.84                     | 0.42              |
| 10:U:593:ARG:CD   | 11:V:182:TRP:CZ3   | 3.03                     | 0.42              |
| 10:U:612:VAL:O    | 10:U:616:ASN:N     | 2.47                     | 0.42              |
| 10:U:968:ASN:OD1  | 10:U:969:LEU:N     | 2.52                     | 0.42              |
| 11:V:298:ILE:HG21 | 11:V:364:TRP:HA    | 2.02                     | 0.42              |
| 11:V:527:GLN:HA   | 11:V:530:ARG:NH1   | 2.34                     | 0.42              |
| 11:V:647:LYS:HA   | 11:V:650:GLU:CG    | 2.49                     | 0.42              |
| 11:V:686:LEU:HD23 | 11:V:686:LEU:HA    | 1.86                     | 0.42              |
| 11:V:1227:THR:O   | 11:V:1231:PHE:HB2  | 2.19                     | 0.42              |
| 11:V:1277:ILE:O   | 11:V:1281:LEU:HD13 | 2.20                     | 0.42              |
| 1:A:495:HIS:HB3   | 1:A:496:PRO:HD3    | 2.01                     | 0.42              |
| 1:A:663:SER:HB3   | 1:A:676:GLN:HE22   | 1.85                     | 0.42              |
| 1:A:1362:LEU:HD12 | 1:A:1363:LYS:N     | 2.35                     | 0.42              |
| 1:A:1368:PHE:CD2  | 1:A:1392:PRO:HB2   | 2.55                     | 0.42              |
| 2:B:488:VAL:HG21  | 2:B:654:ALA:HB2    | 2.02                     | 0.42              |
| 4:E:133:LEU:HD12  | 4:E:133:LEU:HA     | 1.80                     | 0.42              |
| 5:F:11:PHE:CZ     | 5:F:89:CYS:HB2     | 2.54                     | 0.42              |
| 5:F:14:LEU:HD11   | 5:F:26:TRP:CH2     | 2.55                     | 0.42              |
| 5:F:69:GLU:HA     | 5:F:74:ARG:HH22    | 1.84                     | 0.42              |
| 6:G:430:LYS:CE    | 8:P:328:TRP:HB2    | 2.50                     | 0.42              |
| 6:G:522:LEU:HD21  | 6:G:553:HIS:CE1    | 2.55                     | 0.42              |
| 6:H:37:LEU:O      | 6:H:40:GLN:HG3     | 2.18                     | 0.42              |
| 7:L:226:ARG:HD3   | 7:L:226:ARG:HA     | 1.82                     | 0.42              |
| 2:O:303:PHE:HB2   | 2:O:307:ASN:OD1    | 2.20                     | 0.42              |
| 2:O:777:ILE:O     | 2:O:781:GLU:HG3    | 2.20                     | 0.42              |
| 8:P:393:MET:CE    | 8:P:434:LEU:HD21   | 2.50                     | 0.42              |
| 8:Q:563:ILE:HG22  | 8:Q:565:TYR:CE1    | 2.55                     | 0.42              |
| 8:Q:736:LEU:HD23  | 8:Q:807:ARG:HH21   | 1.85                     | 0.42              |
| 1:S:929:TYR:CE2   | 1:S:933:LEU:HD11   | 2.55                     | 0.42              |
| 1:S:1331:LEU:N    | 1:S:1332:PRO:HD2   | 2.35                     | 0.42              |
| 1:S:1398:LYS:HA   | 1:S:1401:LEU:HG    | 2.01                     | 0.42              |
| 10:U:186:LEU:HD22 | 10:U:190:GLU:HB3   | 2.02                     | 0.42              |
| 10:U:277:PHE:O    | 10:U:281:LEU:HG    | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:U:283:TYR:CD1  | 10:U:321:ARG:HD3  | 2.54                     | 0.42              |
| 10:U:295:VAL:HG13 | 10:U:296:GLY:H    | 1.85                     | 0.42              |
| 10:U:831:VAL:O    | 10:U:834:SER:OG   | 2.36                     | 0.42              |
| 11:V:46:SER:OG    | 11:V:49:VAL:HG12  | 2.20                     | 0.42              |
| 11:V:682:ALA:HB2  | 11:V:761:PHE:CE1  | 2.55                     | 0.42              |
| 11:V:686:LEU:HG   | 11:V:815:ARG:CZ   | 2.50                     | 0.42              |
| 11:V:767:PRO:HA   | 11:V:828:LYS:NZ   | 2.35                     | 0.42              |
| 11:V:807:GLU:HG2  | 11:V:808:MET:N    | 2.35                     | 0.42              |
| 11:V:814:THR:HA   | 11:V:817:LYS:HG2  | 2.02                     | 0.42              |
| 1:A:61:LEU:HD12   | 1:A:77:VAL:HG22   | 2.02                     | 0.42              |
| 1:A:342:MET:HB3   | 1:A:346:TRP:CE2   | 2.55                     | 0.42              |
| 1:A:485:SER:O     | 1:A:485:SER:OG    | 2.29                     | 0.42              |
| 1:A:914:ARG:O     | 1:A:917:ARG:N     | 2.53                     | 0.42              |
| 2:B:15:LEU:HB2    | 2:B:327:LEU:HD13  | 2.02                     | 0.42              |
| 3:C:72:ALA:HB2    | 3:C:113:TRP:HZ2   | 1.85                     | 0.42              |
| 3:C:188:VAL:HB    | 3:C:189:PRO:HD3   | 2.02                     | 0.42              |
| 6:G:256:HIS:HA    | 6:G:259:MET:CG    | 2.50                     | 0.42              |
| 6:H:397:PHE:HB2   | 6:H:420:LEU:HD22  | 2.00                     | 0.42              |
| 7:M:84:MET:C      | 7:M:88:LYS:HZ3    | 2.23                     | 0.42              |
| 7:M:257:ASP:OD1   | 7:M:258:HIS:N     | 2.53                     | 0.42              |
| 2:O:480:TYR:CZ    | 2:O:620:VAL:HG23  | 2.54                     | 0.42              |
| 1:S:411:VAL:O     | 1:S:415:MET:HG3   | 2.20                     | 0.42              |
| 1:S:944:ASP:OD1   | 1:S:947:SER:HA    | 2.20                     | 0.42              |
| 1:S:1174:TRP:CD2  | 1:S:1200:LEU:HD22 | 2.55                     | 0.42              |
| 1:S:1339:LEU:HD11 | 1:S:1343:HIS:ND1  | 2.35                     | 0.42              |
| 10:U:106:VAL:HG22 | 10:U:137:LEU:HD21 | 2.02                     | 0.42              |
| 10:U:239:ALA:O    | 10:U:243:GLN:HG2  | 2.20                     | 0.42              |
| 10:U:310:ILE:O    | 10:U:314:LEU:HD23 | 2.20                     | 0.42              |
| 11:V:190:LYS:H    | 11:V:190:LYS:CE   | 2.33                     | 0.42              |
| 1:A:795:ARG:HG2   | 1:A:796:SER:N     | 2.35                     | 0.41              |
| 1:A:818:PHE:HE1   | 1:A:836:PHE:HE2   | 1.66                     | 0.41              |
| 1:A:1194:PRO:HG2  | 1:A:1197:LEU:HD13 | 2.02                     | 0.41              |
| 2:B:106:GLU:O     | 2:B:107:TYR:HB2   | 2.20                     | 0.41              |
| 2:B:402:PHE:O     | 2:B:405:PHE:HB3   | 2.21                     | 0.41              |
| 3:C:232:ILE:HG23  | 3:C:233:SER:N     | 2.35                     | 0.41              |
| 4:E:298:LEU:HD21  | 4:E:347:TRP:CZ2   | 2.54                     | 0.41              |
| 6:G:374:LEU:HD13  | 6:G:393:MET:HE1   | 2.01                     | 0.41              |
| 7:M:16:LEU:HD11   | 2:O:422:SER:CB    | 2.50                     | 0.41              |
| 7:M:226:ARG:O     | 7:M:238:ILE:HG12  | 2.19                     | 0.41              |
| 2:O:41:PRO:HB2    | 2:O:74:LEU:HD12   | 2.02                     | 0.41              |
| 2:O:675:TRP:CH2   | 2:O:734:LEU:HB2   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:P:258:LEU:HD13  | 8:P:271:LEU:HD21   | 2.01                     | 0.41              |
| 8:P:531:ASN:HB2   | 8:P:572:LEU:HD21   | 2.01                     | 0.41              |
| 8:Q:165:ARG:HE    | 8:Q:166:PRO:CD     | 2.33                     | 0.41              |
| 8:Q:280:GLU:OE2   | 8:Q:319:GLY:N      | 2.50                     | 0.41              |
| 1:S:485:SER:HB2   | 1:S:521:LEU:HD13   | 2.02                     | 0.41              |
| 1:S:660:LEU:HD12  | 1:S:660:LEU:HA     | 1.91                     | 0.41              |
| 1:S:769:LEU:HD21  | 1:S:784:LEU:HD23   | 2.02                     | 0.41              |
| 1:S:851:GLN:HG2   | 1:S:853:ARG:HH21   | 1.85                     | 0.41              |
| 1:S:1326:GLN:HG2  | 1:S:1327:HIS:CD2   | 2.54                     | 0.41              |
| 10:U:202:PHE:CD1  | 10:U:210:ILE:HG23  | 2.55                     | 0.41              |
| 10:U:295:VAL:HG13 | 10:U:296:GLY:N     | 2.35                     | 0.41              |
| 10:U:1102:LEU:HB3 | 10:U:1134:ILE:HD11 | 2.01                     | 0.41              |
| 11:V:378:LYS:HE3  | 11:V:378:LYS:HB3   | 1.86                     | 0.41              |
| 1:A:167:CYS:SG    | 1:A:168:GLN:N      | 2.93                     | 0.41              |
| 2:B:657:LYS:HD2   | 2:B:720:TYR:CZ     | 2.55                     | 0.41              |
| 3:C:303:LEU:HD21  | 3:C:391:PHE:CZ     | 2.55                     | 0.41              |
| 2:O:13:GLU:HG3    | 2:O:353:CYS:SG     | 2.60                     | 0.41              |
| 2:O:604:ARG:HH12  | 8:Q:551:SER:C      | 2.24                     | 0.41              |
| 1:S:563:ASN:ND2   | 1:S:1275:SER:OG    | 2.53                     | 0.41              |
| 1:S:1053:ARG:HA   | 1:S:1056:LEU:HD12  | 2.02                     | 0.41              |
| 1:S:1109:PHE:HB3  | 1:S:1163:CYS:HB2   | 2.01                     | 0.41              |
| 1:S:1262:PHE:CE2  | 1:S:1319:LEU:HD22  | 2.55                     | 0.41              |
| 1:S:1404:LEU:HD21 | 1:S:1432:VAL:HG12  | 2.02                     | 0.41              |
| 10:U:40:GLY:HA3   | 10:U:85:ILE:HG21   | 2.02                     | 0.41              |
| 10:U:678:TYR:HA   | 10:U:682:VAL:HG23  | 2.02                     | 0.41              |
| 10:U:1136:MET:CE  | 10:U:1193:ASN:HD21 | 2.33                     | 0.41              |
| 11:V:171:ASN:OD1  | 11:V:171:ASN:N     | 2.50                     | 0.41              |
| 11:V:212:ILE:HG13 | 11:V:215:LEU:HD12  | 2.02                     | 0.41              |
| 11:V:456:LEU:HD12 | 11:V:460:TYR:HE2   | 1.84                     | 0.41              |
| 11:V:787:PHE:CE1  | 11:V:924:PHE:HB3   | 2.55                     | 0.41              |
| 1:A:60:LEU:O      | 1:A:64:VAL:HG22    | 2.21                     | 0.41              |
| 1:A:278:LEU:HD11  | 1:A:327:ILE:HG12   | 2.03                     | 0.41              |
| 1:A:1416:SER:HG   | 1:A:1417:HIS:HD1   | 1.53                     | 0.41              |
| 2:B:14:ARG:HD2    | 2:B:79:CYS:SG      | 2.60                     | 0.41              |
| 3:C:216:GLN:HA    | 3:C:217:PRO:HD3    | 1.87                     | 0.41              |
| 3:C:343:TYR:HD1   | 3:C:344:THR:HG23   | 1.85                     | 0.41              |
| 6:H:198:GLN:OE1   | 6:H:323:ILE:HB     | 2.20                     | 0.41              |
| 6:H:551:TYR:HE1   | 6:H:570:LEU:HD22   | 1.84                     | 0.41              |
| 2:O:132:ASP:HB2   | 2:O:145:ARG:O      | 2.19                     | 0.41              |
| 2:O:216:SER:HB2   | 2:O:220:GLN:HB2    | 2.01                     | 0.41              |
| 8:P:250:LEU:O     | 8:P:250:LEU:HG     | 2.19                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:P:467:GLU:C     | 8:P:470:SER:HG     | 2.14                     | 0.41              |
| 8:Q:165:ARG:HE    | 8:Q:166:PRO:HD3    | 1.85                     | 0.41              |
| 1:S:1128:GLN:HB2  | 1:S:1173:TRP:CE3   | 2.55                     | 0.41              |
| 1:S:1261:PHE:CE1  | 1:S:1265:LEU:HD21  | 2.56                     | 0.41              |
| 10:U:81:LEU:HB2   | 10:U:86:VAL:HG23   | 2.01                     | 0.41              |
| 10:U:591:LEU:HA   | 10:U:594:CYS:SG    | 2.60                     | 0.41              |
| 10:U:1019:ARG:HD2 | 10:U:1019:ARG:HA   | 1.89                     | 0.41              |
| 10:U:1029:MET:HE2 | 10:U:1087:LEU:HD23 | 2.02                     | 0.41              |
| 10:U:1146:HIS:O   | 10:U:1150:GLN:HG3  | 2.20                     | 0.41              |
| 11:V:397:LYS:HB3  | 11:V:401:ARG:HH12  | 1.84                     | 0.41              |
| 11:V:769:GLU:HA   | 11:V:772:GLU:HG2   | 2.01                     | 0.41              |
| 3:C:247:LEU:HB2   | 4:E:132:TRP:CD1    | 2.56                     | 0.41              |
| 5:F:341:VAL:O     | 5:F:344:LEU:HD13   | 2.20                     | 0.41              |
| 7:L:63:LEU:HD23   | 7:L:63:LEU:HA      | 1.77                     | 0.41              |
| 7:M:227:ARG:HA    | 7:M:237:ASN:HA     | 2.02                     | 0.41              |
| 2:O:354:LEU:HG    | 2:O:354:LEU:O      | 2.21                     | 0.41              |
| 2:O:523:CYS:HA    | 2:O:581:VAL:O      | 2.19                     | 0.41              |
| 8:P:38:SER:O      | 8:P:38:SER:OG      | 2.39                     | 0.41              |
| 8:Q:736:LEU:HD23  | 8:Q:807:ARG:NH2    | 2.35                     | 0.41              |
| 1:S:153:GLN:NE2   | 1:S:188:GLN:HB3    | 2.35                     | 0.41              |
| 1:S:481:VAL:O     | 1:S:485:SER:HB3    | 2.19                     | 0.41              |
| 1:S:1349:ARG:HA   | 1:S:1353:PHE:CG    | 2.55                     | 0.41              |
| 10:U:72:CYS:SG    | 10:U:93:LEU:HD11   | 2.60                     | 0.41              |
| 10:U:197:LYS:O    | 10:U:201:MET:HG2   | 2.20                     | 0.41              |
| 10:U:879:ARG:HH12 | 10:U:933:ALA:HB1   | 1.84                     | 0.41              |
| 10:U:1180:TYR:HB3 | 10:U:1267:LEU:HD11 | 2.01                     | 0.41              |
| 11:V:178:SER:OG   | 11:V:179:GLN:NE2   | 2.53                     | 0.41              |
| 11:V:190:LYS:O    | 11:V:194:THR:HG23  | 2.20                     | 0.41              |
| 1:A:758:LEU:O     | 1:A:762:LEU:HG     | 2.21                     | 0.41              |
| 1:A:937:LEU:HA    | 1:A:1014:ASN:OD1   | 2.20                     | 0.41              |
| 2:B:421:LYS:HE3   | 2:B:421:LYS:HB2    | 1.93                     | 0.41              |
| 3:C:19:LEU:HD23   | 3:C:22:TRP:CE3     | 2.55                     | 0.41              |
| 3:C:456:MET:O     | 3:C:459:SER:OG     | 2.29                     | 0.41              |
| 4:E:288:LEU:N     | 4:E:289:PRO:HD2    | 2.36                     | 0.41              |
| 4:E:442:LEU:O     | 4:E:475:LYS:NZ     | 2.23                     | 0.41              |
| 6:G:21:ASP:OD1    | 6:G:195:LEU:HD23   | 2.20                     | 0.41              |
| 6:G:54:LEU:HD21   | 6:G:58:GLN:NE2     | 2.36                     | 0.41              |
| 6:G:151:LEU:HD21  | 6:G:214:ARG:HD3    | 2.02                     | 0.41              |
| 6:G:501:GLN:HG3   | 6:G:502:GLY:N      | 2.35                     | 0.41              |
| 6:H:88:PHE:CD1    | 6:H:149:LEU:HD23   | 2.55                     | 0.41              |
| 7:L:126:LEU:HA    | 7:L:138:LEU:HD23   | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:L:295:ARG:HD2   | 7:L:298:LEU:CD2    | 2.46                     | 0.41              |
| 2:O:765:LYS:NZ    | 2:O:848:LYS:HB2    | 2.36                     | 0.41              |
| 8:P:543:LEU:HD12  | 8:P:601:THR:O      | 2.20                     | 0.41              |
| 8:Q:148:ALA:O     | 8:Q:180:PRO:HD2    | 2.20                     | 0.41              |
| 8:Q:539:GLN:OE1   | 8:Q:609:VAL:HG22   | 2.20                     | 0.41              |
| 1:S:114:ALA:HB1   | 1:S:166:PHE:HA     | 2.02                     | 0.41              |
| 1:S:564:ILE:HD12  | 1:S:607:LEU:HD23   | 2.02                     | 0.41              |
| 1:S:1437:GLN:O    | 1:S:1441:GLN:HG2   | 2.20                     | 0.41              |
| 9:W:83:LYS:HE3    | 9:W:85:PHE:HZ      | 1.86                     | 0.41              |
| 10:U:412:ARG:HD2  | 10:U:413:MET:N     | 2.35                     | 0.41              |
| 10:U:950:SER:OG   | 10:U:951:VAL:N     | 2.52                     | 0.41              |
| 11:V:283:LYS:HG3  | 11:V:287:HIS:CE1   | 2.55                     | 0.41              |
| 2:B:229:ILE:HD12  | 2:B:237:VAL:HG21   | 2.03                     | 0.41              |
| 5:F:193:TRP:CH2   | 5:F:198:GLN:HB3    | 2.56                     | 0.41              |
| 7:L:117:GLU:OE1   | 7:L:158:TYR:OH     | 2.13                     | 0.41              |
| 7:L:171:VAL:HG22  | 7:L:197:LEU:HD11   | 2.01                     | 0.41              |
| 2:O:126:LEU:HD23  | 2:O:126:LEU:HA     | 1.90                     | 0.41              |
| 8:P:17:PRO:HD2    | 8:P:21:LEU:HD23    | 2.02                     | 0.41              |
| 8:P:150:TRP:CD2   | 8:P:178:TYR:CE2    | 3.08                     | 0.41              |
| 8:P:328:TRP:HA    | 8:P:334:LEU:HA     | 2.02                     | 0.41              |
| 1:S:169:GLU:HG3   | 1:S:172:LYS:HD2    | 2.03                     | 0.41              |
| 1:S:316:LEU:HG    | 1:S:320:PHE:CE2    | 2.55                     | 0.41              |
| 1:S:1080:ARG:HA   | 1:S:1080:ARG:HH21  | 1.86                     | 0.41              |
| 1:S:1422:LEU:HD21 | 1:S:1433:SER:HB3   | 2.03                     | 0.41              |
| 10:U:32:LEU:HD12  | 10:U:71:CYS:SG     | 2.60                     | 0.41              |
| 10:U:65:ARG:HA    | 10:U:68:ILE:HG22   | 2.01                     | 0.41              |
| 11:V:265:LEU:HD12 | 11:V:265:LEU:HA    | 1.90                     | 0.41              |
| 11:V:443:LEU:HD22 | 11:V:451:ILE:HG23  | 2.03                     | 0.41              |
| 11:V:1001:PHE:HD2 | 11:V:1004:LEU:HD22 | 1.86                     | 0.41              |
| 11:V:1041:ASN:OD1 | 11:V:1042:HIS:N    | 2.54                     | 0.41              |
| 1:A:376:GLN:HG3   | 1:A:410:TRP:CE3    | 2.56                     | 0.41              |
| 1:A:471:VAL:HG22  | 1:A:510:TYR:OH     | 2.21                     | 0.41              |
| 2:B:279:LEU:HD23  | 2:B:303:PHE:CE1    | 2.55                     | 0.41              |
| 2:B:756:ILE:HG23  | 8:P:866:LEU:CD1    | 2.51                     | 0.41              |
| 4:E:524:ARG:HG2   | 4:E:525:LYS:N      | 2.35                     | 0.41              |
| 6:G:345:GLN:O     | 6:G:349:ILE:HG12   | 2.21                     | 0.41              |
| 6:H:63:ALA:O      | 6:H:67:LEU:HD12    | 2.19                     | 0.41              |
| 7:M:218:LYS:O     | 7:M:218:LYS:HD3    | 2.20                     | 0.41              |
| 2:O:94:ILE:O      | 2:O:109:LEU:HD12   | 2.20                     | 0.41              |
| 2:O:323:GLU:O     | 2:O:324:LYS:CG     | 2.69                     | 0.41              |
| 8:P:384:GLU:O     | 8:P:385:GLU:HG2    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:809:GLN:O     | 8:P:813:THR:HG23  | 2.21                     | 0.41              |
| 8:Q:191:PRO:HD2   | 8:Q:194:LEU:HD22  | 2.03                     | 0.41              |
| 1:S:446:LEU:HB3   | 1:S:449:ALA:HB3   | 2.02                     | 0.41              |
| 1:S:1128:GLN:HB2  | 1:S:1173:TRP:CD2  | 2.54                     | 0.41              |
| 10:U:819:ARG:HA   | 10:U:819:ARG:HD2  | 1.93                     | 0.41              |
| 11:V:242:THR:HG22 | 11:V:246:LEU:CD1  | 2.51                     | 0.41              |
| 11:V:817:LYS:HA   | 11:V:820:VAL:HG12 | 2.02                     | 0.41              |
| 2:B:836:ARG:O     | 2:B:840:LEU:HG    | 2.21                     | 0.41              |
| 5:F:122:ARG:NE    | 5:F:122:ARG:HA    | 2.34                     | 0.41              |
| 2:O:331:ASP:OD1   | 2:O:332:ASP:N     | 2.48                     | 0.41              |
| 2:O:762:THR:HA    | 2:O:765:LYS:HE3   | 2.03                     | 0.41              |
| 8:P:32:GLU:HG3    | 8:P:33:ALA:H      | 1.86                     | 0.41              |
| 8:P:399:LEU:O     | 8:P:399:LEU:HD23  | 2.20                     | 0.41              |
| 8:Q:70:LEU:O      | 8:Q:74:ARG:N      | 2.54                     | 0.41              |
| 8:Q:287:ALA:C     | 8:Q:288:LEU:HD22  | 2.40                     | 0.41              |
| 1:S:193:LEU:HB3   | 1:S:241:MET:SD    | 2.60                     | 0.41              |
| 1:S:722:LEU:O     | 1:S:725:SER:OG    | 2.26                     | 0.41              |
| 1:S:1359:ASP:HA   | 1:S:1362:LEU:HD12 | 2.03                     | 0.41              |
| 10:U:421:LEU:O    | 10:U:422:GLY:C    | 2.59                     | 0.41              |
| 10:U:500:LEU:HA   | 10:U:503:VAL:HG12 | 2.03                     | 0.41              |
| 10:U:619:LEU:HD23 | 10:U:619:LEU:HA   | 1.94                     | 0.41              |
| 10:U:635:TYR:CE2  | 10:U:705:ILE:HG23 | 2.56                     | 0.41              |
| 11:V:296:GLU:HG2  | 11:V:297:VAL:N    | 2.36                     | 0.41              |
| 11:V:423:VAL:HG12 | 11:V:424:HIS:ND1  | 2.36                     | 0.41              |
| 11:V:477:LEU:HD23 | 11:V:477:LEU:HA   | 1.91                     | 0.41              |
| 11:V:646:PRO:HA   | 11:V:649:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:30:VAL:HG11   | 6:H:372:ALA:CB    | 2.51                     | 0.41              |
| 1:A:236:SER:HA    | 1:A:239:VAL:HG12  | 2.03                     | 0.41              |
| 1:A:410:TRP:O     | 1:A:414:LEU:HD23  | 2.21                     | 0.41              |
| 1:A:424:LEU:HD23  | 1:A:424:LEU:HA    | 1.93                     | 0.41              |
| 1:A:753:MET:SD    | 1:A:761:VAL:HG21  | 2.61                     | 0.41              |
| 1:A:1173:TRP:O    | 1:A:1177:LEU:HG   | 2.21                     | 0.41              |
| 1:A:1193:LEU:HD21 | 1:A:1197:LEU:HB2  | 2.03                     | 0.41              |
| 1:A:1272:HIS:CA   | 1:A:1281:LEU:HD21 | 2.50                     | 0.41              |
| 1:A:1293:GLU:HA   | 1:A:1296:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:1325:ASP:OD1  | 1:A:1326:GLN:NE2  | 2.54                     | 0.41              |
| 2:B:481:ARG:HD3   | 2:B:632:TYR:O     | 2.21                     | 0.41              |
| 2:B:725:THR:HG22  | 2:O:585:SER:HB3   | 2.01                     | 0.41              |
| 4:E:408:GLN:OE1   | 4:E:445:PRO:HD2   | 2.21                     | 0.41              |
| 6:G:31:GLN:O      | 6:G:39:ARG:NH1    | 2.49                     | 0.41              |
| 6:G:77:PHE:HE2    | 6:G:95:ASP:OD2    | 2.04                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:483:LEU:HD23  | 6:G:513:ARG:CG    | 2.51                     | 0.41              |
| 6:G:518:ILE:HD11  | 6:G:550:THR:HG22  | 2.02                     | 0.41              |
| 6:H:21:ASP:O      | 6:H:25:ARG:HD3    | 2.21                     | 0.41              |
| 6:H:90:GLU:OE1    | 6:H:90:GLU:N      | 2.51                     | 0.41              |
| 6:H:524:TRP:CE3   | 6:H:524:TRP:HA    | 2.56                     | 0.41              |
| 7:L:168:ASP:OD1   | 7:L:169:PHE:N     | 2.54                     | 0.41              |
| 7:M:29:ILE:HD11   | 7:M:88:LYS:HE3    | 2.03                     | 0.41              |
| 7:M:101:LEU:HD23  | 7:M:101:LEU:HA    | 1.88                     | 0.41              |
| 2:O:134:LEU:HD12  | 2:O:135:ARG:N     | 2.35                     | 0.41              |
| 2:O:146:HIS:CE1   | 2:O:149:ALA:HB3   | 2.56                     | 0.41              |
| 2:O:657:LYS:HE3   | 2:O:718:ILE:HG21  | 2.03                     | 0.41              |
| 8:P:136:LEU:HD21  | 8:P:199:SER:HB2   | 2.03                     | 0.41              |
| 8:Q:253:VAL:HG21  | 8:Q:258:LEU:HD12  | 2.03                     | 0.41              |
| 8:Q:325:LYS:HB3   | 8:Q:337:GLU:HG3   | 2.03                     | 0.41              |
| 8:Q:763:ASN:OD1   | 8:Q:764:VAL:N     | 2.53                     | 0.41              |
| 1:S:287:GLU:OE1   | 1:S:287:GLU:N     | 2.53                     | 0.41              |
| 1:S:393:VAL:HA    | 1:S:396:LEU:HD12  | 2.02                     | 0.41              |
| 1:S:722:LEU:HD21  | 1:S:753:MET:SD    | 2.61                     | 0.41              |
| 1:S:915:THR:HA    | 1:S:918:GLU:HG2   | 2.03                     | 0.41              |
| 1:S:1351:GLU:O    | 1:S:1414:SER:OG   | 2.31                     | 0.41              |
| 1:S:1392:PRO:O    | 1:S:1395:LEU:HB3  | 2.21                     | 0.41              |
| 10:U:75:LEU:HD12  | 10:U:81:LEU:HD11  | 2.03                     | 0.41              |
| 10:U:236:PHE:CE2  | 10:U:240:LEU:HD11 | 2.56                     | 0.41              |
| 10:U:606:TYR:HB3  | 10:U:670:CYS:SG   | 2.60                     | 0.41              |
| 10:U:757:ASN:ND2  | 10:U:770:ASP:HB2  | 2.35                     | 0.41              |
| 10:U:761:SER:OG   | 10:U:762:SER:N    | 2.53                     | 0.41              |
| 11:V:108:ASP:OD1  | 11:V:109:SER:N    | 2.54                     | 0.41              |
| 11:V:110:PHE:HZ   | 11:V:176:ILE:HD13 | 1.86                     | 0.41              |
| 11:V:387:ILE:HG12 | 11:V:431:MET:HE3  | 2.03                     | 0.41              |
| 11:V:791:ASN:HB3  | 11:V:926:ARG:HG2  | 2.02                     | 0.41              |
| 11:V:1128:PHE:HE2 | 11:V:1181:GLN:HB3 | 1.85                     | 0.41              |
| 11:V:1303:GLU:O   | 11:V:1307:LYS:HG2 | 2.21                     | 0.41              |
| 1:A:473:LEU:O     | 1:A:476:PHE:HB3   | 2.21                     | 0.41              |
| 1:A:662:ALA:O     | 1:A:665:THR:HG23  | 2.21                     | 0.41              |
| 1:A:1176:SER:HA   | 1:S:964:LEU:HD21  | 2.03                     | 0.41              |
| 1:A:1354:LEU:O    | 1:A:1358:VAL:HG13 | 2.21                     | 0.41              |
| 2:B:84:ASP:OD1    | 2:B:85:PHE:N      | 2.54                     | 0.41              |
| 2:B:324:LYS:O     | 2:B:325:LEU:HB2   | 2.21                     | 0.41              |
| 3:C:146:TYR:HD1   | 3:C:146:TYR:HA    | 1.81                     | 0.41              |
| 4:E:373:LEU:HD23  | 4:E:373:LEU:HA    | 1.92                     | 0.41              |
| 6:G:541:VAL:HG21  | 6:G:554:LEU:CD2   | 2.51                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:L:237:ASN:O     | 7:L:251:CYS:HA     | 2.21                     | 0.41              |
| 7:M:167:VAL:HG21  | 7:M:169:PHE:CE2    | 2.55                     | 0.41              |
| 2:O:522:LYS:C     | 2:O:523:CYS:SG     | 2.99                     | 0.41              |
| 1:S:45:GLU:HA     | 1:S:48:VAL:HG12    | 2.03                     | 0.41              |
| 1:S:362:LEU:HD23  | 1:S:365:MET:SD     | 2.61                     | 0.41              |
| 10:U:910:GLU:OE2  | 10:U:914:LYS:HE3   | 2.21                     | 0.41              |
| 1:A:310:VAL:O     | 8:P:831:ARG:NE     | 2.54                     | 0.40              |
| 1:A:1017:ILE:HD13 | 1:A:1017:ILE:HA    | 1.94                     | 0.40              |
| 2:B:279:LEU:HD23  | 2:B:303:PHE:HZ     | 1.84                     | 0.40              |
| 2:B:690:GLU:H     | 2:B:690:GLU:CD     | 2.23                     | 0.40              |
| 2:B:780:HIS:NE2   | 2:B:831:SER:HB3    | 2.36                     | 0.40              |
| 3:C:328:LYS:HE3   | 3:C:329:ALA:HB2    | 2.03                     | 0.40              |
| 5:F:238:VAL:HG12  | 5:F:270:LEU:HD21   | 2.03                     | 0.40              |
| 6:G:38:ARG:O      | 6:G:42:LEU:HD13    | 2.21                     | 0.40              |
| 6:G:178:LEU:HD12  | 6:G:178:LEU:HA     | 1.91                     | 0.40              |
| 6:G:388:PRO:O     | 6:G:501:GLN:NE2    | 2.54                     | 0.40              |
| 7:M:134:SER:OG    | 7:M:135:THR:N      | 2.54                     | 0.40              |
| 7:M:147:GLU:OE1   | 7:M:147:GLU:N      | 2.54                     | 0.40              |
| 2:O:106:GLU:O     | 2:O:107:TYR:HB2    | 2.20                     | 0.40              |
| 8:P:367:CYS:HA    | 8:P:392:PRO:HA     | 2.04                     | 0.40              |
| 8:Q:86:TYR:CE2    | 8:Q:123:CYS:HB2    | 2.57                     | 0.40              |
| 8:Q:232:ASP:OD1   | 8:Q:233:ALA:N      | 2.49                     | 0.40              |
| 8:Q:582:LEU:O     | 8:Q:582:LEU:HG     | 2.21                     | 0.40              |
| 1:S:156:LEU:HD23  | 1:S:190:ILE:HD13   | 2.03                     | 0.40              |
| 1:S:1071:ARG:O    | 1:S:1075:LEU:HG    | 2.21                     | 0.40              |
| 10:U:270:THR:HA   | 10:U:273:LEU:HD12  | 2.01                     | 0.40              |
| 10:U:611:ASP:OD1  | 10:U:614:ARG:NH1   | 2.44                     | 0.40              |
| 11:V:668:SER:HA   | 11:V:761:PHE:HZ    | 1.86                     | 0.40              |
| 11:V:927:GLU:OE2  | 11:V:1001:PHE:HA   | 2.21                     | 0.40              |
| 11:V:1289:PRO:HA  | 11:V:1352:ARG:HH12 | 1.85                     | 0.40              |
| 1:A:363:PHE:HB3   | 1:A:400:PHE:CZ     | 2.56                     | 0.40              |
| 1:A:931:ASP:O     | 1:A:935:LEU:HG     | 2.20                     | 0.40              |
| 1:A:1392:PRO:HA   | 1:A:1395:LEU:CG    | 2.50                     | 0.40              |
| 2:B:774:SER:HB2   | 8:P:834:HIS:ND1    | 2.36                     | 0.40              |
| 3:C:364:TRP:CH2   | 3:C:538:ILE:HG13   | 2.54                     | 0.40              |
| 4:E:351:LEU:HG    | 4:E:352:SER:O      | 2.21                     | 0.40              |
| 4:E:356:SER:HB3   | 7:M:73:ARG:HD2     | 2.02                     | 0.40              |
| 6:H:137:SER:OG    | 6:H:190:GLU:HG3    | 2.21                     | 0.40              |
| 6:H:395:GLU:HA    | 6:H:398:LEU:HD12   | 2.02                     | 0.40              |
| 7:M:226:ARG:HD3   | 7:M:226:ARG:HA     | 1.97                     | 0.40              |
| 8:P:67:LEU:HD22   | 8:P:76:LEU:HD21    | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Q:588:GLU:HB3   | 8:Q:591:GLY:HA3   | 2.03                     | 0.40              |
| 10:U:15:ASP:OD1   | 10:U:16:LYS:HG2   | 2.21                     | 0.40              |
| 10:U:66:ARG:HH12  | 10:U:70:THR:HG23  | 1.87                     | 0.40              |
| 10:U:102:GLY:HA3  | 10:U:144:LEU:HD11 | 2.02                     | 0.40              |
| 10:U:365:LEU:HB3  | 10:U:369:LYS:NZ   | 2.36                     | 0.40              |
| 10:U:968:ASN:HA   | 10:U:971:SER:HG   | 1.86                     | 0.40              |
| 11:V:211:ILE:O    | 11:V:214:SER:OG   | 2.29                     | 0.40              |
| 11:V:281:ILE:O    | 11:V:284:PHE:HB3  | 2.20                     | 0.40              |
| 11:V:568:PHE:CD2  | 11:V:851:THR:HG21 | 2.54                     | 0.40              |
| 11:V:794:ARG:NE   | 11:V:926:ARG:O    | 2.42                     | 0.40              |
| 11:V:1031:HIS:CE1 | 11:V:1062:TYR:HB2 | 2.57                     | 0.40              |
| 1:A:1048:LEU:HD23 | 1:A:1048:LEU:HA   | 1.95                     | 0.40              |
| 2:B:73:HIS:NE2    | 2:B:101:LYS:HE2   | 2.36                     | 0.40              |
| 2:B:90:ASN:C      | 2:B:91:LEU:HG     | 2.41                     | 0.40              |
| 3:C:415:ALA:HB1   | 3:C:450:LEU:HD21  | 2.03                     | 0.40              |
| 4:E:141:ARG:HB3   | 4:E:147:GLY:HA3   | 2.03                     | 0.40              |
| 6:G:251:ALA:O     | 6:G:254:SER:OG    | 2.26                     | 0.40              |
| 6:G:389:PRO:HA    | 6:G:501:GLN:HE22  | 1.86                     | 0.40              |
| 6:G:457:LEU:HB2   | 6:G:479:CYS:SG    | 2.62                     | 0.40              |
| 6:G:473:ILE:HG21  | 6:G:524:TRP:CH2   | 2.56                     | 0.40              |
| 6:G:565:ASP:OD1   | 6:G:566:GLU:HG3   | 2.21                     | 0.40              |
| 7:M:207:ILE:HD11  | 7:M:280:VAL:HG21  | 2.02                     | 0.40              |
| 8:P:77:TYR:HE1    | 8:P:87:CYS:SG     | 2.43                     | 0.40              |
| 8:P:250:LEU:HD21  | 8:P:276:HIS:HB3   | 2.04                     | 0.40              |
| 1:S:555:ILE:HD11  | 1:S:599:SER:HB2   | 2.03                     | 0.40              |
| 1:S:822:LEU:HD21  | 1:S:824:CYS:SG    | 2.62                     | 0.40              |
| 10:U:290:VAL:O    | 10:U:294:LYS:N    | 2.55                     | 0.40              |
| 10:U:369:LYS:O    | 10:U:372:VAL:HG12 | 2.22                     | 0.40              |
| 11:V:792:TRP:NE1  | 11:V:796:ILE:HD11 | 2.35                     | 0.40              |
| 11:V:1010:GLN:NE2 | 11:V:1075:TRP:HE1 | 2.19                     | 0.40              |
| 11:V:1056:HIS:O   | 11:V:1059:SER:OG  | 2.36                     | 0.40              |
| 1:A:29:ARG:HD3    | 1:A:29:ARG:N      | 2.37                     | 0.40              |
| 1:A:214:LEU:HD13  | 1:A:273:MET:SD    | 2.61                     | 0.40              |
| 1:A:1134:PHE:CZ   | 1:A:1138:LEU:HD21 | 2.56                     | 0.40              |
| 1:A:1334:ALA:O    | 1:A:1338:LEU:HD23 | 2.22                     | 0.40              |
| 2:B:356:SER:OG    | 2:B:356:SER:O     | 2.39                     | 0.40              |
| 2:B:822:LYS:HA    | 2:B:825:GLN:HG3   | 2.02                     | 0.40              |
| 3:C:62:GLU:OE1    | 3:C:63:ARG:NH2    | 2.54                     | 0.40              |
| 6:H:237:SER:O     | 6:H:237:SER:OG    | 2.37                     | 0.40              |
| 7:L:125:LYS:HE2   | 7:L:187:TYR:CE2   | 2.56                     | 0.40              |
| 2:O:105:PHE:O     | 2:O:126:LEU:N     | 2.53                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:170:ILE:HG23   | 2:O:170:ILE:O      | 2.22                     | 0.40              |
| 2:O:237:VAL:CG2    | 2:O:258:ALA:HB1    | 2.51                     | 0.40              |
| 2:O:520:LEU:CD2    | 8:P:518:GLN:HB3    | 2.49                     | 0.40              |
| 2:O:749:SER:O      | 2:O:755:LEU:HD11   | 2.22                     | 0.40              |
| 8:P:27:ARG:C       | 8:P:400:ASN:ND2    | 2.71                     | 0.40              |
| 8:P:221:GLU:HG3    | 8:P:308:HIS:HB3    | 2.03                     | 0.40              |
| 8:P:572:LEU:HA     | 8:P:572:LEU:HD12   | 1.85                     | 0.40              |
| 8:Q:30:CYS:HB3     | 8:Q:35:VAL:HG12    | 2.02                     | 0.40              |
| 8:Q:192:HIS:HD2    | 8:Q:193:PHE:CE2    | 2.39                     | 0.40              |
| 1:S:92:SER:HA      | 1:S:154:TYR:CE2    | 2.55                     | 0.40              |
| 1:S:1243:ARG:HE    | 1:S:1286:HIS:CE1   | 2.39                     | 0.40              |
| 1:S:1319:LEU:HA    | 1:S:1322:VAL:HG12  | 2.03                     | 0.40              |
| 1:S:1336:TYR:HD2   | 1:S:1364:LEU:HD13  | 1.87                     | 0.40              |
| 10:U:605:LEU:HD13  | 10:U:605:LEU:HA    | 1.95                     | 0.40              |
| 10:U:718:LEU:HD23  | 10:U:725:LYS:HE2   | 2.04                     | 0.40              |
| 10:U:895:SER:OG    | 10:U:896:GLY:N     | 2.55                     | 0.40              |
| 10:U:1089:LEU:O    | 10:U:1093:GLU:HG3  | 2.21                     | 0.40              |
| 11:V:222:SER:HG    | 11:V:223:GLN:H     | 1.69                     | 0.40              |
| 11:V:794:ARG:HA    | 11:V:797:VAL:HG22  | 2.04                     | 0.40              |
| 11:V:1359:LEU:HA   | 11:V:1362:LYS:HE2  | 2.03                     | 0.40              |
| 1:A:1139:LEU:HD23  | 1:A:1143:LEU:HD12  | 2.03                     | 0.40              |
| 1:A:1155:ILE:HD13  | 1:A:1158:LYS:NZ    | 2.36                     | 0.40              |
| 1:A:1255:GLU:HG3   | 1:A:1259:PHE:CE2   | 2.57                     | 0.40              |
| 3:C:72:ALA:O       | 3:C:76:TRP:HE3     | 2.04                     | 0.40              |
| 3:C:127:PHE:HA     | 5:F:147:ARG:NH2    | 2.37                     | 0.40              |
| 3:C:287:HIS:ND1    | 3:C:289:ALA:HB3    | 2.36                     | 0.40              |
| 4:E:37:PRO:C       | 4:E:39:GLY:H       | 2.24                     | 0.40              |
| 4:E:140:LEU:HA     | 4:E:140:LEU:HD12   | 1.82                     | 0.40              |
| 4:E:313:LEU:HA     | 4:E:313:LEU:HD12   | 1.89                     | 0.40              |
| 4:E:396:TYR:HB3    | 4:E:397:PRO:HD3    | 2.03                     | 0.40              |
| 5:F:260:LEU:O      | 5:F:264:THR:HG23   | 2.21                     | 0.40              |
| 6:G:414:LEU:HD21   | 6:G:462:ALA:HB3    | 2.02                     | 0.40              |
| 6:H:342:THR:O      | 6:H:345:GLN:N      | 2.55                     | 0.40              |
| 2:O:509:LEU:O      | 2:O:595:CYS:HA     | 2.22                     | 0.40              |
| 8:Q:673:ARG:HG2    | 8:Q:677:ALA:CB     | 2.52                     | 0.40              |
| 1:S:428:VAL:HG22   | 1:S:476:PHE:CZ     | 2.56                     | 0.40              |
| 10:U:1060:ILE:HG13 | 10:U:1061:ASP:N    | 2.35                     | 0.40              |
| 11:V:765:LEU:HD22  | 11:V:786:ILE:HG13  | 2.03                     | 0.40              |
| 11:V:1037:LEU:O    | 11:V:1041:ASN:ND2  | 2.55                     | 0.40              |
| 11:V:1089:SER:O    | 11:V:1093:VAL:HG23 | 2.21                     | 0.40              |
| 11:V:1234:PHE:O    | 11:V:1238:MET:HB2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed          | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1160/1477 (78%)   | 1066 (92%) | 86 (7%)  | 8 (1%)   | 22          | 62  |
| 1   | S     | 1224/1477 (83%)   | 1126 (92%) | 98 (8%)  | 0        | 100         | 100 |
| 2   | B     | 685/884 (78%)     | 595 (87%)  | 75 (11%) | 15 (2%)  | 6           | 38  |
| 2   | O     | 685/884 (78%)     | 592 (86%)  | 84 (12%) | 9 (1%)   | 12          | 48  |
| 3   | C     | 546/583 (94%)     | 496 (91%)  | 48 (9%)  | 2 (0%)   | 34          | 72  |
| 4   | E     | 411/555 (74%)     | 400 (97%)  | 9 (2%)   | 2 (0%)   | 29          | 68  |
| 5   | F     | 336/399 (84%)     | 316 (94%)  | 20 (6%)  | 0        | 100         | 100 |
| 6   | G     | 567/641 (88%)     | 514 (91%)  | 52 (9%)  | 1 (0%)   | 47          | 80  |
| 6   | H     | 532/641 (83%)     | 491 (92%)  | 40 (8%)  | 1 (0%)   | 47          | 80  |
| 7   | L     | 368/394 (93%)     | 334 (91%)  | 33 (9%)  | 1 (0%)   | 41          | 76  |
| 7   | M     | 368/394 (93%)     | 333 (90%)  | 32 (9%)  | 3 (1%)   | 19          | 60  |
| 8   | P     | 726/906 (80%)     | 626 (86%)  | 80 (11%) | 20 (3%)  | 5           | 33  |
| 8   | Q     | 732/906 (81%)     | 644 (88%)  | 74 (10%) | 14 (2%)  | 8           | 41  |
| 9   | W     | 21/39 (54%)       | 13 (62%)   | 8 (38%)  | 0        | 100         | 100 |
| 10  | U     | 1150/1328 (87%)   | 1056 (92%) | 88 (8%)  | 6 (0%)   | 29          | 68  |
| 11  | V     | 1131/1451 (78%)   | 1060 (94%) | 65 (6%)  | 6 (0%)   | 29          | 68  |
| All | All   | 10642/12959 (82%) | 9662 (91%) | 892 (8%) | 88 (1%)  | 24          | 60  |

All (88) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 754 | CYS  |
| 2   | B     | 148 | LYS  |
| 2   | B     | 324 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 353 | PRO  |
| 2   | O     | 147 | VAL  |
| 2   | O     | 324 | LYS  |
| 2   | O     | 637 | PRO  |
| 8   | P     | 449 | GLU  |
| 8   | P     | 572 | LEU  |
| 8   | P     | 721 | ASP  |
| 8   | Q     | 49  | GLN  |
| 8   | Q     | 720 | LYS  |
| 8   | Q     | 782 | ILE  |
| 1   | A     | 288 | GLU  |
| 1   | A     | 947 | SER  |
| 1   | A     | 972 | GLY  |
| 2   | B     | 133 | GLY  |
| 2   | B     | 147 | VAL  |
| 2   | B     | 316 | PHE  |
| 2   | B     | 325 | LEU  |
| 3   | C     | 23  | ASP  |
| 4   | E     | 77  | PRO  |
| 7   | M     | 108 | PRO  |
| 2   | O     | 83  | SER  |
| 2   | O     | 638 | LYS  |
| 8   | P     | 32  | GLU  |
| 8   | P     | 720 | LYS  |
| 8   | P     | 750 | ALA  |
| 8   | P     | 781 | PRO  |
| 8   | P     | 782 | ILE  |
| 8   | Q     | 572 | LEU  |
| 8   | Q     | 649 | MET  |
| 8   | Q     | 781 | PRO  |
| 10  | U     | 296 | GLY  |
| 10  | U     | 356 | HIS  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 313 | LYS  |
| 2   | B     | 354 | LEU  |
| 3   | C     | 279 | SER  |
| 7   | L     | 216 | PRO  |
| 7   | M     | 105 | PRO  |
| 7   | M     | 216 | PRO  |
| 8   | P     | 384 | GLU  |
| 8   | P     | 860 | CYS  |
| 8   | Q     | 518 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | Q     | 538  | ASP  |
| 8   | Q     | 586  | PRO  |
| 11  | V     | 307  | LEU  |
| 11  | V     | 414  | GLU  |
| 11  | V     | 753  | ASP  |
| 11  | V     | 767  | PRO  |
| 11  | V     | 777  | LYS  |
| 1   | A     | 287  | GLU  |
| 1   | A     | 1221 | ASN  |
| 2   | B     | 78   | CYS  |
| 6   | H     | 239  | LEU  |
| 2   | O     | 217  | LEU  |
| 8   | P     | 63   | GLN  |
| 8   | P     | 387  | PRO  |
| 8   | P     | 727  | PRO  |
| 8   | P     | 875  | HIS  |
| 8   | Q     | 557  | ASP  |
| 10  | U     | 120  | SER  |
| 10  | U     | 978  | ASN  |
| 2   | B     | 140  | PRO  |
| 6   | G     | 192  | ASP  |
| 2   | O     | 84   | ASP  |
| 8   | P     | 557  | ASP  |
| 8   | Q     | 674  | ASP  |
| 8   | Q     | 721  | ASP  |
| 1   | A     | 755  | GLY  |
| 8   | P     | 148  | ALA  |
| 8   | P     | 166  | PRO  |
| 8   | P     | 595  | PRO  |
| 8   | Q     | 595  | PRO  |
| 10  | U     | 376  | ASP  |
| 2   | B     | 273  | PRO  |
| 2   | B     | 637  | PRO  |
| 8   | P     | 822  | ALA  |
| 10  | U     | 27   | GLY  |
| 1   | A     | 1222 | PRO  |
| 2   | B     | 712  | PRO  |
| 2   | O     | 140  | PRO  |
| 2   | O     | 636  | PHE  |
| 8   | P     | 161  | GLY  |
| 11  | V     | 379  | VAL  |
| 8   | Q     | 573  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 610 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |    |
|-----|-------|------------------|-------------|----------|-------------|----|
| 1   | A     | 1034/1282 (81%)  | 1028 (99%)  | 6 (1%)   | 86          | 92 |
| 1   | S     | 1092/1282 (85%)  | 1090 (100%) | 2 (0%)   | 93          | 96 |
| 2   | B     | 644/810 (80%)    | 640 (99%)   | 4 (1%)   | 86          | 92 |
| 2   | O     | 641/810 (79%)    | 635 (99%)   | 6 (1%)   | 78          | 87 |
| 3   | C     | 480/507 (95%)    | 477 (99%)   | 3 (1%)   | 86          | 92 |
| 4   | E     | 358/467 (77%)    | 354 (99%)   | 4 (1%)   | 73          | 84 |
| 5   | F     | 288/336 (86%)    | 287 (100%)  | 1 (0%)   | 92          | 95 |
| 6   | G     | 483/538 (90%)    | 480 (99%)   | 3 (1%)   | 86          | 92 |
| 6   | H     | 454/538 (84%)    | 451 (99%)   | 3 (1%)   | 84          | 90 |
| 7   | L     | 334/354 (94%)    | 331 (99%)   | 3 (1%)   | 78          | 87 |
| 7   | M     | 334/354 (94%)    | 333 (100%)  | 1 (0%)   | 92          | 95 |
| 8   | P     | 627/749 (84%)    | 614 (98%)   | 13 (2%)  | 53          | 71 |
| 8   | Q     | 630/749 (84%)    | 627 (100%)  | 3 (0%)   | 88          | 93 |
| 9   | W     | 22/22 (100%)     | 21 (96%)    | 1 (4%)   | 27          | 54 |
| 10  | U     | 1066/1204 (88%)  | 1052 (99%)  | 14 (1%)  | 69          | 82 |
| 11  | V     | 1065/1324 (80%)  | 1049 (98%)  | 16 (2%)  | 65          | 80 |
| All | All   | 9552/11326 (84%) | 9469 (99%)  | 83 (1%)  | 79          | 87 |

All (83) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 29  | ARG  |
| 1   | A     | 30  | VAL  |
| 1   | A     | 714 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 845  | LEU  |
| 1   | A     | 1032 | GLN  |
| 1   | A     | 1308 | LEU  |
| 2   | B     | 353  | CYS  |
| 2   | B     | 401  | CYS  |
| 2   | B     | 521  | LEU  |
| 2   | B     | 523  | CYS  |
| 3   | C     | 66   | THR  |
| 3   | C     | 146  | TYR  |
| 3   | C     | 343  | TYR  |
| 4   | E     | 90   | LEU  |
| 4   | E     | 98   | LEU  |
| 4   | E     | 295  | LEU  |
| 4   | E     | 524  | ARG  |
| 5   | F     | 101  | ARG  |
| 6   | G     | 23   | LEU  |
| 6   | G     | 89   | THR  |
| 6   | G     | 594  | GLU  |
| 6   | H     | 12   | CYS  |
| 6   | H     | 373  | LEU  |
| 6   | H     | 538  | LEU  |
| 7   | L     | 30   | SER  |
| 7   | L     | 46   | LEU  |
| 7   | L     | 152  | LEU  |
| 7   | M     | 297  | ILE  |
| 2   | O     | 9    | SER  |
| 2   | O     | 477  | LYS  |
| 2   | O     | 505  | THR  |
| 2   | O     | 611  | LYS  |
| 2   | O     | 640  | LYS  |
| 2   | O     | 779  | LYS  |
| 8   | P     | 16   | CYS  |
| 8   | P     | 199  | SER  |
| 8   | P     | 201  | SER  |
| 8   | P     | 219  | THR  |
| 8   | P     | 315  | PHE  |
| 8   | P     | 390  | LEU  |
| 8   | P     | 399  | LEU  |
| 8   | P     | 402  | CYS  |
| 8   | P     | 567  | ILE  |
| 8   | P     | 607  | ARG  |
| 8   | P     | 643  | SER  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 8   | P     | 655  | PHE  |
| 8   | P     | 839  | THR  |
| 8   | Q     | 222  | ASP  |
| 8   | Q     | 252  | CYS  |
| 8   | Q     | 339  | ARG  |
| 1   | S     | 32   | ARG  |
| 1   | S     | 460  | ARG  |
| 9   | W     | 79   | THR  |
| 10  | U     | 11   | GLU  |
| 10  | U     | 306  | SER  |
| 10  | U     | 307  | PRO  |
| 10  | U     | 369  | LYS  |
| 10  | U     | 435  | MET  |
| 10  | U     | 483  | GLU  |
| 10  | U     | 495  | THR  |
| 10  | U     | 615  | ARG  |
| 10  | U     | 750  | CYS  |
| 10  | U     | 753  | LEU  |
| 10  | U     | 898  | LYS  |
| 10  | U     | 905  | SER  |
| 10  | U     | 976  | ASP  |
| 10  | U     | 1199 | LYS  |
| 11  | V     | 91   | LYS  |
| 11  | V     | 135  | LEU  |
| 11  | V     | 185  | ARG  |
| 11  | V     | 302  | ARG  |
| 11  | V     | 310  | CYS  |
| 11  | V     | 342  | CYS  |
| 11  | V     | 371  | THR  |
| 11  | V     | 378  | LYS  |
| 11  | V     | 436  | LEU  |
| 11  | V     | 562  | GLN  |
| 11  | V     | 729  | CYS  |
| 11  | V     | 774  | MET  |
| 11  | V     | 1015 | CYS  |
| 11  | V     | 1130 | CYS  |
| 11  | V     | 1228 | ARG  |
| 11  | V     | 1364 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (163) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 55   | GLN  |
| 1   | A     | 123  | GLN  |
| 1   | A     | 158  | HIS  |
| 1   | A     | 200  | HIS  |
| 1   | A     | 248  | GLN  |
| 1   | A     | 292  | HIS  |
| 1   | A     | 343  | GLN  |
| 1   | A     | 352  | HIS  |
| 1   | A     | 417  | GLN  |
| 1   | A     | 423  | GLN  |
| 1   | A     | 669  | GLN  |
| 1   | A     | 767  | GLN  |
| 1   | A     | 771  | HIS  |
| 1   | A     | 913  | HIS  |
| 1   | A     | 1057 | GLN  |
| 1   | A     | 1118 | ASN  |
| 1   | A     | 1128 | GLN  |
| 1   | A     | 1190 | GLN  |
| 1   | A     | 1272 | HIS  |
| 1   | A     | 1355 | HIS  |
| 1   | A     | 1437 | GLN  |
| 2   | B     | 73   | HIS  |
| 2   | B     | 99   | ASN  |
| 2   | B     | 306  | ASN  |
| 2   | B     | 431  | GLN  |
| 2   | B     | 525  | ASN  |
| 2   | B     | 656  | HIS  |
| 2   | B     | 670  | ASN  |
| 2   | B     | 679  | HIS  |
| 2   | B     | 846  | GLN  |
| 3   | C     | 107  | GLN  |
| 3   | C     | 212  | GLN  |
| 3   | C     | 441  | GLN  |
| 3   | C     | 468  | GLN  |
| 3   | C     | 493  | ASN  |
| 4   | E     | 123  | GLN  |
| 4   | E     | 163  | GLN  |
| 4   | E     | 359  | ASN  |
| 4   | E     | 455  | GLN  |
| 5   | F     | 7    | HIS  |
| 5   | F     | 43   | HIS  |
| 5   | F     | 63   | HIS  |
| 5   | F     | 144  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 149 | ASN  |
| 5   | F     | 211 | GLN  |
| 5   | F     | 244 | ASN  |
| 5   | F     | 283 | GLN  |
| 6   | G     | 20  | ASN  |
| 6   | G     | 31  | GLN  |
| 6   | G     | 94  | GLN  |
| 6   | G     | 140 | HIS  |
| 6   | G     | 201 | GLN  |
| 6   | G     | 501 | GLN  |
| 6   | G     | 510 | GLN  |
| 6   | G     | 511 | GLN  |
| 6   | G     | 547 | ASN  |
| 6   | G     | 553 | HIS  |
| 6   | H     | 20  | ASN  |
| 6   | H     | 31  | GLN  |
| 6   | H     | 224 | ASN  |
| 6   | H     | 456 | HIS  |
| 6   | H     | 461 | GLN  |
| 7   | L     | 37  | HIS  |
| 7   | L     | 99  | GLN  |
| 7   | L     | 189 | GLN  |
| 7   | L     | 272 | HIS  |
| 7   | L     | 331 | GLN  |
| 7   | M     | 37  | HIS  |
| 7   | M     | 76  | HIS  |
| 7   | M     | 148 | HIS  |
| 7   | M     | 331 | GLN  |
| 7   | M     | 335 | GLN  |
| 7   | M     | 350 | GLN  |
| 2   | O     | 10  | ASN  |
| 2   | O     | 71  | ASN  |
| 2   | O     | 73  | HIS  |
| 2   | O     | 90  | ASN  |
| 2   | O     | 116 | ASN  |
| 2   | O     | 270 | ASN  |
| 2   | O     | 350 | ASN  |
| 2   | O     | 608 | ASN  |
| 2   | O     | 656 | HIS  |
| 2   | O     | 679 | HIS  |
| 2   | O     | 724 | GLN  |
| 2   | O     | 729 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | O     | 733  | ASN  |
| 2   | O     | 746  | ASN  |
| 8   | P     | 66   | HIS  |
| 8   | P     | 192  | HIS  |
| 8   | P     | 249  | GLN  |
| 8   | P     | 277  | HIS  |
| 8   | P     | 317  | HIS  |
| 8   | P     | 382  | GLN  |
| 8   | P     | 734  | GLN  |
| 8   | P     | 815  | GLN  |
| 8   | P     | 845  | GLN  |
| 8   | Q     | 92   | HIS  |
| 8   | Q     | 192  | HIS  |
| 8   | Q     | 360  | HIS  |
| 8   | Q     | 400  | ASN  |
| 8   | Q     | 531  | ASN  |
| 8   | Q     | 589  | ASN  |
| 8   | Q     | 734  | GLN  |
| 8   | Q     | 815  | GLN  |
| 8   | Q     | 845  | GLN  |
| 1   | S     | 123  | GLN  |
| 1   | S     | 186  | HIS  |
| 1   | S     | 227  | HIS  |
| 1   | S     | 374  | HIS  |
| 1   | S     | 492  | HIS  |
| 1   | S     | 563  | ASN  |
| 1   | S     | 582  | HIS  |
| 1   | S     | 716  | HIS  |
| 1   | S     | 913  | HIS  |
| 1   | S     | 986  | ASN  |
| 1   | S     | 1128 | GLN  |
| 1   | S     | 1437 | GLN  |
| 10  | U     | 110  | ASN  |
| 10  | U     | 172  | GLN  |
| 10  | U     | 266  | HIS  |
| 10  | U     | 298  | GLN  |
| 10  | U     | 304  | ASN  |
| 10  | U     | 320  | GLN  |
| 10  | U     | 325  | GLN  |
| 10  | U     | 345  | GLN  |
| 10  | U     | 373  | HIS  |
| 10  | U     | 417  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | U     | 433  | HIS  |
| 10  | U     | 465  | ASN  |
| 10  | U     | 580  | ASN  |
| 10  | U     | 597  | GLN  |
| 10  | U     | 621  | ASN  |
| 10  | U     | 673  | HIS  |
| 10  | U     | 836  | ASN  |
| 10  | U     | 929  | GLN  |
| 10  | U     | 973  | GLN  |
| 10  | U     | 978  | ASN  |
| 10  | U     | 1071 | HIS  |
| 10  | U     | 1091 | GLN  |
| 10  | U     | 1137 | GLN  |
| 10  | U     | 1193 | ASN  |
| 10  | U     | 1204 | HIS  |
| 10  | U     | 1278 | HIS  |
| 11  | V     | 66   | ASN  |
| 11  | V     | 72   | GLN  |
| 11  | V     | 76   | GLN  |
| 11  | V     | 81   | GLN  |
| 11  | V     | 86   | HIS  |
| 11  | V     | 146  | GLN  |
| 11  | V     | 198  | GLN  |
| 11  | V     | 377  | HIS  |
| 11  | V     | 471  | GLN  |
| 11  | V     | 545  | ASN  |
| 11  | V     | 562  | GLN  |
| 11  | V     | 746  | ASN  |
| 11  | V     | 748  | ASN  |
| 11  | V     | 937  | HIS  |
| 11  | V     | 1010 | GLN  |
| 11  | V     | 1026 | HIS  |
| 11  | V     | 1092 | HIS  |
| 11  | V     | 1258 | GLN  |
| 11  | V     | 1280 | ASN  |
| 11  | V     | 1355 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 9   | W     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | W     | 9:UNK     | C      | 73:GLU    | N      | 36.69        |
| 1     | W     | 95:TRP    | C      | 101:UNK   | N      | 7.00         |

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23086. These allow visual inspection of the internal detail of the map and identification of artifacts.

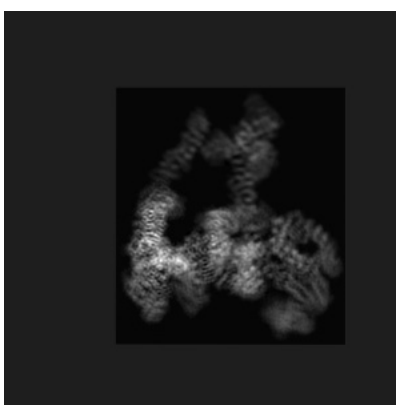
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

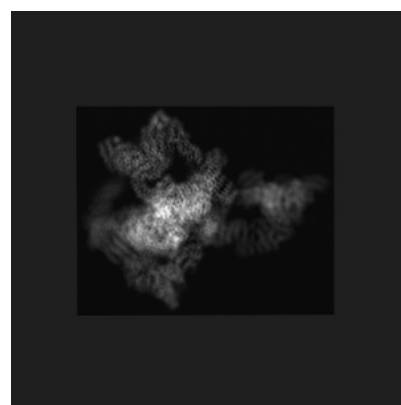
#### 6.1.1 Primary map



X



Y

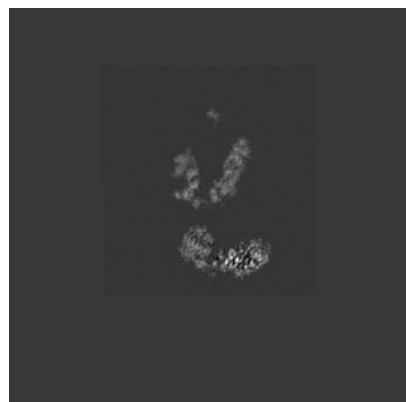


Z

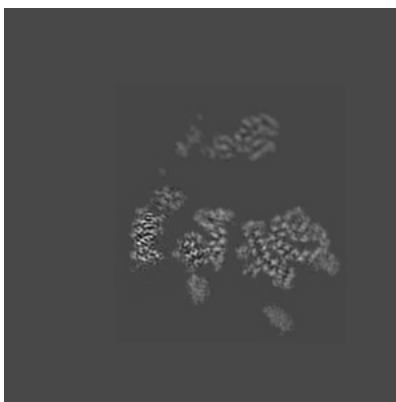
The images above show the map projected in three orthogonal directions.

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

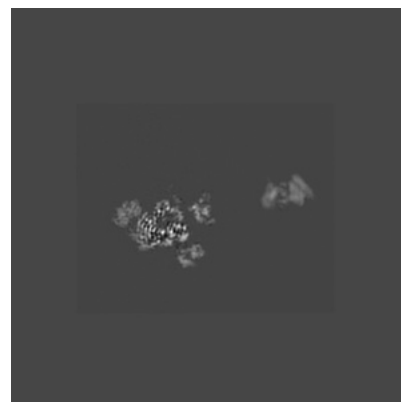
#### 6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

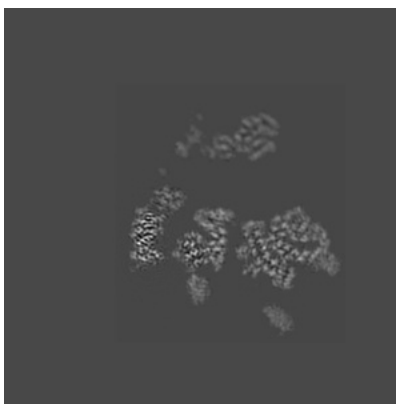
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 168



Y Index: 224



Z Index: 168

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

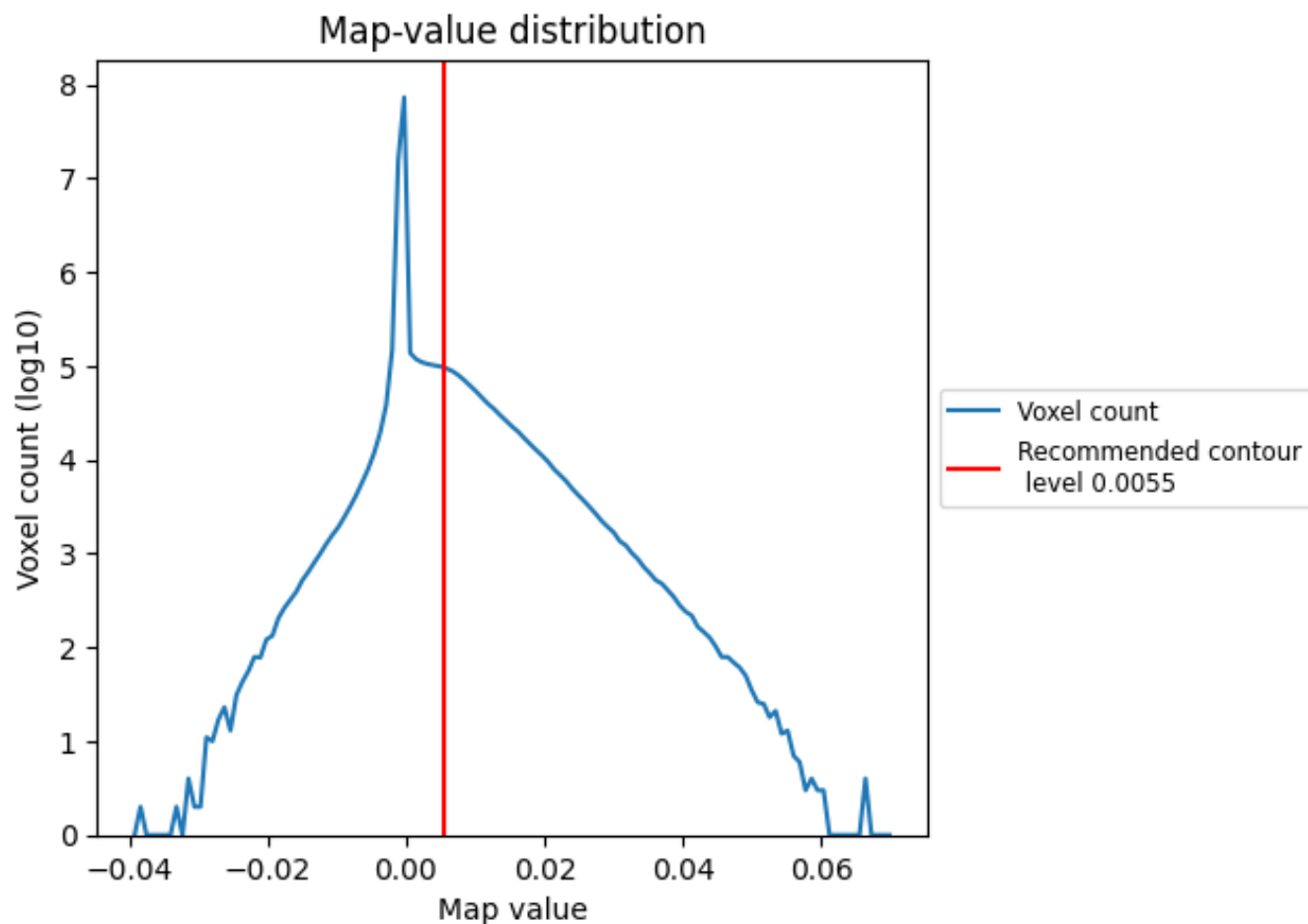
## 6.5 Mask visualisation

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.

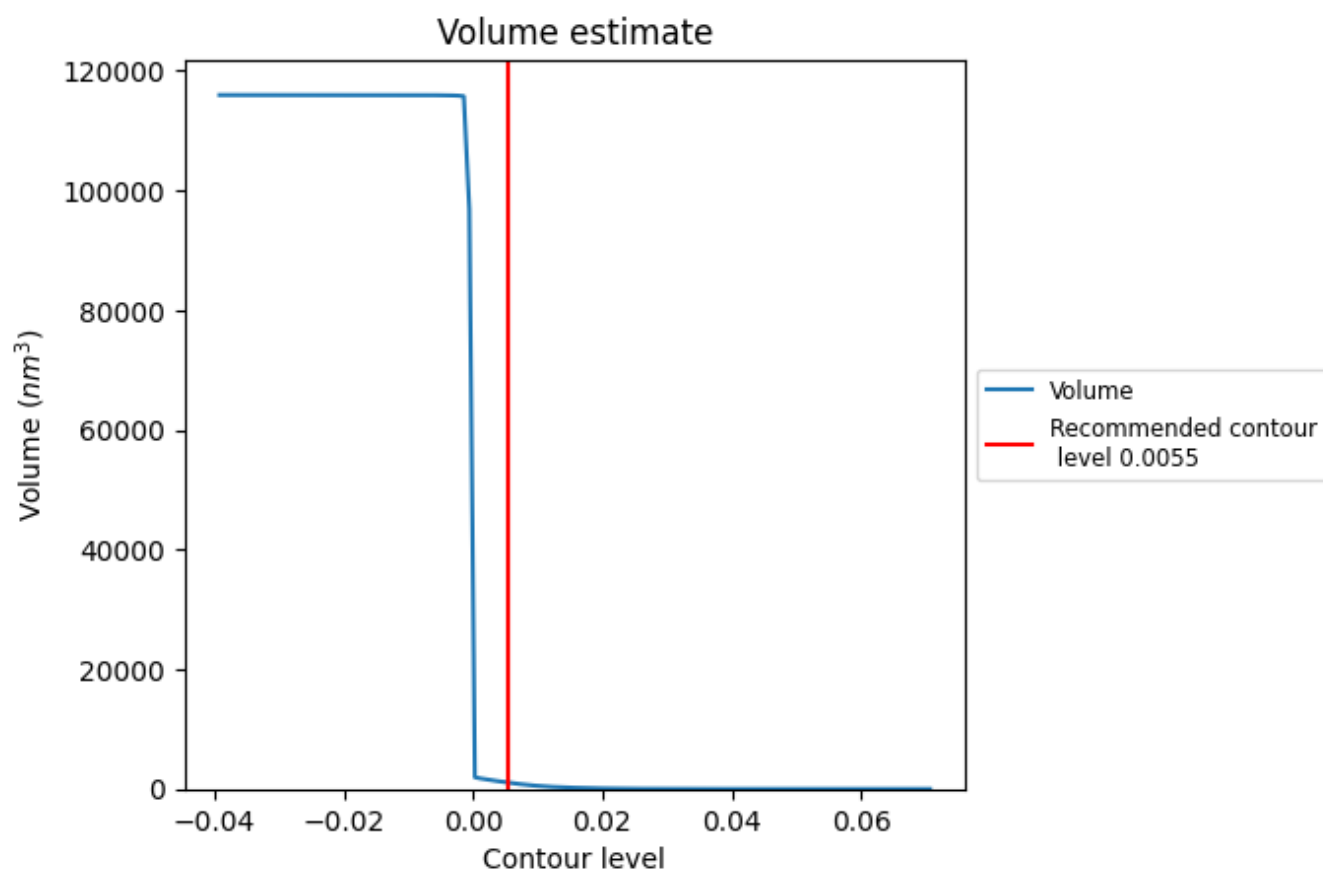
### 7.1 Map-value distribution [i](#)



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.



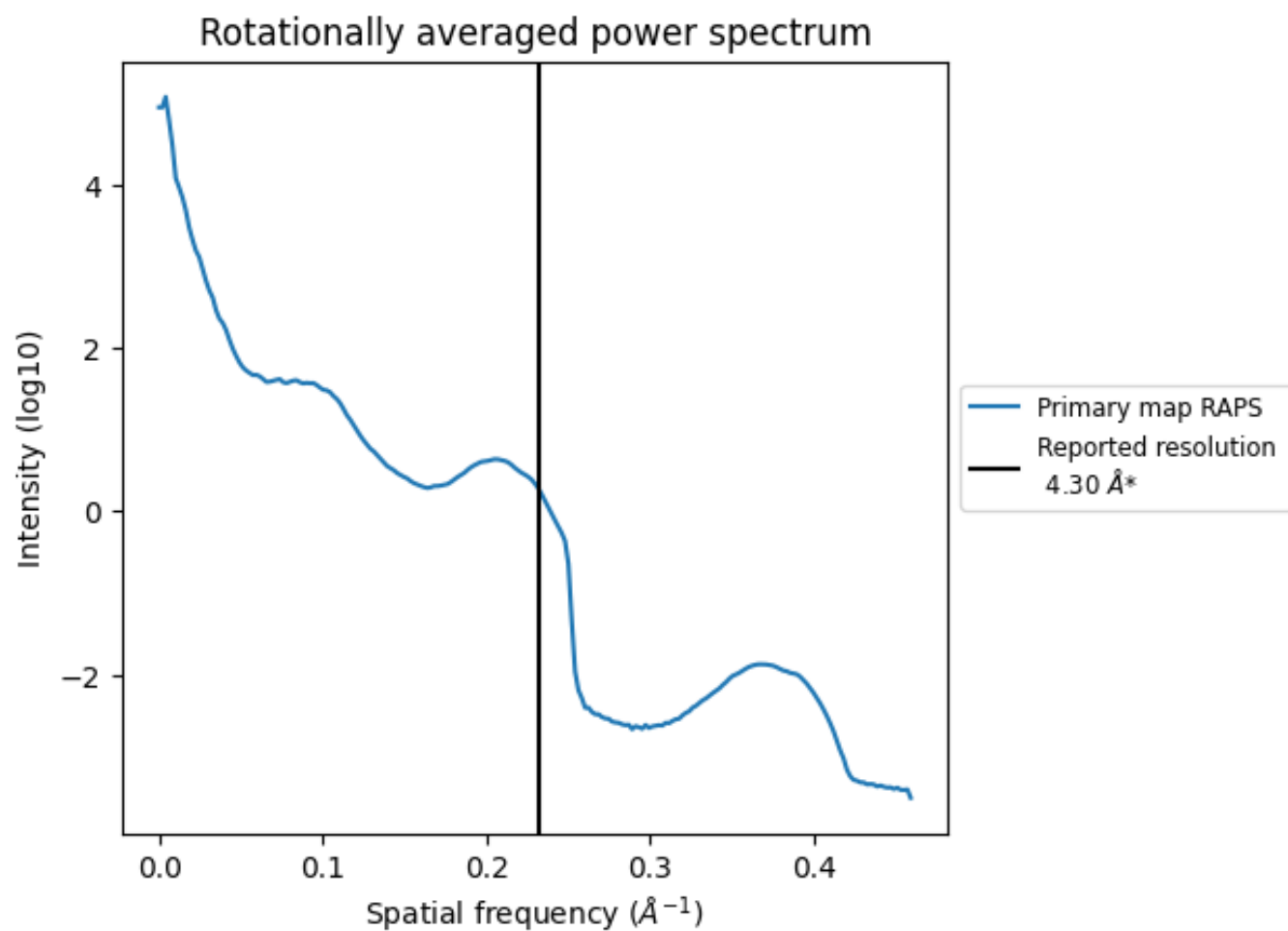
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1056  $\text{nm}^3$ ; this corresponds to an approximate mass of 954 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 0.233 Å<sup>-1</sup>

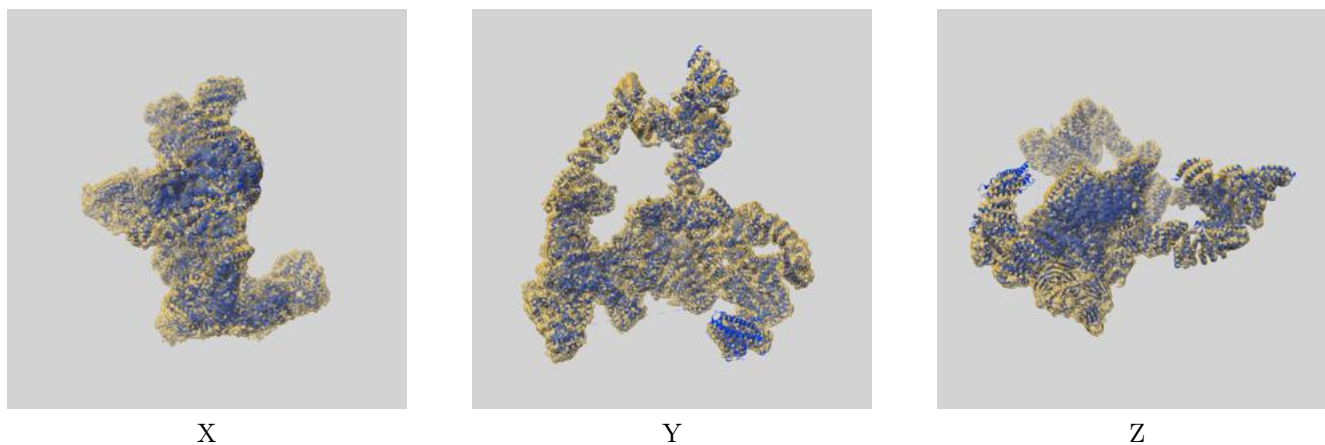
## 8 Fourier-Shell correlation

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

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

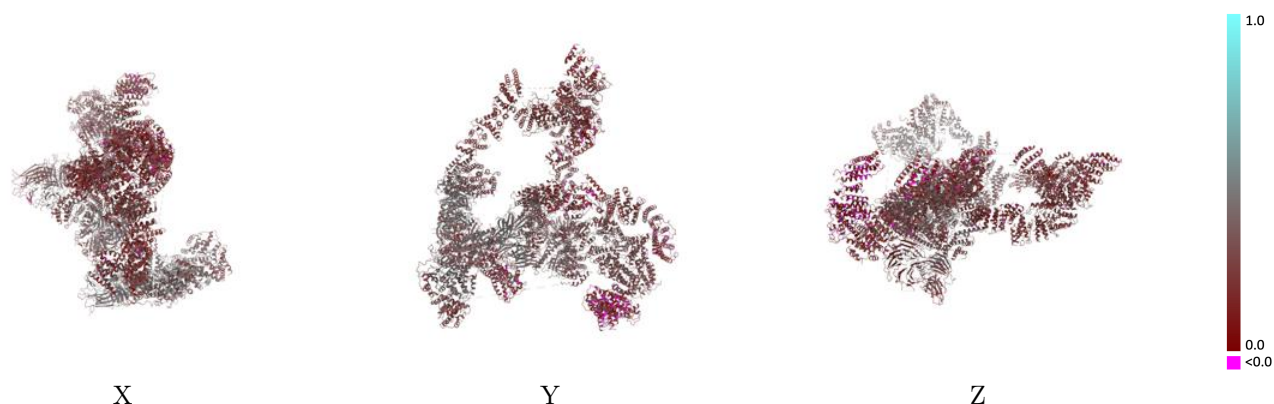
This section contains information regarding the fit between EMDB map EMD-23086 and PDB model 7KZQ. Per-residue inclusion information can be found in section 3 on page 14.

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



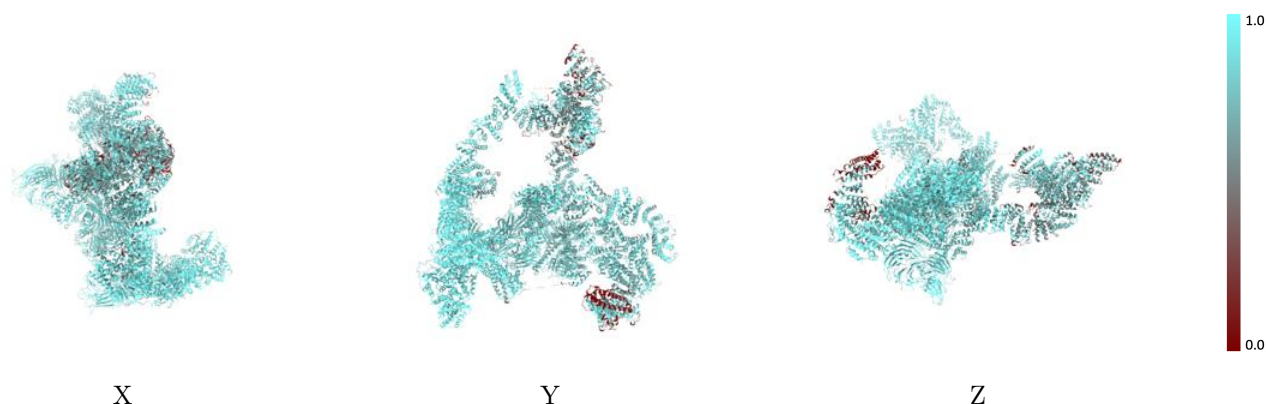
The images above show the 3D surface view of the map at the recommended contour level 0.0055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



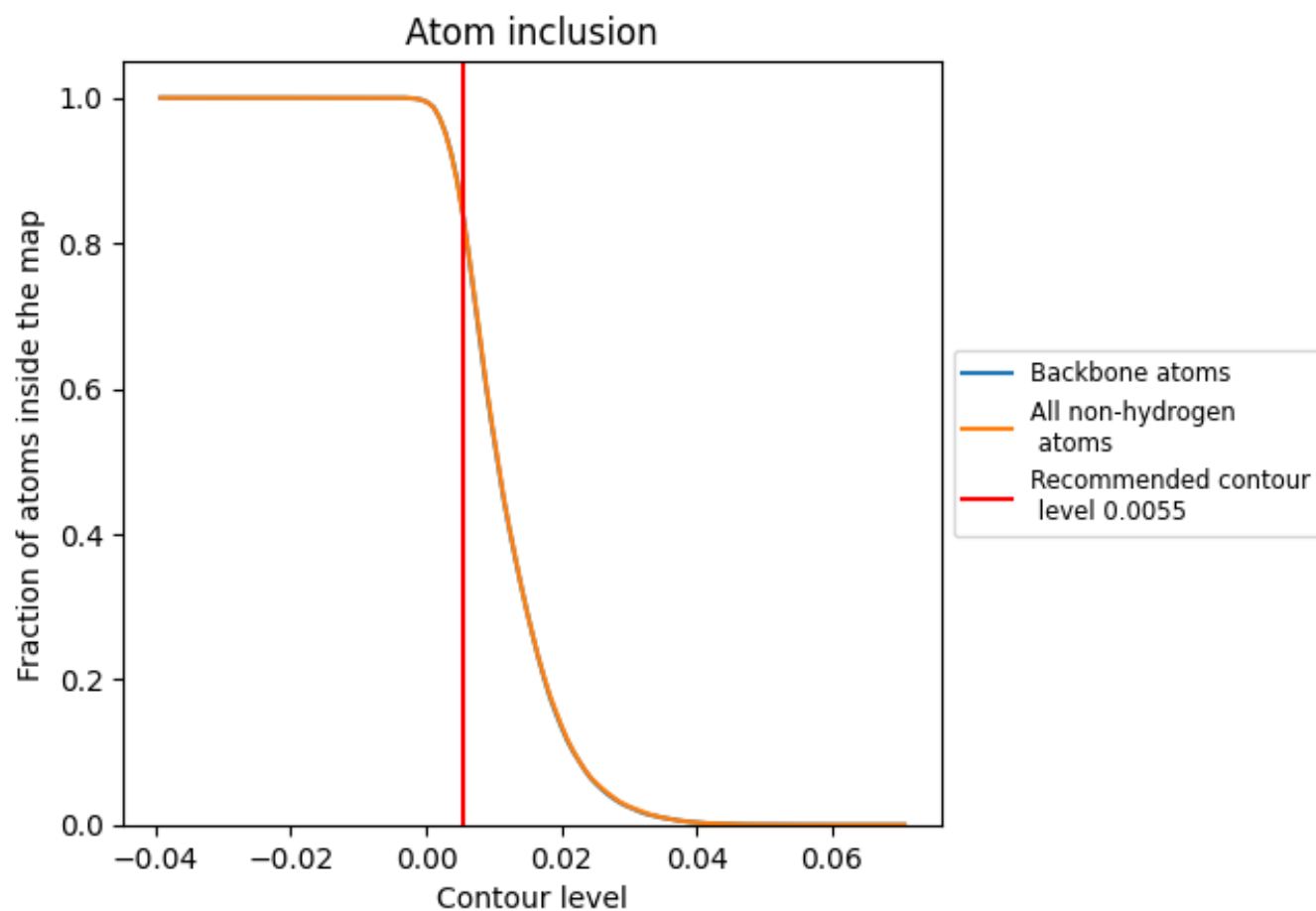
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0055).



































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.0055) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8365   |  0.2980   |
| A     |  0.7386   |  0.2360   |
| B     |  0.9209   |  0.3940   |
| C     |  0.9506   |  0.3710   |
| E     |  0.8730   |  0.3550   |
| F     |  0.9475   |  0.3640   |
| G     |  0.8809   |  0.3380   |
| H     |  0.8484   |  0.2740   |
| L     |  0.9367   |  0.3810   |
| M     |  0.9007   |  0.3080   |
| O     |  0.9103   |  0.3130   |
| P     |  0.9402   |  0.4100   |
| Q     |  0.9047   |  0.2980   |
| S     |  0.7163   |  0.2390   |
| U     |  0.8688  |  0.2570  |
| V     |  0.7186 |  0.2130 |
| W     |  0.7361 |  0.2920 |

