



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:55 PM UTC

PDB ID : 7KZV / pdb\_00007kzv  
EMDB ID : EMD-23090  
Title : Structure of the human fanconi anaemia Core-UBE2T-ID-DNA complex in closed state  
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:

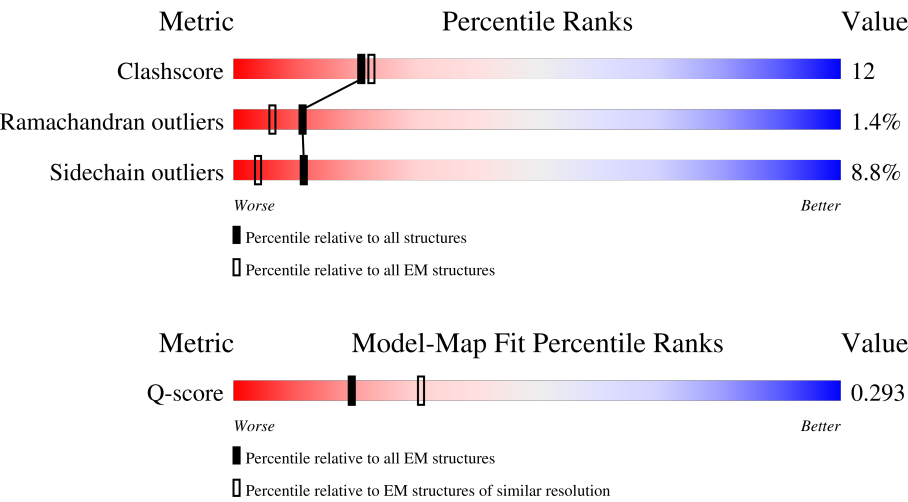
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 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) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 5410 ( 3.70 - 4.70 )                                     |

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

| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 1   | A     | 1477   | <div><div>12%</div><div>52%</div><div>25%</div><div>•</div><div>20%</div></div>            |
| 1   | S     | 1477   | <div><div>6%</div><div>59%</div><div>22%</div><div>•</div><div>15%</div></div>             |
| 2   | B     | 884    | <div><div>•</div><div>41%</div><div>29%</div><div>8%</div><div>•</div><div>21%</div></div> |
| 2   | O     | 884    | <div><div>•</div><div>52%</div><div>22%</div><div>•</div><div>•</div><div>21%</div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 583    |                  |
| 4   | E     | 555    |                  |
| 5   | F     | 399    |                  |
| 6   | G     | 641    |                  |
| 6   | H     | 641    |                  |
| 7   | L     | 394    |                  |
| 7   | M     | 394    |                  |
| 8   | P     | 906    |                  |
| 8   | Q     | 906    |                  |
| 9   | W     | 39     |                  |
| 10  | X     | 197    |                  |
| 11  | U     | 1328   |                  |
| 12  | V     | 1451   |                  |
| 13  | Y     | 58     |                  |
| 14  | Z     | 58     |                  |

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 177592 atoms, of which 89365 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 Ubiquitin-conjugating enzyme E2 T.

| Mol | Chain | Residues | Atoms |     |      |     |     | AltConf | Trace |   |
|-----|-------|----------|-------|-----|------|-----|-----|---------|-------|---|
| 10  | X     | 153      | Total | C   | H    | N   | O   | S       | 0     | 0 |
|     |       |          | 2484  | 789 | 1251 | 216 | 221 | 7       |       |   |

- Molecule 11 is a protein called Fanconi anemia, complementation group I.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 11  | U     | 1198     | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 19367 | 6076 | 9883 | 1592 | 1760 | 56 |         |       |

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 12 is a protein called Fanconi anemia group D2 protein.

| Mol | Chain | Residues | Atoms |      |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|------|----|---------|-------|
| 12  | V     | 1155     | Total | C    | H    | N    | O    | S  | 0       | 0     |
|     |       |          | 18807 | 5993 | 9518 | 1537 | 1706 | 53 |         |       |

- Molecule 13 is a DNA chain called DNA (29-MER).

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 13  | Y     | 29       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 923   | 282 | 326 | 111 | 175 | 29 |         |       |

- Molecule 14 is a DNA chain called DNA (29-MER).

| Mol | Chain | Residues | Atoms |     |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|---------|-------|
| 14  | Z     | 29       | Total | C   | H   | N   | O   | P  | 0       | 0     |
|     |       |          | 917   | 280 | 325 | 110 | 173 | 29 |         |       |

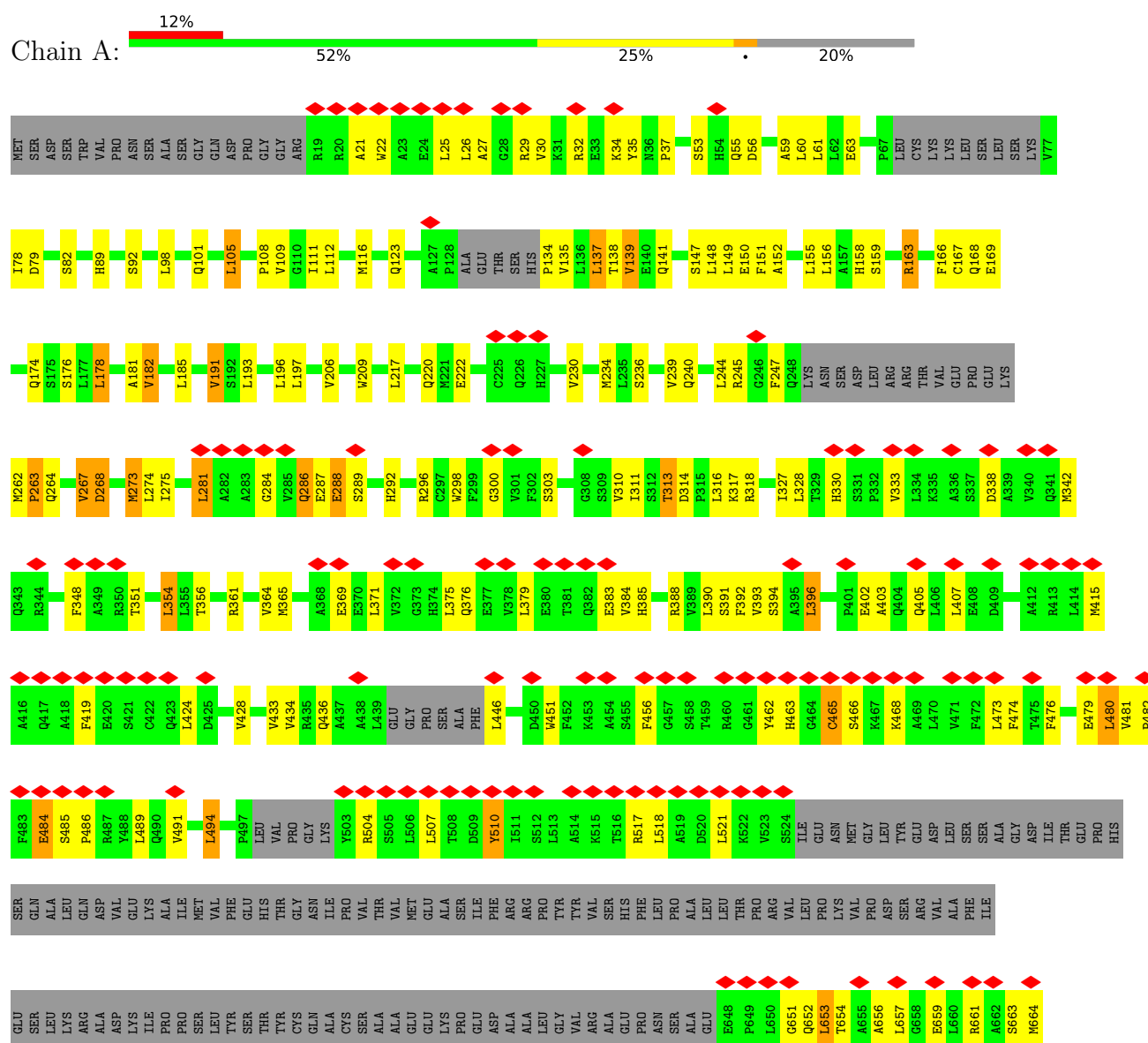
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 15  | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 15  | L     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |
| 15  | M     | 2        | Total | Zn | 0       |
|     |       |          | 2     | 2  |         |

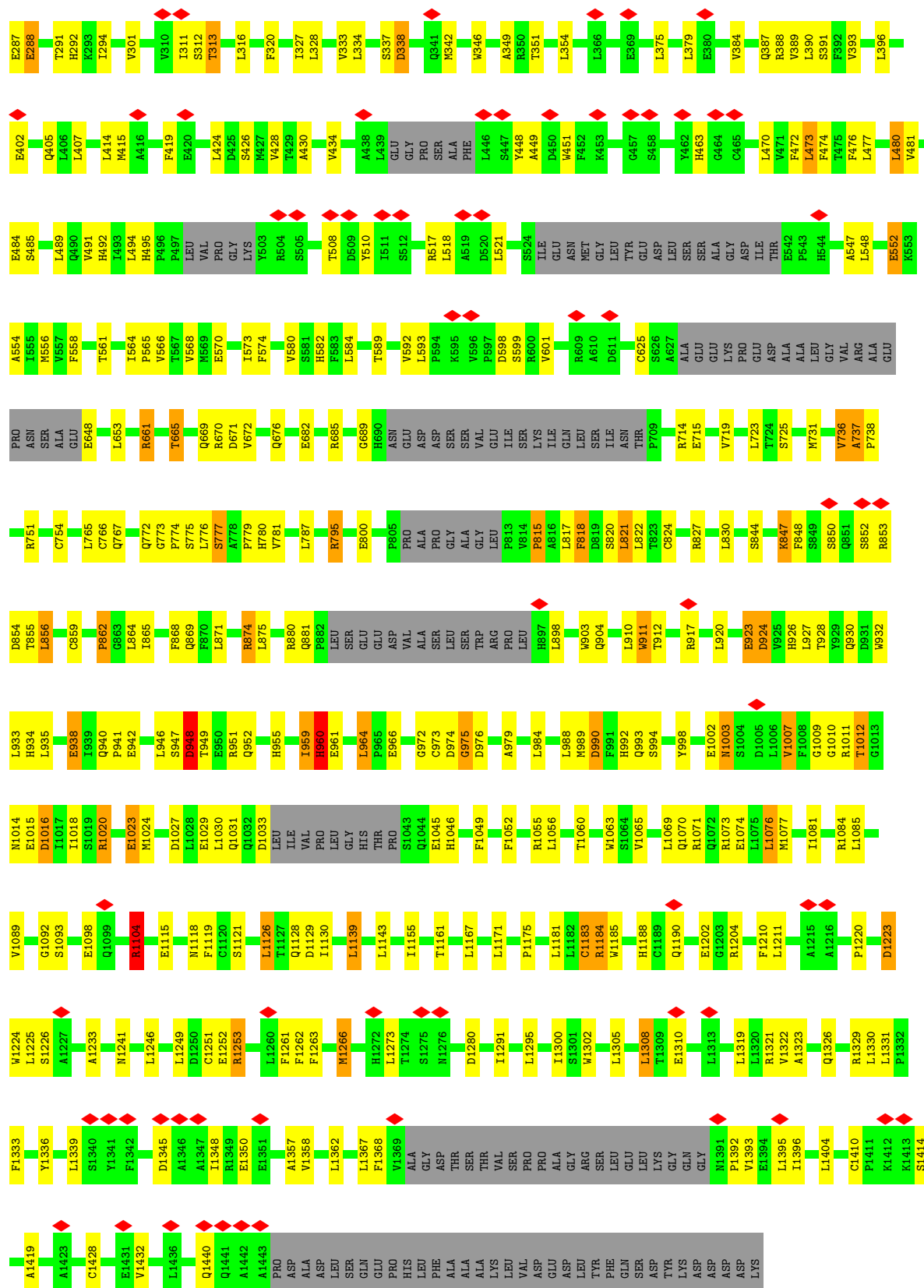
### 3 Residue-property plots [i](#)

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

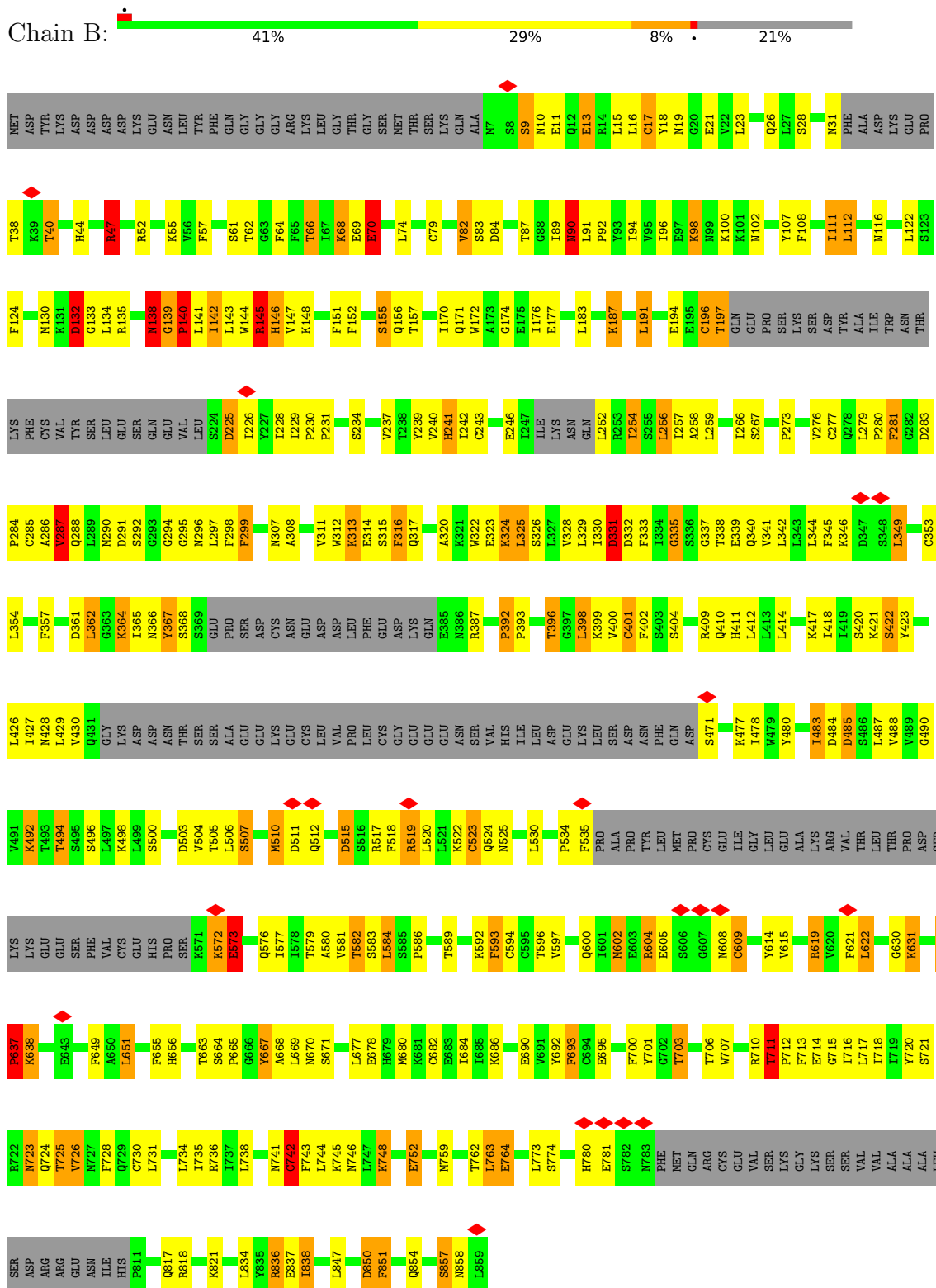
#### • Molecule 1: Fanconi anemia group A protein







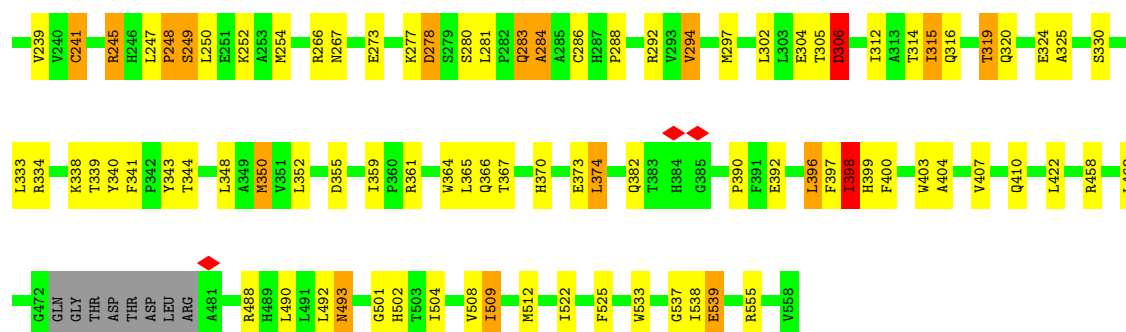
• Molecule 2: Fanconi anemia group B protein



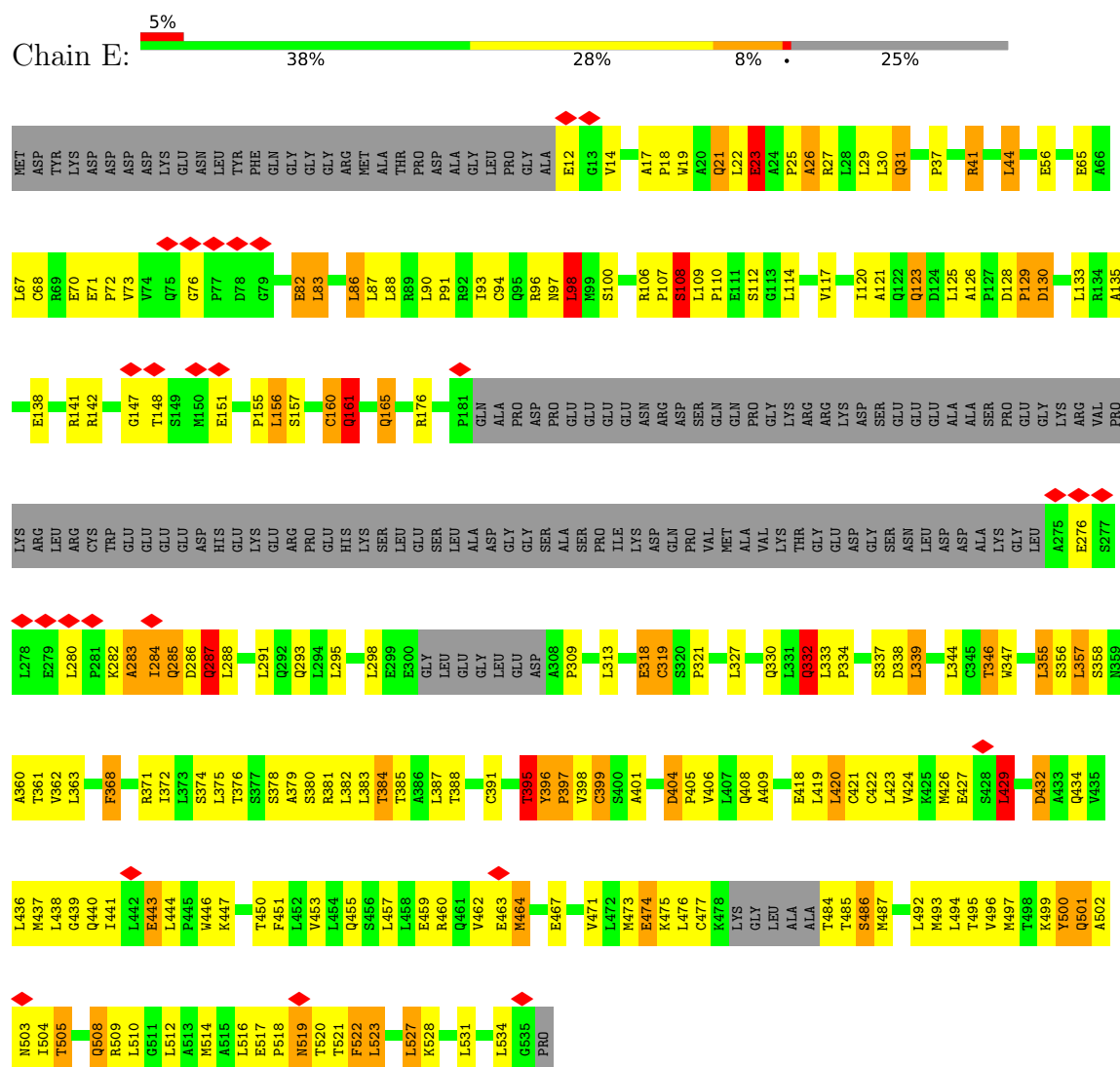
• Molecule 2: Fanconi anemia group B protein



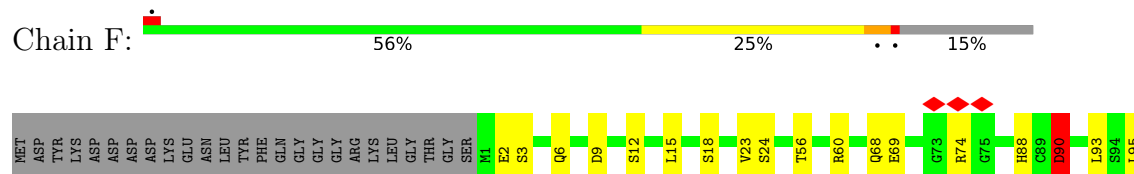


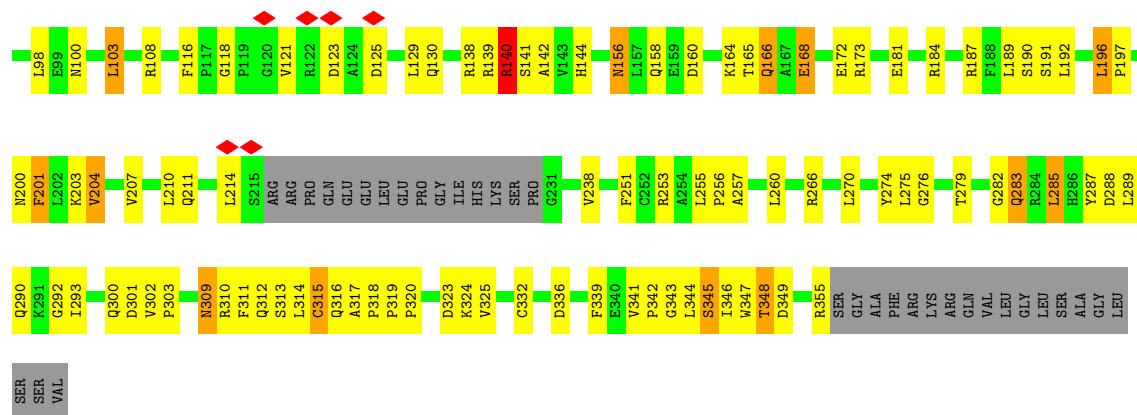


- Molecule 4: Fanconi anemia group E protein

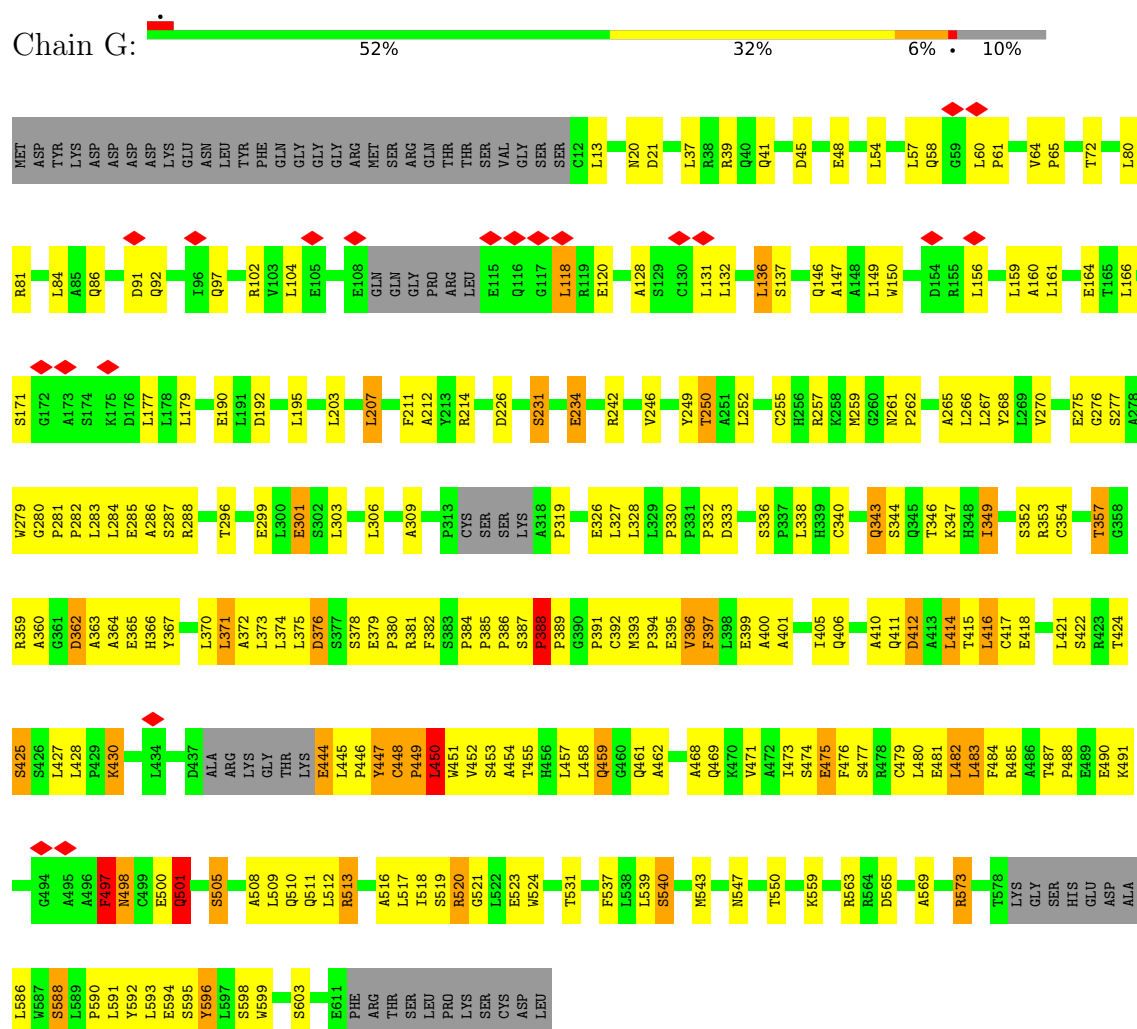


- Molecule 5: Fanconi anemia group F protein





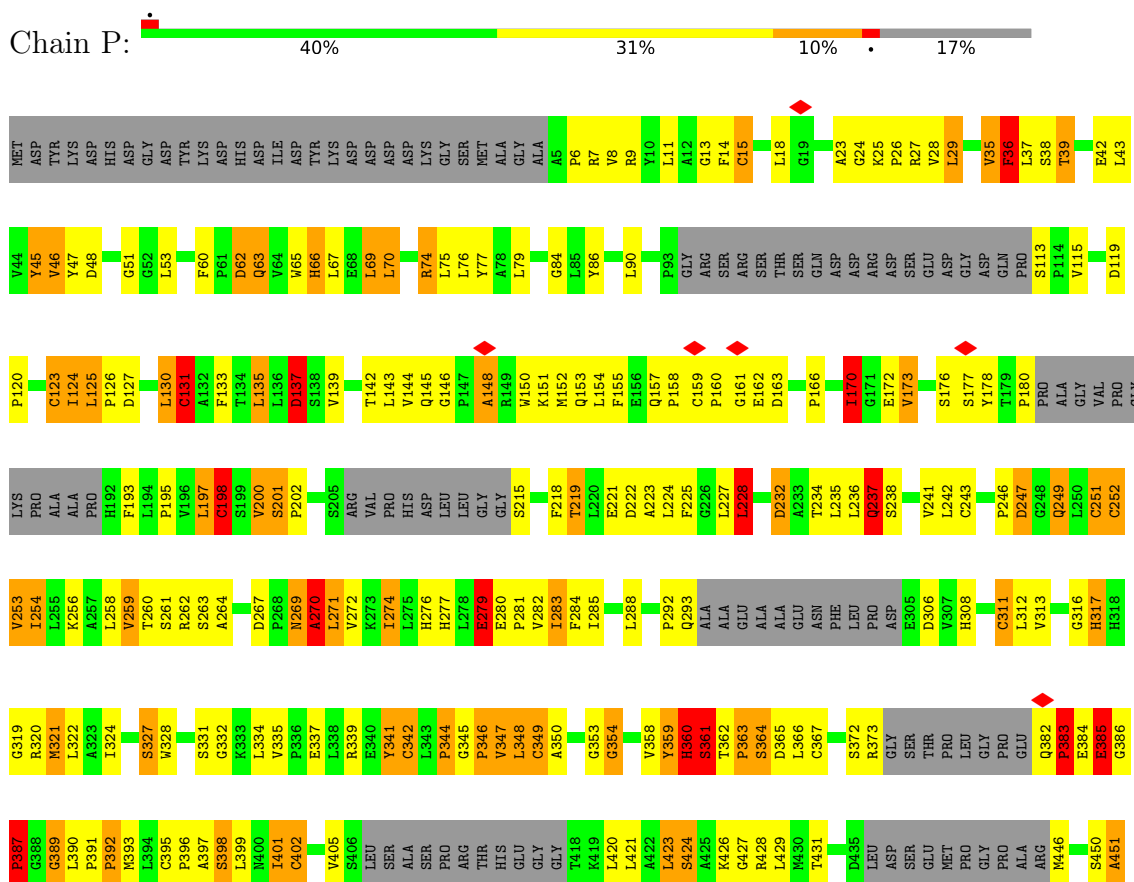
### • Molecule 6: Fanconi anemia group G protein

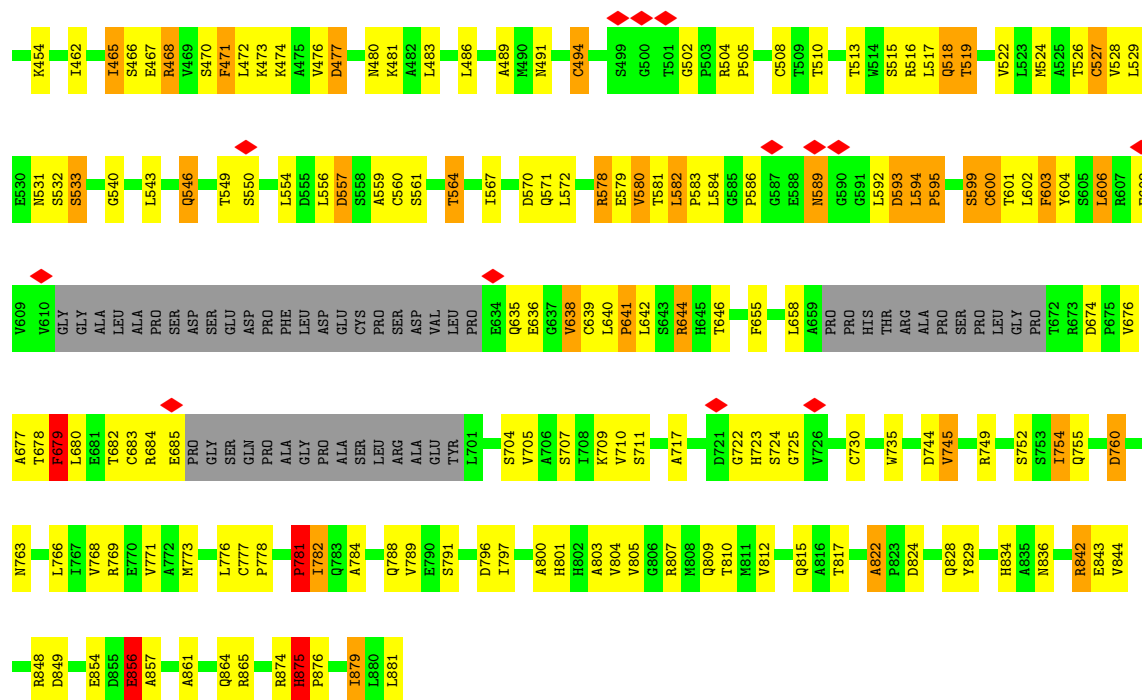


### • Molecule 6: Fanconi anemia group G protein

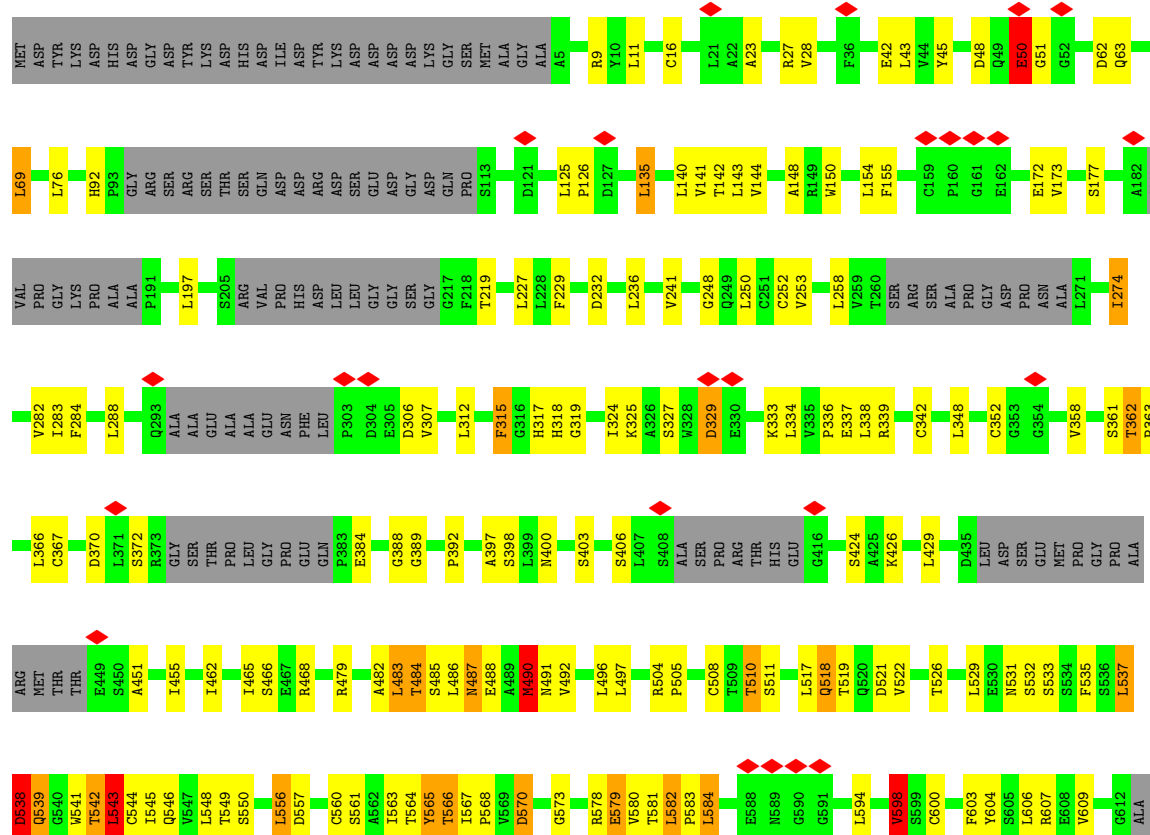


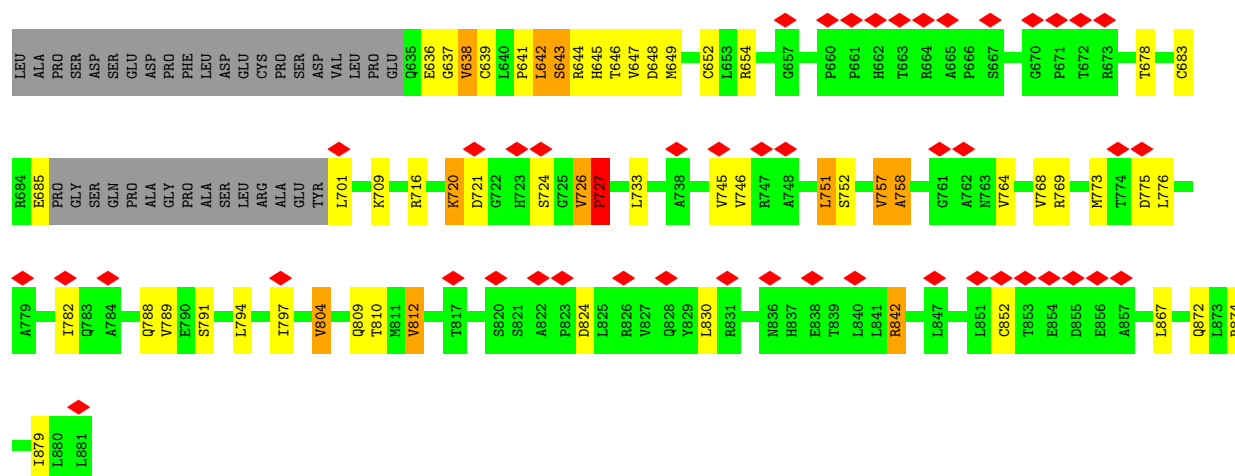




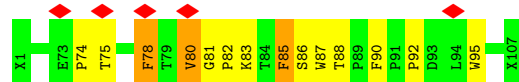


• Molecule 8: Fanconi anemia core complex-associated protein 100

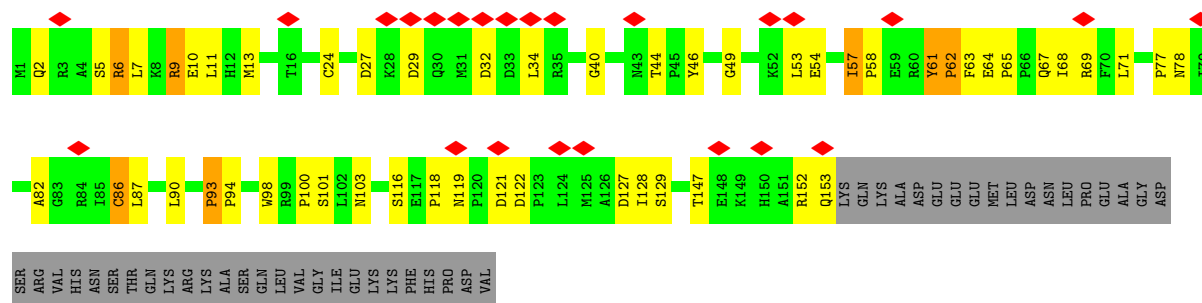




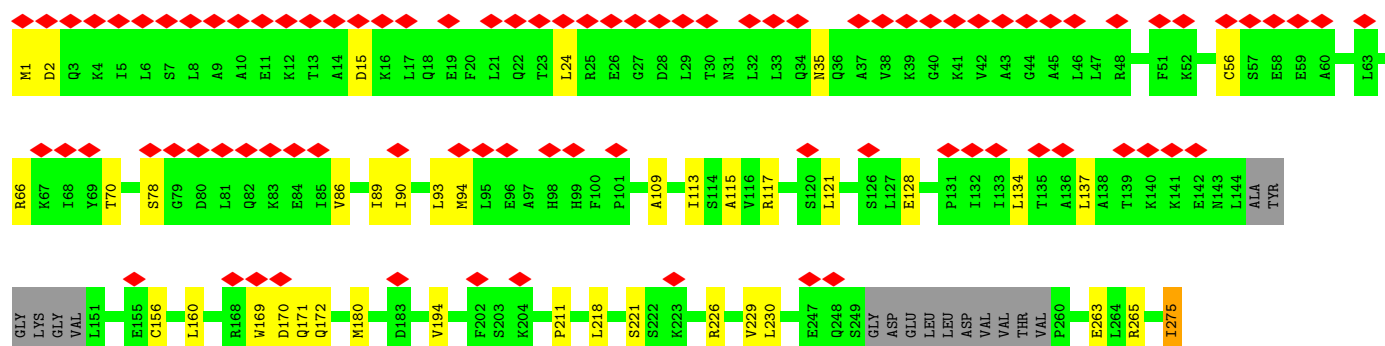
- Molecule 9: Fanconi anemia core complex-associated protein 20



- Molecule 10: Ubiquitin-conjugating enzyme E2 T



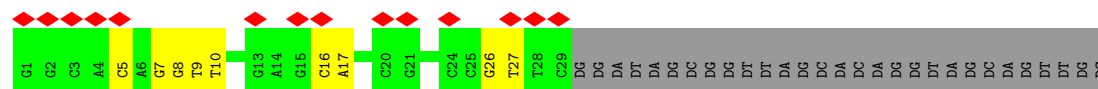
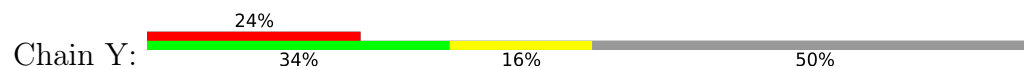
- Molecule 11: Fanconi anemia, complementation group I



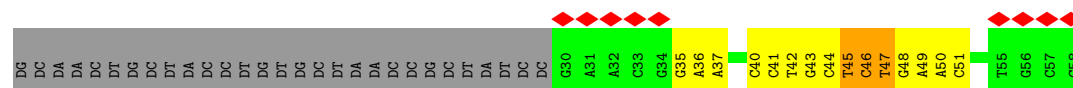




- Molecule 13: DNA (29-MER)



- Molecule 14: DNA (29-MER)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 74481                                   | 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 ( $e^-/\text{\AA}^2$ ) | 36.5                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.049                                   | Depositor |
| Minimum map value                    | -0.023                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.001                                   | Depositor |
| Recommended contour level            | 0.006                                   | Depositor |
| Map size (Å)                         | 473.088, 473.088, 473.088               | wwPDB     |
| Map dimensions                       | 448, 448, 448                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.056, 1.056, 1.056                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 1.14         | 1/9605 (0.0%)   | 1.77        | 54/13008 (0.4%)    |
| 1   | S     | 1.13         | 2/10153 (0.0%)  | 1.78        | 71/13749 (0.5%)    |
| 2   | B     | 1.23         | 8/5707 (0.1%)   | 1.87        | 118/7686 (1.5%)    |
| 2   | O     | 1.16         | 0/5701          | 1.69        | 59/7686 (0.8%)     |
| 3   | C     | 1.18         | 5/4497 (0.1%)   | 1.90        | 78/6103 (1.3%)     |
| 4   | E     | 1.24         | 3/3274 (0.1%)   | 1.96        | 71/4438 (1.6%)     |
| 5   | F     | 1.16         | 1/2791 (0.0%)   | 1.83        | 37/3790 (1.0%)     |
| 6   | G     | 1.20         | 7/4568 (0.2%)   | 1.89        | 65/6215 (1.0%)     |
| 6   | H     | 1.11         | 2/4293 (0.0%)   | 1.85        | 56/5840 (1.0%)     |
| 7   | L     | 1.19         | 5/3050 (0.2%)   | 1.71        | 50/4143 (1.2%)     |
| 7   | M     | 1.16         | 1/3050 (0.0%)   | 1.70        | 29/4143 (0.7%)     |
| 8   | P     | 1.29         | 16/5697 (0.3%)  | 1.91        | 128/7752 (1.7%)    |
| 8   | Q     | 1.19         | 2/5737 (0.0%)   | 1.70        | 56/7810 (0.7%)     |
| 9   | W     | 1.07         | 0/202           | 1.55        | 1/281 (0.4%)       |
| 10  | X     | 1.26         | 0/1267          | 1.81        | 21/1722 (1.2%)     |
| 11  | U     | 1.22         | 1/9629 (0.0%)   | 1.90        | 120/12982 (0.9%)   |
| 12  | V     | 1.19         | 3/9464 (0.0%)   | 1.84        | 92/12798 (0.7%)    |
| 13  | Y     | 0.39         | 0/669           | 1.08        | 7/1031 (0.7%)      |
| 14  | Z     | 0.40         | 0/663           | 1.05        | 7/1020 (0.7%)      |
| All | All   | 1.18         | 57/90017 (0.1%) | 1.81        | 1120/122197 (0.9%) |

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                   | 13                  |
| 1   | S     | 0                   | 12                  |
| 2   | B     | 0                   | 18                  |
| 2   | O     | 0                   | 13                  |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 3   | C     | 0                   | 4                   |
| 4   | E     | 0                   | 7                   |
| 5   | F     | 0                   | 1                   |
| 6   | G     | 0                   | 8                   |
| 6   | H     | 0                   | 6                   |
| 7   | L     | 0                   | 4                   |
| 7   | M     | 0                   | 3                   |
| 8   | P     | 0                   | 38                  |
| 8   | Q     | 0                   | 10                  |
| 10  | X     | 0                   | 5                   |
| 11  | U     | 0                   | 5                   |
| 12  | V     | 0                   | 5                   |
| All | All   | 0                   | 152                 |

All (57) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|--------|-------------|----------|
| 7   | L     | 332  | PRO  | C-N     | -14.24 | 1.15        | 1.33     |
| 7   | L     | 305  | MET  | C-N     | 11.90  | 1.50        | 1.33     |
| 7   | L     | 322  | GLN  | C-N     | 11.68  | 1.49        | 1.33     |
| 7   | L     | 339  | TYR  | C-N     | -11.12 | 1.17        | 1.33     |
| 7   | L     | 313  | TYR  | C-N     | 9.04   | 1.46        | 1.33     |
| 3   | C     | 250  | LEU  | N-CA    | 8.07   | 1.56        | 1.46     |
| 8   | P     | 282  | VAL  | C-O     | -7.91  | 1.16        | 1.24     |
| 2   | B     | 721  | SER  | CA-CB   | -7.87  | 1.42        | 1.53     |
| 6   | H     | 241  | PRO  | C-O     | -6.80  | 1.15        | 1.24     |
| 11  | U     | 683  | ILE  | CA-CB   | 6.72   | 1.57        | 1.54     |
| 8   | P     | 282  | VAL  | C-N     | -6.71  | 1.27        | 1.33     |
| 4   | E     | 96   | ARG  | NE-CZ   | 6.43   | 1.40        | 1.33     |
| 8   | P     | 28   | VAL  | C-O     | 6.40   | 1.30        | 1.24     |
| 12  | V     | 1125 | ILE  | N-CA    | 6.18   | 1.51        | 1.46     |
| 8   | P     | 283  | ILE  | C-O     | 6.14   | 1.29        | 1.23     |
| 12  | V     | 671  | VAL  | N-CA    | 6.13   | 1.51        | 1.46     |
| 8   | P     | 316  | GLY  | C-O     | 5.87   | 1.30        | 1.23     |
| 8   | P     | 583  | PRO  | C-O     | -5.85  | 1.17        | 1.23     |
| 2   | B     | 241  | HIS  | CE1-NE2 | 5.83   | 1.38        | 1.32     |
| 8   | P     | 285  | ILE  | C-O     | 5.76   | 1.29        | 1.24     |
| 3   | C     | 177  | PRO  | C-O     | -5.74  | 1.16        | 1.24     |
| 8   | P     | 361  | SER  | CA-CB   | 5.69   | 1.62        | 1.53     |
| 6   | G     | 418  | GLU  | N-CA    | 5.67   | 1.53        | 1.46     |
| 2   | B     | 752  | GLU  | C-O     | 5.64   | 1.30        | 1.24     |
| 6   | G     | 446  | PRO  | C-O     | -5.58  | 1.16        | 1.23     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 8   | P     | 223  | ALA  | C-O     | 5.58  | 1.30        | 1.24     |
| 4   | E     | 396  | TYR  | N-CA    | 5.48  | 1.50        | 1.46     |
| 3   | C     | 315  | ILE  | N-CA    | 5.40  | 1.52        | 1.46     |
| 8   | Q     | 641  | PRO  | C-O     | -5.40 | 1.17        | 1.23     |
| 2   | B     | 656  | HIS  | CE1-NE2 | 5.40  | 1.38        | 1.32     |
| 6   | H     | 63   | ALA  | C-O     | 5.36  | 1.30        | 1.24     |
| 1   | S     | 961  | GLU  | N-CA    | 5.35  | 1.53        | 1.46     |
| 2   | B     | 651  | LEU  | C-O     | -5.33 | 1.17        | 1.24     |
| 1   | S     | 979  | ALA  | C-O     | 5.28  | 1.30        | 1.24     |
| 3   | C     | 187  | CYS  | N-CA    | 5.27  | 1.53        | 1.46     |
| 8   | P     | 361  | SER  | C-O     | 5.25  | 1.30        | 1.23     |
| 2   | B     | 313  | LYS  | C-O     | -5.25 | 1.17        | 1.24     |
| 6   | G     | 411  | GLN  | N-CA    | 5.24  | 1.53        | 1.46     |
| 8   | P     | 405  | VAL  | N-CA    | 5.23  | 1.52        | 1.46     |
| 2   | B     | 368  | SER  | C-O     | 5.23  | 1.29        | 1.24     |
| 5   | F     | 256  | PRO  | C-O     | -5.22 | 1.17        | 1.24     |
| 3   | C     | 227  | ILE  | N-CA    | 5.21  | 1.52        | 1.46     |
| 12  | V     | 468  | TYR  | N-CA    | 5.18  | 1.52        | 1.46     |
| 6   | G     | 394  | PRO  | C-O     | -5.16 | 1.18        | 1.24     |
| 4   | E     | 18   | PRO  | C-O     | -5.16 | 1.17        | 1.24     |
| 8   | Q     | 543  | LEU  | N-CA    | 5.16  | 1.52        | 1.46     |
| 2   | B     | 194  | GLU  | C-O     | 5.13  | 1.30        | 1.23     |
| 8   | P     | 259  | VAL  | C-O     | 5.12  | 1.29        | 1.24     |
| 8   | P     | 387  | PRO  | C-O     | -5.11 | 1.17        | 1.24     |
| 6   | G     | 483  | LEU  | N-CA    | 5.11  | 1.52        | 1.46     |
| 6   | G     | 422  | SER  | N-CA    | 5.10  | 1.52        | 1.46     |
| 8   | P     | 252  | CYS  | C-O     | 5.09  | 1.30        | 1.23     |
| 8   | P     | 271  | LEU  | C-O     | 5.09  | 1.31        | 1.23     |
| 8   | P     | 317  | HIS  | C-O     | -5.05 | 1.18        | 1.24     |
| 6   | G     | 344  | SER  | CA-CB   | -5.05 | 1.45        | 1.53     |
| 1   | A     | 1348 | ILE  | N-CA    | 5.03  | 1.50        | 1.46     |
| 7   | M     | 297  | ILE  | N-CA    | 5.02  | 1.52        | 1.46     |

All (1120) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 3   | C     | 79  | PHE  | CA-CB-CG  | -15.17 | 98.63       | 113.80   |
| 2   | B     | 703 | THR  | CA-CB-OG1 | -13.33 | 89.61       | 109.60   |
| 7   | L     | 313 | TYR  | O-C-N     | 12.80  | 137.39      | 123.06   |
| 7   | M     | 333 | PHE  | CA-C-N    | 11.67  | 141.66      | 122.87   |
| 7   | M     | 333 | PHE  | C-N-CA    | 11.67  | 141.66      | 122.87   |
| 7   | L     | 321 | ASP  | CA-CB-CG  | 11.55  | 124.15      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 8   | P     | 679  | PHE  | CA-CB-CG    | -11.06 | 102.74      | 113.80   |
| 1   | S     | 737  | ALA  | N-CA-C      | 10.99  | 117.85      | 108.07   |
| 8   | P     | 392  | PRO  | CB-CA-C     | -10.58 | 95.09       | 110.75   |
| 2   | B     | 90   | ASN  | CA-CB-CG    | 10.53  | 123.13      | 112.60   |
| 1   | S     | 1012 | THR  | CB-CA-C     | 10.29  | 126.47      | 111.65   |
| 2   | B     | 503  | ASP  | CA-CB-CG    | 10.26  | 122.86      | 112.60   |
| 8   | P     | 157  | GLN  | CB-CA-C     | 10.12  | 123.62      | 110.16   |
| 7   | L     | 305  | MET  | O-C-N       | 9.85   | 137.16      | 121.89   |
| 7   | L     | 39   | ARG  | CG-CD-NE    | 9.79   | 133.55      | 112.00   |
| 7   | M     | 303  | PHE  | CA-CB-CG    | 9.71   | 123.51      | 113.80   |
| 6   | G     | 388  | PRO  | N-CA-C      | 9.70   | 122.54      | 110.70   |
| 12  | V     | 430  | ASP  | CA-CB-CG    | 9.69   | 122.29      | 112.60   |
| 7   | M     | 333  | PHE  | O-C-N       | -9.68  | 110.24      | 122.73   |
| 2   | B     | 90   | ASN  | CB-CA-C     | 9.51   | 123.27      | 110.06   |
| 2   | B     | 283  | ASP  | CA-CB-CG    | 9.46   | 122.06      | 112.60   |
| 2   | O     | 612  | ASP  | CA-CB-CG    | 9.40   | 122.00      | 112.60   |
| 8   | P     | 346  | PRO  | CB-CA-C     | 9.35   | 124.04      | 110.85   |
| 8   | Q     | 538  | ASP  | CA-CB-CG    | 9.32   | 121.92      | 112.60   |
| 3   | C     | 278  | ASP  | CA-CB-CG    | 9.29   | 121.89      | 112.60   |
| 8   | Q     | 583  | PRO  | CB-CA-C     | -9.13  | 99.06       | 111.21   |
| 6   | G     | 459  | GLN  | CA-C-N      | 9.11   | 129.87      | 119.94   |
| 6   | G     | 459  | GLN  | C-N-CA      | 9.11   | 129.87      | 119.94   |
| 6   | H     | 333  | ASP  | CA-CB-CG    | 9.09   | 121.69      | 112.60   |
| 2   | B     | 764  | GLU  | CB-CG-CD    | 8.86   | 127.66      | 112.60   |
| 6   | G     | 397  | PHE  | CB-CA-C     | -8.82  | 95.68       | 110.68   |
| 6   | G     | 594  | GLU  | CB-CA-C     | -8.74  | 96.33       | 110.84   |
| 8   | P     | 384  | GLU  | CA-C-O      | -8.74  | 111.82      | 121.00   |
| 2   | B     | 196  | CYS  | CA-C-N      | 8.72   | 137.41      | 121.70   |
| 2   | B     | 196  | CYS  | C-N-CA      | 8.72   | 137.41      | 121.70   |
| 6   | H     | 21   | ASP  | CA-CB-CG    | 8.63   | 121.23      | 112.60   |
| 6   | G     | 45   | ASP  | CA-CB-CG    | 8.57   | 121.17      | 112.60   |
| 2   | B     | 152  | PHE  | CA-CB-CG    | 8.55   | 122.35      | 113.80   |
| 6   | G     | 362  | ASP  | CA-CB-CG    | 8.53   | 121.13      | 112.60   |
| 3   | C     | 248  | PRO  | N-CA-C      | 8.53   | 124.92      | 113.84   |
| 13  | Y     | 7    | DG   | C2'-C3'-O3' | 8.47   | 124.21      | 111.50   |
| 13  | Y     | 17   | DA   | C2'-C3'-O3' | 8.46   | 124.19      | 111.50   |
| 6   | G     | 353  | ARG  | CB-CA-C     | 8.31   | 123.93      | 110.88   |
| 7   | M     | 286  | ASP  | CA-CB-CG    | 8.31   | 120.91      | 112.60   |
| 2   | B     | 9    | SER  | CA-C-N      | 8.28   | 131.38      | 120.28   |
| 2   | B     | 9    | SER  | C-N-CA      | 8.28   | 131.38      | 120.28   |
| 8   | P     | 39   | THR  | CA-CB-OG1   | -8.29  | 97.17       | 109.60   |
| 11  | U     | 770  | ASP  | CA-CB-CG    | 8.27   | 120.87      | 112.60   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | C     | 249 | SER  | CA-C-N    | 8.21  | 131.60      | 120.44   |
| 3   | C     | 249 | SER  | C-N-CA    | 8.21  | 131.60      | 120.44   |
| 4   | E     | 96  | ARG  | CB-CA-C   | 8.18  | 124.38      | 110.79   |
| 2   | B     | 291 | ASP  | CA-CB-CG  | 8.16  | 120.77      | 112.60   |
| 7   | L     | 305 | MET  | CA-C-N    | -8.15 | 109.12      | 122.82   |
| 7   | L     | 305 | MET  | C-N-CA    | -8.15 | 109.12      | 122.82   |
| 2   | B     | 752 | GLU  | CB-CA-C   | 8.12  | 123.62      | 110.88   |
| 8   | Q     | 484 | THR  | CB-CA-C   | -8.09 | 98.51       | 110.96   |
| 2   | O     | 518 | PHE  | CA-CB-CG  | 8.07  | 121.87      | 113.80   |
| 8   | P     | 385 | GLU  | CB-CG-CD  | -8.07 | 98.88       | 112.60   |
| 2   | O     | 411 | HIS  | CA-CB-CG  | 8.05  | 121.86      | 113.80   |
| 11  | U     | 783 | ASP  | CA-CB-CG  | 8.01  | 120.61      | 112.60   |
| 7   | L     | 168 | ASP  | CA-CB-CG  | 8.00  | 120.60      | 112.60   |
| 8   | P     | 603 | PHE  | CA-CB-CG  | 7.98  | 121.78      | 113.80   |
| 5   | F     | 90  | ASP  | CA-CB-CG  | 7.98  | 120.58      | 112.60   |
| 7   | M     | 310 | CYS  | CA-C-N    | 7.96  | 135.65      | 123.47   |
| 7   | M     | 310 | CYS  | C-N-CA    | 7.96  | 135.65      | 123.47   |
| 3   | C     | 355 | ASP  | CA-CB-CG  | 7.96  | 120.56      | 112.60   |
| 2   | B     | 725 | THR  | CA-CB-OG1 | 7.95  | 121.52      | 109.60   |
| 8   | P     | 344 | PRO  | N-CA-C    | 7.93  | 123.24      | 111.03   |
| 2   | B     | 735 | ILE  | CA-C-N    | 7.89  | 134.94      | 121.14   |
| 2   | B     | 735 | ILE  | C-N-CA    | 7.89  | 134.94      | 121.14   |
| 8   | P     | 197 | LEU  | CA-C-O    | -7.87 | 112.20      | 120.70   |
| 2   | B     | 519 | ARG  | CB-CA-C   | 7.86  | 122.92      | 110.19   |
| 1   | A     | 480 | LEU  | CA-C-N    | 7.83  | 125.17      | 120.24   |
| 1   | A     | 480 | LEU  | C-N-CA    | 7.83  | 125.17      | 120.24   |
| 6   | H     | 158 | ASP  | CA-CB-CG  | 7.83  | 120.43      | 112.60   |
| 7   | M     | 257 | ASP  | CA-CB-CG  | 7.71  | 120.31      | 112.60   |
| 2   | B     | 366 | ASN  | CA-CB-CG  | 7.70  | 120.30      | 112.60   |
| 6   | G     | 366 | HIS  | N-CA-C    | -7.70 | 101.63      | 111.02   |
| 8   | Q     | 542 | THR  | CA-C-O    | -7.69 | 113.21      | 121.36   |
| 3   | C     | 398 | ILE  | N-CA-CB   | 7.68  | 119.00      | 110.62   |
| 7   | L     | 237 | ASN  | CA-CB-CG  | 7.68  | 120.28      | 112.60   |
| 3   | C     | 341 | PHE  | CA-CB-CG  | 7.67  | 121.47      | 113.80   |
| 6   | H     | 214 | ARG  | CG-CD-NE  | 7.65  | 128.84      | 112.00   |
| 3   | C     | 249 | SER  | CA-C-O    | -7.63 | 112.80      | 120.82   |
| 7   | L     | 205 | ASP  | CA-CB-CG  | 7.62  | 120.22      | 112.60   |
| 3   | C     | 218 | GLU  | CA-C-N    | 7.61  | 130.33      | 120.44   |
| 3   | C     | 218 | GLU  | C-N-CA    | 7.61  | 130.33      | 120.44   |
| 6   | G     | 386 | PRO  | CA-C-N    | 7.61  | 132.24      | 120.60   |
| 6   | G     | 386 | PRO  | C-N-CA    | 7.61  | 132.24      | 120.60   |
| 1   | S     | 517 | ARG  | CG-CD-NE  | 7.61  | 128.73      | 112.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 6   | H     | 241 | PRO  | N-CA-C      | 7.60  | 128.13      | 112.47   |
| 2   | O     | 525 | ASN  | CB-CA-C     | 7.60  | 122.34      | 109.50   |
| 2   | B     | 396 | THR  | CA-CB-OG1   | -7.59 | 98.21       | 109.60   |
| 8   | P     | 875 | HIS  | CA-CB-CG    | -7.58 | 106.22      | 113.80   |
| 8   | P     | 346 | PRO  | N-CA-C      | -7.50 | 98.50       | 111.32   |
| 14  | Z     | 50  | DA   | C2'-C3'-O3' | 7.48  | 122.72      | 111.50   |
| 2   | B     | 621 | PHE  | CA-CB-CG    | 7.46  | 121.25      | 113.80   |
| 6   | G     | 497 | PHE  | CA-CB-CG    | 7.44  | 121.24      | 113.80   |
| 6   | H     | 48  | GLU  | CB-CG-CD    | 7.44  | 125.25      | 112.60   |
| 5   | F     | 342 | PRO  | CB-CA-C     | -7.43 | 101.22      | 110.95   |
| 2   | B     | 736 | ARG  | CA-C-N      | 7.42  | 131.51      | 122.16   |
| 2   | B     | 736 | ARG  | C-N-CA      | 7.42  | 131.51      | 122.16   |
| 5   | F     | 165 | THR  | CA-CB-OG1   | -7.41 | 98.48       | 109.60   |
| 2   | O     | 515 | ASP  | CA-CB-CG    | 7.41  | 120.01      | 112.60   |
| 1   | A     | 923 | GLU  | N-CA-C      | 7.39  | 120.96      | 108.02   |
| 8   | P     | 237 | GLN  | CB-CG-CD    | 7.37  | 125.12      | 112.60   |
| 3   | C     | 273 | GLU  | CB-CG-CD    | 7.35  | 125.09      | 112.60   |
| 8   | P     | 198 | CYS  | CA-C-N      | 7.34  | 132.00      | 121.50   |
| 8   | P     | 198 | CYS  | C-N-CA      | 7.34  | 132.00      | 121.50   |
| 6   | H     | 120 | GLU  | CB-CA-C     | -7.33 | 98.39       | 110.85   |
| 12  | V     | 833 | THR  | CB-CA-C     | 7.29  | 117.00      | 110.44   |
| 3   | C     | 226 | ALA  | CA-C-O      | -7.26 | 111.89      | 120.10   |
| 3   | C     | 127 | PHE  | CA-C-N      | 7.25  | 135.39      | 121.54   |
| 3   | C     | 127 | PHE  | C-N-CA      | 7.25  | 135.39      | 121.54   |
| 2   | B     | 296 | ASN  | CA-CB-CG    | 7.23  | 119.83      | 112.60   |
| 2   | O     | 231 | PRO  | CA-C-N      | 7.23  | 130.30      | 120.54   |
| 2   | O     | 231 | PRO  | C-N-CA      | 7.23  | 130.30      | 120.54   |
| 3   | C     | 195 | ASP  | CA-CB-CG    | 7.22  | 119.82      | 112.60   |
| 10  | X     | 94  | PRO  | N-CA-C      | 7.22  | 127.34      | 112.47   |
| 8   | P     | 249 | GLN  | N-CA-CB     | 7.22  | 120.96      | 110.06   |
| 1   | A     | 288 | GLU  | CB-CA-C     | 7.17  | 121.47      | 111.86   |
| 6   | H     | 45  | ASP  | CA-CB-CG    | 7.14  | 119.74      | 112.60   |
| 2   | B     | 485 | ASP  | CA-CB-CG    | 7.13  | 119.73      | 112.60   |
| 6   | H     | 120 | GLU  | N-CA-CB     | 7.13  | 120.72      | 110.16   |
| 11  | U     | 170 | ASP  | CA-CB-CG    | 7.10  | 119.70      | 112.60   |
| 8   | P     | 119 | ASP  | CA-CB-CG    | 7.09  | 119.69      | 112.60   |
| 1   | A     | 286 | GLN  | CB-CA-C     | 7.08  | 121.98      | 110.37   |
| 1   | A     | 37  | PRO  | CA-C-N      | 7.08  | 130.09      | 120.54   |
| 1   | A     | 37  | PRO  | C-N-CA      | 7.08  | 130.09      | 120.54   |
| 2   | B     | 667 | TYR  | CA-C-O      | -7.08 | 113.74      | 121.31   |
| 8   | P     | 589 | ASN  | CA-CB-CG    | 7.07  | 119.67      | 112.60   |
| 8   | Q     | 727 | PRO  | N-CD-CG     | -7.07 | 92.59       | 103.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 8   | P     | 306 | ASP  | CA-CB-CG    | 7.07  | 119.67      | 112.60   |
| 2   | B     | 90  | ASN  | N-CA-C      | -7.05 | 99.72       | 110.30   |
| 2   | O     | 588 | LEU  | N-CA-C      | -7.05 | 104.68      | 112.72   |
| 7   | L     | 286 | ASP  | CA-CB-CG    | 7.05  | 119.65      | 112.60   |
| 11  | U     | 300 | ASP  | CA-CB-CG    | 7.05  | 119.65      | 112.60   |
| 7   | L     | 237 | ASN  | CB-CA-C     | 7.04  | 121.35      | 109.80   |
| 2   | B     | 477 | LYS  | CA-C-N      | 7.02  | 132.84      | 121.62   |
| 2   | B     | 477 | LYS  | C-N-CA      | 7.02  | 132.84      | 121.62   |
| 1   | S     | 874 | ARG  | CG-CD-NE    | -7.02 | 96.56       | 112.00   |
| 4   | E     | 90  | LEU  | CB-CA-C     | 7.00  | 120.50      | 109.37   |
| 2   | B     | 92  | PRO  | CA-C-O      | -6.99 | 113.94      | 121.27   |
| 5   | F     | 279 | THR  | CB-CA-C     | 6.97  | 122.32      | 110.74   |
| 3   | C     | 227 | ILE  | N-CA-CB     | 6.97  | 118.22      | 110.62   |
| 2   | B     | 670 | ASN  | CB-CA-C     | 6.96  | 119.98      | 109.13   |
| 12  | V     | 386 | PHE  | CA-CB-CG    | 6.96  | 120.76      | 113.80   |
| 13  | Y     | 16  | DC   | C2'-C3'-O3' | 6.96  | 121.94      | 111.50   |
| 11  | U     | 682 | VAL  | CA-C-N      | 6.95  | 127.10      | 120.43   |
| 11  | U     | 682 | VAL  | C-N-CA      | 6.95  | 127.10      | 120.43   |
| 11  | U     | 338 | PHE  | CA-CB-CG    | -6.94 | 106.86      | 113.80   |
| 10  | X     | 57  | ILE  | CB-CA-C     | 6.92  | 118.12      | 110.71   |
| 5   | F     | 319 | PRO  | N-CA-C      | 6.91  | 119.12      | 110.70   |
| 8   | Q     | 565 | TYR  | CA-C-O      | -6.90 | 114.12      | 121.99   |
| 6   | H     | 241 | PRO  | CB-CA-C     | -6.88 | 100.21      | 111.56   |
| 1   | S     | 517 | ARG  | CB-CG-CD    | 6.86  | 127.08      | 111.30   |
| 2   | O     | 579 | THR  | CB-CA-C     | 6.85  | 124.05      | 110.42   |
| 2   | O     | 314 | GLU  | CB-CG-CD    | 6.83  | 124.21      | 112.60   |
| 7   | M     | 35  | ASP  | CB-CA-C     | 6.80  | 120.91      | 109.48   |
| 4   | E     | 98  | LEU  | N-CA-C      | -6.79 | 102.73      | 111.02   |
| 12  | V     | 256 | PRO  | CA-C-N      | 6.78  | 129.69      | 120.54   |
| 12  | V     | 256 | PRO  | C-N-CA      | 6.78  | 129.69      | 120.54   |
| 6   | G     | 394 | PRO  | CB-CA-C     | -6.77 | 102.39      | 112.55   |
| 8   | P     | 395 | CYS  | CB-CA-C     | 6.76  | 119.36      | 108.87   |
| 2   | B     | 593 | PHE  | CA-CB-CG    | -6.76 | 107.04      | 113.80   |
| 8   | P     | 137 | ASP  | CA-CB-CG    | 6.75  | 119.35      | 112.60   |
| 11  | U     | 598 | GLN  | CA-C-N      | 6.75  | 130.17      | 120.79   |
| 11  | U     | 598 | GLN  | C-N-CA      | 6.75  | 130.17      | 120.79   |
| 3   | C     | 343 | TYR  | CB-CA-C     | 6.74  | 121.35      | 110.09   |
| 2   | O     | 485 | ASP  | CA-CB-CG    | 6.74  | 119.34      | 112.60   |
| 2   | B     | 108 | PHE  | CA-C-O      | -6.74 | 113.01      | 120.69   |
| 8   | Q     | 490 | MET  | N-CA-CB     | 6.74  | 120.14      | 110.16   |
| 1   | S     | 338 | ASP  | CA-CB-CG    | 6.74  | 119.34      | 112.60   |
| 8   | P     | 155 | PHE  | CA-CB-CG    | 6.74  | 120.54      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | A     | 1328 | THR  | CB-CA-C     | -6.73 | 99.23       | 110.68   |
| 8   | P     | 817  | THR  | N-CA-CB     | 6.73  | 119.73      | 109.98   |
| 11  | U     | 528  | ASN  | CA-CB-CG    | 6.73  | 119.33      | 112.60   |
| 5   | F     | 336  | ASP  | CA-CB-CG    | 6.72  | 119.33      | 112.60   |
| 6   | G     | 275  | GLU  | CA-C-N      | 6.72  | 127.55      | 120.43   |
| 6   | G     | 275  | GLU  | C-N-CA      | 6.72  | 127.55      | 120.43   |
| 14  | Z     | 51   | DC   | C2'-C3'-O3' | 6.71  | 121.57      | 111.50   |
| 1   | S     | 948  | ASP  | CA-CB-CG    | 6.71  | 119.31      | 112.60   |
| 12  | V     | 357  | GLU  | CA-C-N      | 6.68  | 130.13      | 120.38   |
| 12  | V     | 357  | GLU  | C-N-CA      | 6.68  | 130.13      | 120.38   |
| 4   | E     | 65   | GLU  | CB-CA-C     | -6.67 | 100.37      | 110.90   |
| 11  | U     | 977  | PHE  | CA-CB-CG    | 6.66  | 120.46      | 113.80   |
| 8   | P     | 219  | THR  | CB-CA-C     | -6.65 | 98.89       | 109.80   |
| 8   | P     | 344  | PRO  | CB-CA-C     | -6.65 | 103.26      | 111.64   |
| 1   | S     | 862  | PRO  | CA-C-N      | 6.65  | 128.50      | 120.13   |
| 1   | S     | 862  | PRO  | C-N-CA      | 6.65  | 128.50      | 120.13   |
| 2   | B     | 47   | ARG  | CB-CA-C     | 6.62  | 121.58      | 110.79   |
| 8   | P     | 389  | GLY  | CA-C-O      | -6.62 | 115.63      | 121.58   |
| 12  | V     | 478  | VAL  | CA-C-O      | -6.62 | 114.07      | 120.95   |
| 3   | C     | 194  | THR  | CB-CA-C     | 6.61  | 121.77      | 110.79   |
| 7   | L     | 237  | ASN  | CA-C-N      | 6.59  | 131.96      | 123.13   |
| 7   | L     | 237  | ASN  | C-N-CA      | 6.59  | 131.96      | 123.13   |
| 4   | E     | 31   | GLN  | N-CA-C      | -6.58 | 104.10      | 111.28   |
| 8   | Q     | 637  | GLY  | CA-C-N      | 6.58  | 131.77      | 123.14   |
| 8   | Q     | 637  | GLY  | C-N-CA      | 6.58  | 131.77      | 123.14   |
| 8   | Q     | 721  | ASP  | N-CA-C      | -6.58 | 103.10      | 111.92   |
| 2   | B     | 725  | THR  | N-CA-CB     | 6.57  | 119.73      | 109.94   |
| 8   | P     | 533  | SER  | CA-C-N      | 6.57  | 129.08      | 120.28   |
| 8   | P     | 533  | SER  | C-N-CA      | 6.57  | 129.08      | 120.28   |
| 10  | X     | 29   | ASP  | CA-CB-CG    | 6.57  | 119.17      | 112.60   |
| 8   | P     | 810  | THR  | N-CA-CB     | 6.57  | 119.53      | 110.01   |
| 2   | O     | 226  | ILE  | CA-C-O      | -6.56 | 115.12      | 120.70   |
| 7   | M     | 310  | CYS  | O-C-N       | -6.54 | 113.51      | 122.46   |
| 12  | V     | 1323 | ASP  | CA-CB-CG    | 6.53  | 119.13      | 112.60   |
| 7   | L     | 61   | THR  | CB-CA-C     | -6.53 | 99.59       | 110.68   |
| 6   | G     | 425  | SER  | CA-C-N      | 6.52  | 134.00      | 121.54   |
| 6   | G     | 425  | SER  | C-N-CA      | 6.52  | 134.00      | 121.54   |
| 2   | B     | 368  | SER  | CA-C-N      | 6.52  | 133.44      | 121.70   |
| 2   | B     | 368  | SER  | C-N-CA      | 6.52  | 133.44      | 121.70   |
| 2   | O     | 164  | SER  | CA-C-N      | 6.52  | 126.53      | 120.34   |
| 2   | O     | 164  | SER  | C-N-CA      | 6.52  | 126.53      | 120.34   |
| 11  | U     | 342  | GLN  | CA-C-N      | 6.51  | 129.01      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 11  | U     | 342  | GLN  | C-N-CA    | 6.51  | 129.01      | 120.28   |
| 4   | E     | 508  | GLN  | CB-CG-CD  | 6.51  | 123.67      | 112.60   |
| 8   | P     | 123  | CYS  | CA-C-N    | 6.51  | 131.60      | 122.23   |
| 8   | P     | 123  | CYS  | C-N-CA    | 6.51  | 131.60      | 122.23   |
| 8   | P     | 232  | ASP  | N-CA-C    | -6.50 | 103.09      | 111.02   |
| 12  | V     | 1340 | HIS  | CA-C-N    | 6.50  | 128.99      | 120.28   |
| 12  | V     | 1340 | HIS  | C-N-CA    | 6.50  | 128.99      | 120.28   |
| 1   | S     | 100  | ASP  | CA-CB-CG  | 6.50  | 119.10      | 112.60   |
| 2   | B     | 743  | PHE  | CA-C-O    | -6.49 | 114.91      | 122.37   |
| 3   | C     | 186  | VAL  | CA-C-O    | -6.49 | 113.47      | 120.47   |
| 6   | G     | 211  | PHE  | CA-CB-CG  | -6.48 | 107.32      | 113.80   |
| 5   | F     | 24   | SER  | CA-C-N    | 6.48  | 129.84      | 120.38   |
| 5   | F     | 24   | SER  | C-N-CA    | 6.48  | 129.84      | 120.38   |
| 2   | O     | 291  | ASP  | CA-CB-CG  | 6.47  | 119.07      | 112.60   |
| 8   | P     | 554  | LEU  | CA-C-N    | 6.47  | 129.20      | 120.65   |
| 8   | P     | 554  | LEU  | C-N-CA    | 6.47  | 129.20      | 120.65   |
| 8   | Q     | 362  | THR  | CB-CA-C   | 6.47  | 118.60      | 108.63   |
| 8   | P     | 467  | GLU  | CB-CA-C   | -6.44 | 100.05      | 110.74   |
| 11  | U     | 415  | ASN  | CB-CA-C   | 6.44  | 119.02      | 109.29   |
| 8   | P     | 308  | HIS  | CA-CB-CG  | -6.44 | 107.36      | 113.80   |
| 1   | A     | 1012 | THR  | CB-CA-C   | 6.44  | 123.26      | 109.10   |
| 5   | F     | 339  | PHE  | CB-CA-C   | 6.43  | 121.30      | 109.46   |
| 7   | M     | 107  | PRO  | N-CA-C    | 6.43  | 118.54      | 110.70   |
| 6   | H     | 51   | ARG  | CG-CD-NE  | -6.42 | 97.89       | 112.00   |
| 8   | Q     | 542  | THR  | CA-CB-OG1 | -6.40 | 100.00      | 109.60   |
| 2   | O     | 204  | ASP  | CA-CB-CG  | 6.40  | 119.00      | 112.60   |
| 12  | V     | 276  | GLU  | N-CA-C    | -6.39 | 104.31      | 111.28   |
| 2   | O     | 586  | PRO  | N-CA-CB   | -6.39 | 95.98       | 103.26   |
| 7   | L     | 36   | PHE  | CA-CB-CG  | 6.38  | 120.18      | 113.80   |
| 1   | S     | 1104 | ARG  | CG-CD-NE  | 6.38  | 126.03      | 112.00   |
| 4   | E     | 399  | CYS  | CB-CA-C   | 6.37  | 122.36      | 110.70   |
| 8   | P     | 365  | ASP  | CA-CB-CG  | 6.37  | 118.97      | 112.60   |
| 2   | O     | 296  | ASN  | CA-CB-CG  | 6.36  | 118.96      | 112.60   |
| 6   | H     | 234  | GLU  | CA-C-N    | 6.35  | 129.27      | 120.63   |
| 6   | H     | 234  | GLU  | C-N-CA    | 6.35  | 129.27      | 120.63   |
| 11  | U     | 1144 | PHE  | CA-C-O    | -6.34 | 114.34      | 121.00   |
| 1   | S     | 287  | GLU  | CA-C-N    | 6.34  | 133.65      | 121.54   |
| 1   | S     | 287  | GLU  | C-N-CA    | 6.34  | 133.65      | 121.54   |
| 5   | F     | 266  | ARG  | CA-C-O    | -6.34 | 114.34      | 121.00   |
| 1   | A     | 942  | GLU  | CB-CG-CD  | 6.33  | 123.37      | 112.60   |
| 4   | E     | 397  | PRO  | CA-C-N    | 6.33  | 129.07      | 120.77   |
| 4   | E     | 397  | PRO  | C-N-CA    | 6.33  | 129.07      | 120.77   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 837  | GLU  | CB-CG-CD | 6.33  | 123.37      | 112.60   |
| 6   | H     | 291  | GLN  | CA-C-N   | 6.33  | 129.40      | 120.28   |
| 6   | H     | 291  | GLN  | C-N-CA   | 6.33  | 129.40      | 120.28   |
| 8   | P     | 327  | SER  | CA-C-N   | 6.31  | 131.11      | 122.34   |
| 8   | P     | 327  | SER  | C-N-CA   | 6.31  | 131.11      | 122.34   |
| 2   | B     | 764  | GLU  | N-CA-C   | -6.30 | 103.70      | 111.33   |
| 12  | V     | 690  | ASP  | CA-CB-CG | 6.30  | 118.90      | 112.60   |
| 2   | B     | 511  | ASP  | CA-CB-CG | 6.30  | 118.90      | 112.60   |
| 6   | G     | 540  | SER  | CA-C-N   | 6.30  | 128.57      | 120.70   |
| 6   | G     | 540  | SER  | C-N-CA   | 6.30  | 128.57      | 120.70   |
| 2   | O     | 481  | ARG  | CG-CD-NE | -6.29 | 98.15       | 112.00   |
| 6   | G     | 366  | HIS  | CB-CA-C  | 6.29  | 120.92      | 110.92   |
| 1   | A     | 1368 | PHE  | CA-CB-CG | -6.29 | 107.51      | 113.80   |
| 3   | C     | 85   | GLU  | CB-CG-CD | 6.28  | 123.27      | 112.60   |
| 2   | B     | 858  | ASN  | CA-CB-CG | 6.28  | 118.88      | 112.60   |
| 1   | S     | 1027 | ASP  | CA-CB-CG | 6.28  | 118.88      | 112.60   |
| 3   | C     | 245  | ARG  | CB-CA-C  | 6.26  | 120.95      | 110.44   |
| 4   | E     | 346  | THR  | CB-CA-C  | 6.25  | 120.82      | 110.81   |
| 7   | L     | 263  | LEU  | CA-C-N   | 6.25  | 127.96      | 120.14   |
| 7   | L     | 263  | LEU  | C-N-CA   | 6.25  | 127.96      | 120.14   |
| 8   | P     | 222  | ASP  | N-CA-C   | -6.25 | 104.75      | 112.38   |
| 1   | S     | 661  | ARG  | CG-CD-NE | 6.25  | 125.75      | 112.00   |
| 2   | B     | 723  | ASN  | CA-C-O   | -6.24 | 114.72      | 121.14   |
| 11  | U     | 530  | LEU  | CA-C-N   | 6.24  | 128.92      | 120.38   |
| 11  | U     | 530  | LEU  | C-N-CA   | 6.24  | 128.92      | 120.38   |
| 3   | C     | 84   | ASP  | CA-CB-CG | -6.23 | 106.37      | 112.60   |
| 7   | L     | 316  | ASP  | CA-CB-CG | 6.23  | 118.83      | 112.60   |
| 8   | P     | 270  | ALA  | O-C-N    | 6.23  | 128.75      | 122.08   |
| 8   | Q     | 468  | ARG  | CB-CG-CD | -6.22 | 96.99       | 111.30   |
| 2   | B     | 146  | HIS  | CA-C-N   | 6.22  | 133.17      | 121.97   |
| 2   | B     | 146  | HIS  | C-N-CA   | 6.22  | 133.17      | 121.97   |
| 6   | G     | 401  | ALA  | CA-C-O   | -6.21 | 113.97      | 120.55   |
| 10  | X     | 2    | GLN  | CA-C-N   | 6.20  | 128.91      | 120.54   |
| 10  | X     | 2    | GLN  | C-N-CA   | 6.20  | 128.91      | 120.54   |
| 4   | E     | 23   | GLU  | CB-CA-C  | 6.20  | 119.57      | 109.90   |
| 6   | H     | 136  | LEU  | CA-C-N   | 6.20  | 128.87      | 120.38   |
| 6   | H     | 136  | LEU  | C-N-CA   | 6.20  | 128.87      | 120.38   |
| 11  | U     | 518  | ILE  | CA-C-N   | 6.19  | 128.90      | 120.54   |
| 11  | U     | 518  | ILE  | C-N-CA   | 6.19  | 128.90      | 120.54   |
| 12  | V     | 1351 | THR  | CB-CA-C  | 6.19  | 120.68      | 110.90   |
| 8   | P     | 163  | ASP  | CA-CB-CG | 6.19  | 118.79      | 112.60   |
| 2   | O     | 642  | ILE  | CB-CA-C  | 6.17  | 117.90      | 111.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 21   | GLU  | CB-CA-C     | 6.17  | 122.44      | 109.79   |
| 4   | E     | 501  | GLN  | CA-C-N      | 6.17  | 128.55      | 120.28   |
| 4   | E     | 501  | GLN  | C-N-CA      | 6.17  | 128.55      | 120.28   |
| 7   | M     | 346  | LEU  | CA-C-N      | 6.17  | 128.84      | 120.38   |
| 7   | M     | 346  | LEU  | C-N-CA      | 6.17  | 128.84      | 120.38   |
| 6   | H     | 281  | PRO  | N-CA-C      | 6.17  | 118.22      | 110.70   |
| 6   | G     | 171  | SER  | CA-C-N      | 6.16  | 126.78      | 120.00   |
| 6   | G     | 171  | SER  | C-N-CA      | 6.16  | 126.78      | 120.00   |
| 3   | C     | 32   | GLN  | CB-CA-C     | -6.16 | 100.96      | 110.81   |
| 1   | A     | 510  | TYR  | CB-CA-C     | -6.16 | 100.39      | 110.85   |
| 8   | P     | 760  | ASP  | CA-CB-CG    | 6.16  | 118.76      | 112.60   |
| 12  | V     | 429  | LYS  | CA-C-N      | 6.16  | 128.85      | 120.54   |
| 12  | V     | 429  | LYS  | C-N-CA      | 6.16  | 128.85      | 120.54   |
| 10  | X     | 119  | ASN  | CB-CA-C     | 6.15  | 118.23      | 109.38   |
| 3   | C     | 204  | LEU  | CA-C-N      | -6.14 | 114.54      | 121.85   |
| 3   | C     | 204  | LEU  | C-N-CA      | -6.14 | 114.54      | 121.85   |
| 2   | O     | 525  | ASN  | CA-CB-CG    | -6.14 | 106.46      | 112.60   |
| 11  | U     | 1218 | ASN  | CA-CB-CG    | 6.13  | 118.73      | 112.60   |
| 8   | P     | 342  | CYS  | CB-CA-C     | 6.13  | 120.28      | 111.82   |
| 8   | P     | 606  | LEU  | CA-C-N      | 6.13  | 128.78      | 120.38   |
| 8   | P     | 606  | LEU  | C-N-CA      | 6.13  | 128.78      | 120.38   |
| 6   | G     | 450  | LEU  | CA-C-O      | -6.13 | 114.06      | 120.92   |
| 1   | S     | 94   | ILE  | CA-C-N      | 6.13  | 126.74      | 119.94   |
| 1   | S     | 94   | ILE  | C-N-CA      | 6.13  | 126.74      | 119.94   |
| 1   | S     | 781  | VAL  | CA-C-O      | -6.13 | 114.36      | 120.85   |
| 1   | A     | 924  | ASP  | CA-CB-CG    | 6.12  | 118.72      | 112.60   |
| 8   | P     | 386  | GLY  | CA-C-N      | 6.12  | 127.49      | 119.84   |
| 8   | P     | 386  | GLY  | C-N-CA      | 6.12  | 127.49      | 119.84   |
| 3   | C     | 227  | ILE  | CB-CA-C     | -6.11 | 104.17      | 111.81   |
| 2   | B     | 492  | LYS  | CB-CA-C     | 6.10  | 120.88      | 109.71   |
| 7   | M     | 60   | ARG  | CB-CG-CD    | 6.10  | 125.33      | 111.30   |
| 2   | B     | 589  | THR  | CB-CA-C     | 6.10  | 122.82      | 110.38   |
| 1   | S     | 852  | SER  | CA-C-N      | 6.10  | 129.42      | 120.82   |
| 1   | S     | 852  | SER  | C-N-CA      | 6.10  | 129.42      | 120.82   |
| 4   | E     | 519  | ASN  | CA-C-N      | 6.09  | 128.94      | 120.29   |
| 4   | E     | 519  | ASN  | C-N-CA      | 6.09  | 128.94      | 120.29   |
| 8   | P     | 359  | TYR  | CA-C-O      | -6.09 | 113.94      | 120.46   |
| 1   | A     | 897  | HIS  | CA-CB-CG    | 6.09  | 119.89      | 113.80   |
| 8   | Q     | 579  | GLU  | CB-CG-CD    | 6.09  | 122.95      | 112.60   |
| 1   | A     | 338  | ASP  | CA-CB-CG    | 6.09  | 118.69      | 112.60   |
| 5   | F     | 320  | PRO  | CB-CA-C     | -6.07 | 103.23      | 111.85   |
| 13  | Y     | 8    | DG   | C2'-C3'-O3' | 6.07  | 120.60      | 111.50   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 12  | V     | 1275 | PHE  | CA-C-O   | -6.07 | 114.45      | 120.82   |
| 8   | P     | 200  | VAL  | CA-C-O   | -6.06 | 113.20      | 120.78   |
| 8   | P     | 423  | LEU  | CA-C-N   | 6.06  | 129.32      | 120.71   |
| 8   | P     | 423  | LEU  | C-N-CA   | 6.06  | 129.32      | 120.71   |
| 11  | U     | 1048 | ASP  | CA-CB-CG | 6.06  | 118.66      | 112.60   |
| 12  | V     | 1205 | GLY  | CA-C-N   | 6.06  | 129.13      | 122.77   |
| 12  | V     | 1205 | GLY  | C-N-CA   | 6.06  | 129.13      | 122.77   |
| 2   | B     | 744  | LEU  | CA-C-O   | -6.06 | 115.21      | 121.87   |
| 4   | E     | 422  | CYS  | CA-C-O   | -6.05 | 114.13      | 120.55   |
| 8   | Q     | 490  | MET  | CA-C-O   | -6.05 | 114.01      | 120.42   |
| 1   | S     | 959  | ILE  | CA-C-O   | -6.05 | 114.66      | 120.95   |
| 12  | V     | 276  | GLU  | CB-CA-C  | 6.05  | 120.83      | 110.79   |
| 4   | E     | 309  | PRO  | N-CA-C   | 6.04  | 118.08      | 110.70   |
| 6   | H     | 233  | HIS  | CB-CA-C  | 6.04  | 121.82      | 109.67   |
| 2   | O     | 654  | ALA  | CA-C-N   | 6.04  | 129.41      | 120.95   |
| 2   | O     | 654  | ALA  | C-N-CA   | 6.04  | 129.41      | 120.95   |
| 12  | V     | 962  | PRO  | N-CA-C   | 6.04  | 118.07      | 110.70   |
| 7   | L     | 297  | ILE  | CB-CA-C  | 6.04  | 118.33      | 110.12   |
| 6   | H     | 192  | ASP  | CA-CB-CG | 6.03  | 118.63      | 112.60   |
| 8   | P     | 364  | SER  | O-C-N    | 6.03  | 128.55      | 122.03   |
| 8   | P     | 221  | GLU  | O-C-N    | 6.03  | 130.25      | 123.19   |
| 4   | E     | 56   | GLU  | CB-CG-CD | 6.03  | 122.85      | 112.60   |
| 10  | X     | 129  | SER  | CA-C-N   | 6.03  | 128.28      | 120.44   |
| 10  | X     | 129  | SER  | C-N-CA   | 6.03  | 128.28      | 120.44   |
| 12  | V     | 1304 | ALA  | CA-C-N   | 6.02  | 128.35      | 120.28   |
| 12  | V     | 1304 | ALA  | C-N-CA   | 6.02  | 128.35      | 120.28   |
| 8   | P     | 803  | ALA  | O-C-N    | 6.02  | 128.29      | 122.03   |
| 2   | O     | 477  | LYS  | CA-C-N   | 6.02  | 131.52      | 122.91   |
| 2   | O     | 477  | LYS  | C-N-CA   | 6.02  | 131.52      | 122.91   |
| 4   | E     | 18   | PRO  | CB-CA-C  | -6.02 | 101.63      | 111.56   |
| 1   | S     | 32   | ARG  | CA-C-O   | -6.01 | 114.19      | 120.92   |
| 6   | G     | 301  | GLU  | CB-CG-CD | 6.01  | 122.81      | 112.60   |
| 2   | B     | 320  | ALA  | O-C-N    | 6.00  | 129.40      | 123.46   |
| 1   | S     | 480  | LEU  | CA-C-N   | 6.00  | 124.02      | 120.24   |
| 1   | S     | 480  | LEU  | C-N-CA   | 6.00  | 124.02      | 120.24   |
| 1   | S     | 960  | HIS  | CA-C-N   | 6.00  | 133.47      | 122.79   |
| 1   | S     | 960  | HIS  | C-N-CA   | 6.00  | 133.47      | 122.79   |
| 2   | B     | 851  | PHE  | CA-CB-CG | -5.99 | 107.81      | 113.80   |
| 4   | E     | 321  | PRO  | CA-C-N   | 5.99  | 128.23      | 120.44   |
| 4   | E     | 321  | PRO  | C-N-CA   | 5.99  | 128.23      | 120.44   |
| 8   | P     | 477  | ASP  | CB-CA-C  | -5.99 | 101.47      | 110.88   |
| 3   | C     | 204  | LEU  | CA-C-O   | -5.99 | 111.28      | 119.12   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 6   | H     | 164  | GLU  | CB-CG-CD   | 5.99  | 122.77      | 112.60   |
| 2   | B     | 718  | ILE  | CA-C-O     | -5.98 | 113.98      | 120.67   |
| 8   | P     | 451  | ALA  | CA-C-N     | 5.97  | 126.57      | 119.94   |
| 8   | P     | 451  | ALA  | C-N-CA     | 5.97  | 126.57      | 119.94   |
| 10  | X     | 128  | ILE  | CA-C-O     | -5.97 | 114.32      | 120.71   |
| 1   | S     | 824  | CYS  | CB-CA-C    | 5.96  | 120.46      | 110.44   |
| 12  | V     | 967  | PHE  | CA-CB-CG   | 5.96  | 119.76      | 113.80   |
| 11  | U     | 1042 | PRO  | N-CA-CB    | -5.95 | 97.00       | 103.25   |
| 2   | B     | 44   | HIS  | CA-CB-CG   | -5.95 | 107.85      | 113.80   |
| 6   | H     | 13   | LEU  | CA-C-N     | 5.95  | 129.05      | 120.79   |
| 6   | H     | 13   | LEU  | C-N-CA     | 5.95  | 129.05      | 120.79   |
| 12  | V     | 309  | HIS  | CA-C-N     | 5.95  | 129.06      | 120.38   |
| 12  | V     | 309  | HIS  | C-N-CA     | 5.95  | 129.06      | 120.38   |
| 13  | Y     | 27   | DT   | N1-C1'-C2' | 5.94  | 122.41      | 113.50   |
| 3   | C     | 127  | PHE  | CB-CA-C    | 5.94  | 123.13      | 110.07   |
| 8   | Q     | 583  | PRO  | N-CA-C     | 5.94  | 120.51      | 111.19   |
| 11  | U     | 15   | ASP  | CA-CB-CG   | 5.94  | 118.54      | 112.60   |
| 2   | B     | 57   | PHE  | CA-CB-CG   | 5.93  | 119.73      | 113.80   |
| 6   | G     | 391  | PRO  | CA-C-N     | 5.93  | 132.20      | 121.06   |
| 6   | G     | 391  | PRO  | C-N-CA     | 5.93  | 132.20      | 121.06   |
| 6   | H     | 250  | THR  | CA-CB-OG1  | 5.93  | 118.49      | 109.60   |
| 8   | Q     | 537  | LEU  | CA-C-N     | 5.93  | 128.50      | 120.44   |
| 8   | Q     | 537  | LEU  | C-N-CA     | 5.93  | 128.50      | 120.44   |
| 2   | O     | 757  | ASP  | CA-C-N     | 5.92  | 128.50      | 120.44   |
| 2   | O     | 757  | ASP  | C-N-CA     | 5.92  | 128.50      | 120.44   |
| 2   | O     | 522  | LYS  | CA-C-N     | 5.92  | 130.40      | 121.40   |
| 2   | O     | 522  | LYS  | C-N-CA     | 5.92  | 130.40      | 121.40   |
| 2   | B     | 64   | PHE  | CA-CB-CG   | 5.92  | 119.72      | 113.80   |
| 3   | C     | 128  | ASP  | CA-CB-CG   | 5.92  | 118.52      | 112.60   |
| 11  | U     | 1061 | ASP  | CA-CB-CG   | 5.92  | 118.52      | 112.60   |
| 1   | A     | 862  | PRO  | CA-C-N     | 5.91  | 126.67      | 119.99   |
| 1   | A     | 862  | PRO  | C-N-CA     | 5.91  | 126.67      | 119.99   |
| 8   | Q     | 388  | GLY  | CA-C-N     | 5.91  | 127.31      | 121.57   |
| 8   | Q     | 388  | GLY  | C-N-CA     | 5.91  | 127.31      | 121.57   |
| 1   | A     | 158  | HIS  | CA-C-N     | 5.91  | 130.52      | 122.19   |
| 1   | A     | 158  | HIS  | C-N-CA     | 5.91  | 130.52      | 122.19   |
| 8   | P     | 178  | TYR  | CA-CB-CG   | -5.91 | 103.27      | 113.90   |
| 8   | Q     | 126  | PRO  | CA-C-N     | 5.91  | 128.19      | 120.28   |
| 8   | Q     | 126  | PRO  | C-N-CA     | 5.91  | 128.19      | 120.28   |
| 4   | E     | 161  | GLN  | CA-C-N     | 5.90  | 128.47      | 120.44   |
| 4   | E     | 161  | GLN  | C-N-CA     | 5.90  | 128.47      | 120.44   |
| 12  | V     | 275  | LEU  | CA-C-N     | 5.90  | 128.19      | 120.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | V     | 275  | LEU  | C-N-CA      | 5.90  | 128.19      | 120.28   |
| 1   | S     | 960  | HIS  | CB-CA-C     | 5.90  | 119.34      | 111.14   |
| 2   | B     | 174  | GLY  | CA-C-N      | 5.90  | 129.22      | 120.90   |
| 2   | B     | 174  | GLY  | C-N-CA      | 5.90  | 129.22      | 120.90   |
| 4   | E     | 339  | LEU  | CA-C-N      | 5.90  | 126.37      | 119.94   |
| 4   | E     | 339  | LEU  | C-N-CA      | 5.90  | 126.37      | 119.94   |
| 6   | H     | 252  | LEU  | CA-C-N      | 5.89  | 126.52      | 119.98   |
| 6   | H     | 252  | LEU  | C-N-CA      | 5.89  | 126.52      | 119.98   |
| 6   | G     | 234  | GLU  | CB-CG-CD    | 5.89  | 122.62      | 112.60   |
| 7   | L     | 303  | PHE  | CA-CB-CG    | 5.89  | 119.69      | 113.80   |
| 2   | O     | 522  | LYS  | O-C-N       | 5.89  | 129.54      | 122.94   |
| 8   | Q     | 545  | ILE  | CA-C-O      | -5.89 | 114.93      | 121.23   |
| 8   | P     | 337  | GLU  | CB-CA-C     | 5.89  | 119.62      | 110.67   |
| 1   | S     | 1003 | ASN  | CA-CB-CG    | 5.89  | 118.49      | 112.60   |
| 11  | U     | 878  | THR  | CA-CB-OG1   | -5.89 | 100.77      | 109.60   |
| 6   | G     | 410  | ALA  | CA-C-O      | -5.88 | 114.32      | 120.55   |
| 7   | L     | 133  | PHE  | N-CA-C      | -5.87 | 105.42      | 112.58   |
| 5   | F     | 283  | GLN  | CB-CG-CD    | 5.87  | 122.58      | 112.60   |
| 6   | G     | 449  | PRO  | CB-CA-C     | 5.87  | 119.03      | 111.46   |
| 6   | H     | 91   | ASP  | CA-CB-CG    | 5.85  | 118.45      | 112.60   |
| 6   | H     | 254  | SER  | CA-C-O      | -5.85 | 114.87      | 120.90   |
| 8   | P     | 595  | PRO  | N-CD-CG     | -5.85 | 94.43       | 103.20   |
| 2   | O     | 766  | GLU  | CA-C-N      | 5.85  | 128.12      | 120.28   |
| 2   | O     | 766  | GLU  | C-N-CA      | 5.85  | 128.12      | 120.28   |
| 12  | V     | 1273 | ARG  | CA-C-O      | -5.85 | 114.22      | 120.42   |
| 12  | V     | 765  | LEU  | CA-C-N      | 5.84  | 128.29      | 120.58   |
| 12  | V     | 765  | LEU  | C-N-CA      | 5.84  | 128.29      | 120.58   |
| 7   | L     | 258  | HIS  | CA-CB-CG    | 5.84  | 119.64      | 113.80   |
| 4   | E     | 129  | PRO  | CB-CA-C     | 5.83  | 120.03      | 111.22   |
| 2   | B     | 582  | THR  | CA-CB-OG1   | -5.83 | 100.85      | 109.60   |
| 2   | B     | 743  | PHE  | CA-CB-CG    | 5.83  | 119.63      | 113.80   |
| 11  | U     | 540  | PHE  | CA-C-O      | -5.83 | 114.69      | 120.70   |
| 11  | U     | 830  | SER  | CA-C-N      | 5.83  | 128.02      | 120.56   |
| 11  | U     | 830  | SER  | C-N-CA      | 5.83  | 128.02      | 120.56   |
| 4   | E     | 332  | GLN  | CB-CA-C     | 5.83  | 119.56      | 111.63   |
| 14  | Z     | 49   | DA   | C2'-C3'-O3' | 5.83  | 120.24      | 111.50   |
| 2   | B     | 726  | VAL  | N-CA-C      | -5.82 | 103.81      | 111.09   |
| 7   | M     | 44   | GLU  | CB-CG-CD    | 5.82  | 122.50      | 112.60   |
| 12  | V     | 480  | HIS  | CA-CB-CG    | -5.82 | 107.98      | 113.80   |
| 4   | E     | 156  | LEU  | CA-C-N      | 5.82  | 130.07      | 120.94   |
| 4   | E     | 156  | LEU  | C-N-CA      | 5.82  | 130.07      | 120.94   |
| 4   | E     | 129  | PRO  | N-CA-C      | -5.81 | 103.08      | 111.22   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | H     | 238  | GLY  | CA-C-O      | -5.81 | 116.55      | 122.59   |
| 2   | B     | 287  | VAL  | CA-CB-CG2   | 5.81  | 120.27      | 110.40   |
| 6   | H     | 77   | PHE  | CA-CB-CG    | 5.80  | 119.60      | 113.80   |
| 8   | P     | 28   | VAL  | CA-C-N      | 5.80  | 131.02      | 121.86   |
| 8   | P     | 28   | VAL  | C-N-CA      | 5.80  | 131.02      | 121.86   |
| 8   | P     | 341  | TYR  | CA-C-O      | -5.80 | 115.48      | 122.03   |
| 8   | P     | 221  | GLU  | N-CA-CB     | 5.79  | 120.08      | 110.52   |
| 11  | U     | 665  | ASP  | CA-C-N      | 5.79  | 128.52      | 120.29   |
| 11  | U     | 665  | ASP  | C-N-CA      | 5.79  | 128.52      | 120.29   |
| 1   | S     | 942  | GLU  | CB-CG-CD    | 5.79  | 122.44      | 112.60   |
| 1   | S     | 854  | ASP  | CA-CB-CG    | 5.78  | 118.38      | 112.60   |
| 6   | G     | 418  | GLU  | CB-CA-C     | -5.77 | 102.00      | 110.95   |
| 8   | P     | 561  | SER  | O-C-N       | 5.77  | 128.02      | 122.07   |
| 4   | E     | 395  | THR  | CA-C-O      | -5.77 | 114.75      | 120.70   |
| 1   | S     | 934  | HIS  | CA-CB-CG    | -5.77 | 108.03      | 113.80   |
| 3   | C     | 283  | GLN  | CB-CA-C     | 5.77  | 121.90      | 110.42   |
| 8   | P     | 320  | ARG  | CB-CA-C     | -5.77 | 101.13      | 110.77   |
| 12  | V     | 924  | PHE  | CA-CB-CG    | 5.77  | 119.57      | 113.80   |
| 12  | V     | 1305 | PHE  | CA-CB-CG    | 5.76  | 119.56      | 113.80   |
| 6   | G     | 91   | ASP  | CA-CB-CG    | 5.76  | 118.36      | 112.60   |
| 8   | P     | 228  | LEU  | CB-CA-C     | -5.76 | 102.02      | 110.95   |
| 8   | Q     | 804  | VAL  | CA-C-O      | -5.76 | 114.74      | 120.85   |
| 8   | Q     | 487  | ASN  | CA-CB-CG    | 5.76  | 118.36      | 112.60   |
| 11  | U     | 376  | ASP  | CA-CB-CG    | 5.75  | 118.36      | 112.60   |
| 2   | O     | 248  | ILE  | CA-C-O      | -5.75 | 116.33      | 121.97   |
| 6   | G     | 414  | LEU  | CA-C-O      | -5.75 | 113.86      | 120.24   |
| 7   | L     | 204  | MET  | CA-C-N      | 5.75  | 127.91      | 120.44   |
| 7   | L     | 204  | MET  | C-N-CA      | 5.75  | 127.91      | 120.44   |
| 4   | E     | 287  | GLN  | CB-CG-CD    | 5.75  | 122.37      | 112.60   |
| 11  | U     | 1036 | HIS  | CA-C-N      | 5.75  | 128.63      | 120.53   |
| 11  | U     | 1036 | HIS  | C-N-CA      | 5.75  | 128.63      | 120.53   |
| 6   | G     | 513  | ARG  | CB-CG-CD    | 5.74  | 124.51      | 111.30   |
| 8   | P     | 36   | PHE  | CA-CB-CG    | -5.74 | 108.06      | 113.80   |
| 11  | U     | 868  | GLU  | CB-CG-CD    | 5.74  | 122.36      | 112.60   |
| 1   | S     | 1223 | ASP  | CA-CB-CG    | 5.74  | 118.34      | 112.60   |
| 6   | H     | 167  | ASN  | CA-CB-CG    | 5.72  | 118.32      | 112.60   |
| 14  | Z     | 46   | DC   | C2'-C3'-O3' | 5.72  | 120.08      | 111.50   |
| 3   | C     | 324  | GLU  | CB-CA-C     | 5.72  | 120.55      | 110.37   |
| 5   | F     | 123  | ASP  | CA-CB-CG    | 5.71  | 118.31      | 112.60   |
| 8   | P     | 810  | THR  | CB-CA-C     | -5.71 | 101.91      | 110.88   |
| 11  | U     | 478  | SER  | CA-C-N      | 5.71  | 128.73      | 120.79   |
| 11  | U     | 478  | SER  | C-N-CA      | 5.71  | 128.73      | 120.79   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 211  | PRO  | N-CA-C   | 5.71  | 117.66      | 110.70   |
| 10  | X     | 6    | ARG  | CA-C-N   | 5.71  | 127.93      | 120.28   |
| 10  | X     | 6    | ARG  | C-N-CA   | 5.71  | 127.93      | 120.28   |
| 11  | U     | 425  | ILE  | N-CA-CB  | 5.71  | 117.23      | 110.55   |
| 12  | V     | 1354 | THR  | CA-C-N   | 5.71  | 127.86      | 120.44   |
| 12  | V     | 1354 | THR  | C-N-CA   | 5.71  | 127.86      | 120.44   |
| 8   | P     | 198  | CYS  | O-C-N    | 5.71  | 129.89      | 123.27   |
| 2   | B     | 111  | ILE  | CB-CA-C  | 5.70  | 119.12      | 110.62   |
| 4   | E     | 420  | LEU  | CA-C-N   | 5.70  | 128.17      | 120.65   |
| 4   | E     | 420  | LEU  | C-N-CA   | 5.70  | 128.17      | 120.65   |
| 8   | Q     | 496  | LEU  | CA-C-O   | -5.70 | 114.46      | 120.55   |
| 2   | B     | 287  | VAL  | CA-C-O   | -5.69 | 115.03      | 121.75   |
| 3   | C     | 153  | MET  | O-C-N    | 5.69  | 128.01      | 122.09   |
| 3   | C     | 163  | GLU  | CB-CG-CD | 5.69  | 122.27      | 112.60   |
| 2   | B     | 594  | CYS  | CB-CA-C  | 5.68  | 119.60      | 110.16   |
| 3   | C     | 200  | VAL  | N-CA-C   | -5.68 | 104.32      | 110.23   |
| 3   | C     | 314  | THR  | CA-C-O   | -5.68 | 113.68      | 120.10   |
| 8   | P     | 401  | ILE  | CA-C-O   | -5.68 | 115.70      | 121.67   |
| 6   | G     | 417  | CYS  | CA-C-N   | 5.68  | 128.35      | 120.63   |
| 6   | G     | 417  | CYS  | C-N-CA   | 5.68  | 128.35      | 120.63   |
| 12  | V     | 224  | HIS  | CA-C-N   | 5.68  | 127.82      | 120.44   |
| 12  | V     | 224  | HIS  | C-N-CA   | 5.68  | 127.82      | 120.44   |
| 1   | A     | 820  | SER  | CA-C-N   | 5.67  | 128.15      | 120.38   |
| 1   | A     | 820  | SER  | C-N-CA   | 5.67  | 128.15      | 120.38   |
| 2   | B     | 582  | THR  | CA-C-O   | -5.67 | 115.04      | 120.94   |
| 2   | O     | 768  | VAL  | CA-C-O   | -5.67 | 115.15      | 121.17   |
| 6   | G     | 394  | PRO  | N-CA-C   | 5.67  | 120.99      | 113.40   |
| 8   | P     | 70   | LEU  | CA-C-N   | 5.67  | 127.85      | 120.26   |
| 8   | P     | 70   | LEU  | C-N-CA   | 5.67  | 127.85      | 120.26   |
| 2   | O     | 108  | PHE  | CA-C-O   | -5.66 | 114.82      | 121.16   |
| 8   | P     | 361  | SER  | CB-CA-C  | 5.66  | 118.99      | 109.48   |
| 10  | X     | 10   | GLU  | CA-C-O   | -5.66 | 115.06      | 121.00   |
| 6   | H     | 124  | SER  | CA-C-N   | 5.66  | 127.69      | 120.56   |
| 6   | H     | 124  | SER  | C-N-CA   | 5.66  | 127.69      | 120.56   |
| 2   | B     | 693  | PHE  | CB-CA-C  | 5.66  | 120.06      | 109.71   |
| 8   | Q     | 726  | VAL  | CA-C-N   | 5.66  | 126.91      | 119.84   |
| 8   | Q     | 726  | VAL  | C-N-CA   | 5.66  | 126.91      | 119.84   |
| 1   | S     | 941  | PRO  | CA-C-N   | 5.66  | 128.65      | 120.79   |
| 1   | S     | 941  | PRO  | C-N-CA   | 5.66  | 128.65      | 120.79   |
| 11  | U     | 1176 | LEU  | CA-C-N   | 5.66  | 127.90      | 120.60   |
| 11  | U     | 1176 | LEU  | C-N-CA   | 5.66  | 127.90      | 120.60   |
| 2   | B     | 21   | GLU  | CA-C-N   | 5.65  | 130.70      | 123.13   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | B     | 21   | GLU  | C-N-CA      | 5.65  | 130.70      | 123.13   |
| 12  | V     | 191  | ASP  | CA-C-N      | 5.65  | 128.17      | 120.54   |
| 12  | V     | 191  | ASP  | C-N-CA      | 5.65  | 128.17      | 120.54   |
| 1   | A     | 1154 | PHE  | CA-CB-CG    | 5.64  | 119.44      | 113.80   |
| 6   | H     | 565  | ASP  | N-CA-C      | -5.64 | 105.03      | 111.07   |
| 11  | U     | 377  | HIS  | CA-C-N      | 5.64  | 128.16      | 120.77   |
| 11  | U     | 377  | HIS  | C-N-CA      | 5.64  | 128.16      | 120.77   |
| 8   | P     | 153  | GLN  | CB-CA-C     | -5.64 | 100.70      | 110.45   |
| 14  | Z     | 47   | DT   | C2'-C3'-O3' | 5.64  | 119.96      | 111.50   |
| 8   | Q     | 468  | ARG  | CG-CD-NE    | 5.63  | 124.39      | 112.00   |
| 6   | H     | 321  | PHE  | CB-CA-C     | 5.63  | 120.40      | 112.07   |
| 1   | A     | 1223 | ASP  | CA-C-N      | 5.63  | 128.09      | 120.38   |
| 1   | A     | 1223 | ASP  | C-N-CA      | 5.63  | 128.09      | 120.38   |
| 2   | B     | 686  | LYS  | CA-C-N      | 5.63  | 128.38      | 120.28   |
| 2   | B     | 686  | LYS  | C-N-CA      | 5.63  | 128.38      | 120.28   |
| 6   | H     | 154  | ASP  | CA-CB-CG    | 5.63  | 118.23      | 112.60   |
| 8   | P     | 595  | PRO  | N-CA-C      | 5.63  | 124.07      | 112.47   |
| 3   | C     | 294  | VAL  | CA-C-O      | -5.63 | 115.56      | 121.41   |
| 4   | E     | 285  | GLN  | CA-C-N      | 5.63  | 128.08      | 120.65   |
| 4   | E     | 285  | GLN  | C-N-CA      | 5.63  | 128.08      | 120.65   |
| 6   | G     | 487  | THR  | N-CA-C      | -5.62 | 102.55      | 110.31   |
| 8   | Q     | 483  | LEU  | CA-C-O      | -5.62 | 114.88      | 120.90   |
| 4   | E     | 318  | GLU  | CB-CG-CD    | 5.62  | 122.16      | 112.60   |
| 6   | H     | 76   | ASN  | CB-CA-C     | 5.62  | 120.24      | 110.68   |
| 2   | B     | 477  | LYS  | O-C-N       | 5.62  | 129.88      | 123.48   |
| 2   | O     | 593  | PHE  | CA-CB-CG    | 5.62  | 119.42      | 113.80   |
| 10  | X     | 121  | ASP  | CA-CB-CG    | 5.62  | 118.22      | 112.60   |
| 2   | B     | 362  | LEU  | CA-C-N      | 5.61  | 132.41      | 121.41   |
| 2   | B     | 362  | LEU  | C-N-CA      | 5.61  | 132.41      | 121.41   |
| 2   | B     | 742  | CYS  | CA-C-N      | 5.61  | 130.58      | 122.16   |
| 2   | B     | 742  | CYS  | C-N-CA      | 5.61  | 130.58      | 122.16   |
| 12  | V     | 168  | ASP  | CA-CB-CG    | 5.61  | 118.21      | 112.60   |
| 8   | P     | 127  | ASP  | CA-CB-CG    | 5.61  | 118.21      | 112.60   |
| 8   | P     | 153  | GLN  | N-CA-CB     | 5.61  | 119.16      | 110.46   |
| 12  | V     | 1120 | ASN  | CA-CB-CG    | 5.61  | 118.21      | 112.60   |
| 4   | E     | 440  | GLN  | CA-C-O      | -5.61 | 114.55      | 120.55   |
| 1   | A     | 990  | ASP  | CA-CB-CG    | 5.60  | 118.20      | 112.60   |
| 1   | A     | 247  | PHE  | CB-CA-C     | 5.60  | 117.75      | 109.29   |
| 8   | P     | 360  | HIS  | CA-CB-CG    | 5.60  | 119.40      | 113.80   |
| 8   | P     | 402  | CYS  | CA-C-O      | -5.60 | 115.46      | 121.45   |
| 2   | B     | 287  | VAL  | O-C-N       | 5.60  | 128.96      | 122.97   |
| 2   | B     | 392  | PRO  | N-CA-CB     | 5.60  | 108.51      | 103.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | U     | 263  | GLU  | CA-C-N      | 5.59  | 128.09      | 120.54   |
| 11  | U     | 263  | GLU  | C-N-CA      | 5.59  | 128.09      | 120.54   |
| 1   | S     | 1266 | MET  | CA-C-N      | 5.59  | 126.03      | 119.94   |
| 1   | S     | 1266 | MET  | C-N-CA      | 5.59  | 126.03      | 119.94   |
| 12  | V     | 683  | LEU  | CA-C-N      | 5.59  | 130.06      | 122.07   |
| 12  | V     | 683  | LEU  | C-N-CA      | 5.59  | 130.06      | 122.07   |
| 2   | B     | 781  | GLU  | CA-C-N      | 5.59  | 127.77      | 120.28   |
| 2   | B     | 781  | GLU  | C-N-CA      | 5.59  | 127.77      | 120.28   |
| 4   | E     | 284  | ILE  | CA-C-O      | -5.59 | 114.92      | 120.85   |
| 6   | H     | 353  | ARG  | CA-C-N      | 5.59  | 128.22      | 120.29   |
| 6   | H     | 353  | ARG  | C-N-CA      | 5.59  | 128.22      | 120.29   |
| 7   | L     | 128  | TYR  | CB-CA-C     | 5.59  | 120.41      | 109.35   |
| 2   | O     | 230  | PRO  | N-CA-C      | 5.58  | 117.51      | 110.70   |
| 8   | P     | 405  | VAL  | CA-C-N      | 5.58  | 131.75      | 121.70   |
| 8   | P     | 405  | VAL  | C-N-CA      | 5.58  | 131.75      | 121.70   |
| 7   | M     | 73   | ARG  | CB-CA-C     | 5.58  | 120.06      | 110.79   |
| 8   | P     | 119  | ASP  | CB-CA-C     | 5.58  | 116.89      | 108.86   |
| 8   | Q     | 560  | CYS  | CA-C-N      | 5.58  | 128.07      | 120.54   |
| 8   | Q     | 560  | CYS  | C-N-CA      | 5.58  | 128.07      | 120.54   |
| 2   | O     | 842  | VAL  | CA-C-O      | -5.56 | 115.17      | 120.95   |
| 7   | L     | 114  | LEU  | CA-C-O      | -5.56 | 114.66      | 120.55   |
| 8   | P     | 222  | ASP  | CB-CA-C     | 5.55  | 122.04      | 110.32   |
| 8   | Q     | 504  | ARG  | CB-CA-C     | 5.55  | 117.11      | 108.61   |
| 9   | W     | 78   | PHE  | CA-CB-CG    | 5.55  | 119.35      | 113.80   |
| 2   | B     | 135  | ARG  | CG-CD-NE    | 5.55  | 124.20      | 112.00   |
| 11  | U     | 422  | GLY  | CA-C-N      | 5.55  | 127.65      | 120.44   |
| 11  | U     | 422  | GLY  | C-N-CA      | 5.55  | 127.65      | 120.44   |
| 14  | Z     | 44   | DC   | C2'-C3'-O3' | 5.55  | 119.82      | 111.50   |
| 11  | U     | 302  | ASN  | CA-CB-CG    | 5.54  | 118.14      | 112.60   |
| 4   | E     | 286  | ASP  | CA-CB-CG    | 5.54  | 118.14      | 112.60   |
| 8   | Q     | 484  | THR  | N-CA-CB     | 5.54  | 118.00      | 109.91   |
| 10  | X     | 27   | ASP  | CA-CB-CG    | 5.54  | 118.14      | 112.60   |
| 11  | U     | 1209 | CYS  | N-CA-CB     | 5.54  | 118.19      | 109.94   |
| 6   | G     | 447  | TYR  | CA-C-O      | -5.54 | 114.35      | 120.38   |
| 8   | Q     | 521  | ASP  | CB-CA-C     | 5.53  | 118.66      | 109.53   |
| 11  | U     | 450  | THR  | CA-CB-OG1   | -5.53 | 101.30      | 109.60   |
| 5   | F     | 303  | PRO  | CA-C-N      | 5.53  | 128.00      | 120.54   |
| 5   | F     | 303  | PRO  | C-N-CA      | 5.53  | 128.00      | 120.54   |
| 2   | O     | 518  | PHE  | CB-CA-C     | 5.53  | 120.60      | 111.31   |
| 1   | S     | 928  | THR  | CB-CA-C     | -5.53 | 98.21       | 109.65   |
| 2   | B     | 584  | LEU  | CA-C-O      | -5.52 | 115.09      | 120.89   |
| 2   | O     | 660  | PHE  | CA-CB-CG    | -5.52 | 108.28      | 113.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 527  | ALA  | CA-C-N   | 5.52  | 129.82      | 120.88   |
| 11  | U     | 527  | ALA  | C-N-CA   | 5.52  | 129.82      | 120.88   |
| 2   | O     | 754  | PHE  | CA-C-O   | -5.52 | 114.70      | 120.55   |
| 8   | P     | 358  | VAL  | CA-C-O   | -5.52 | 114.48      | 120.71   |
| 1   | A     | 1263 | PHE  | CA-CB-CG | 5.51  | 119.31      | 113.80   |
| 12  | V     | 1360 | LEU  | CA-C-N   | 5.51  | 127.61      | 120.44   |
| 12  | V     | 1360 | LEU  | C-N-CA   | 5.51  | 127.61      | 120.44   |
| 2   | O     | 573  | GLU  | CB-CG-CD | 5.51  | 121.97      | 112.60   |
| 2   | B     | 720  | TYR  | CA-C-O   | -5.51 | 114.81      | 120.54   |
| 2   | O     | 303  | PHE  | CA-CB-CG | 5.51  | 119.31      | 113.80   |
| 11  | U     | 682  | VAL  | CA-C-O   | -5.51 | 114.94      | 121.05   |
| 2   | B     | 156  | GLN  | CA-C-N   | 5.50  | 127.92      | 120.65   |
| 2   | B     | 156  | GLN  | C-N-CA   | 5.50  | 127.92      | 120.65   |
| 7   | L     | 123  | TRP  | CA-C-N   | 5.50  | 128.21      | 120.28   |
| 7   | L     | 123  | TRP  | C-N-CA   | 5.50  | 128.21      | 120.28   |
| 4   | E     | 18   | PRO  | N-CA-C   | 5.50  | 123.79      | 112.47   |
| 8   | P     | 269  | ASN  | CA-CB-CG | -5.49 | 107.11      | 112.60   |
| 8   | Q     | 556  | LEU  | O-C-N    | 5.49  | 127.96      | 122.03   |
| 8   | P     | 396  | PRO  | N-CA-C   | -5.49 | 101.16      | 112.47   |
| 8   | P     | 176  | SER  | CA-C-N   | 5.49  | 128.18      | 120.28   |
| 8   | P     | 176  | SER  | C-N-CA   | 5.49  | 128.18      | 120.28   |
| 2   | O     | 687  | GLU  | CB-CG-CD | 5.49  | 121.93      | 112.60   |
| 1   | S     | 661  | ARG  | CB-CG-CD | -5.49 | 98.68       | 111.30   |
| 3   | C     | 316  | GLN  | CB-CA-C  | 5.48  | 120.17      | 110.85   |
| 6   | H     | 483  | LEU  | N-CA-CB  | -5.48 | 101.47      | 110.40   |
| 12  | V     | 781  | PHE  | CA-CB-CG | 5.48  | 119.28      | 113.80   |
| 1   | A     | 1270 | SER  | CA-C-N   | 5.47  | 127.56      | 120.44   |
| 1   | A     | 1270 | SER  | C-N-CA   | 5.47  | 127.56      | 120.44   |
| 8   | P     | 293  | GLN  | CB-CA-C  | 5.47  | 120.50      | 110.10   |
| 2   | B     | 331  | ASP  | CA-CB-CG | 5.47  | 118.07      | 112.60   |
| 8   | Q     | 566  | THR  | CB-CA-C  | -5.47 | 100.44      | 110.62   |
| 2   | B     | 573  | GLU  | CB-CG-CD | 5.47  | 121.90      | 112.60   |
| 8   | P     | 349  | CYS  | CA-CB-SG | -5.47 | 101.82      | 114.40   |
| 1   | S     | 54   | HIS  | CA-CB-CG | -5.46 | 108.33      | 113.80   |
| 11  | U     | 680  | ASN  | CA-C-O   | -5.46 | 115.06      | 120.80   |
| 2   | B     | 142  | ILE  | N-CA-CB  | 5.46  | 117.23      | 111.00   |
| 8   | P     | 279  | GLU  | CB-CG-CD | 5.46  | 121.89      | 112.60   |
| 7   | M     | 67   | HIS  | CA-C-N   | 5.46  | 128.04      | 120.29   |
| 7   | M     | 67   | HIS  | C-N-CA   | 5.46  | 128.04      | 120.29   |
| 11  | U     | 919  | VAL  | N-CA-CB  | 5.46  | 116.57      | 110.51   |
| 1   | S     | 1129 | ASP  | CA-CB-CG | 5.46  | 118.06      | 112.60   |
| 4   | E     | 130  | ASP  | CA-CB-CG | -5.46 | 107.14      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5   | F     | 257  | ALA  | CA-C-N      | 5.46  | 126.14      | 120.03   |
| 5   | F     | 257  | ALA  | C-N-CA      | 5.46  | 126.14      | 120.03   |
| 1   | S     | 1049 | PHE  | CB-CA-C     | 5.46  | 121.51      | 110.38   |
| 8   | Q     | 556  | LEU  | CA-C-N      | 5.45  | 131.96      | 121.54   |
| 8   | Q     | 556  | LEU  | C-N-CA      | 5.45  | 131.96      | 121.54   |
| 3   | C     | 20   | SER  | CA-C-N      | 5.45  | 127.52      | 120.70   |
| 3   | C     | 20   | SER  | C-N-CA      | 5.45  | 127.52      | 120.70   |
| 11  | U     | 424  | ASN  | CA-C-O      | -5.45 | 114.64      | 120.42   |
| 8   | Q     | 636  | GLU  | O-C-N       | 5.45  | 126.74      | 120.58   |
| 11  | U     | 430  | PHE  | CA-C-O      | -5.45 | 115.10      | 120.82   |
| 11  | U     | 749  | VAL  | CA-C-O      | -5.45 | 115.39      | 121.17   |
| 1   | A     | 263  | PRO  | CA-C-N      | 5.44  | 127.89      | 120.54   |
| 1   | A     | 263  | PRO  | C-N-CA      | 5.44  | 127.89      | 120.54   |
| 1   | S     | 1184 | ARG  | CG-CD-NE    | -5.44 | 100.03      | 112.00   |
| 11  | U     | 1146 | HIS  | CA-C-O      | -5.44 | 114.82      | 120.92   |
| 1   | S     | 481  | VAL  | N-CA-CB     | 5.44  | 113.93      | 110.50   |
| 1   | A     | 989  | MET  | CA-C-N      | 5.44  | 127.88      | 120.54   |
| 1   | A     | 989  | MET  | C-N-CA      | 5.44  | 127.88      | 120.54   |
| 14  | Z     | 45   | DT   | C2'-C3'-O3' | 5.44  | 119.66      | 111.50   |
| 2   | B     | 730  | CYS  | CA-C-O      | -5.43 | 112.74      | 120.51   |
| 4   | E     | 451  | PHE  | CA-CB-CG    | 5.43  | 119.23      | 113.80   |
| 5   | F     | 256  | PRO  | CB-CA-C     | -5.43 | 102.60      | 111.56   |
| 6   | G     | 421  | LEU  | CA-C-N      | 5.43  | 128.00      | 120.29   |
| 6   | G     | 421  | LEU  | C-N-CA      | 5.43  | 128.00      | 120.29   |
| 7   | L     | 35   | ASP  | CA-CB-CG    | 5.43  | 118.03      | 112.60   |
| 7   | L     | 128  | TYR  | N-CA-C      | -5.43 | 100.17      | 109.24   |
| 3   | C     | 200  | VAL  | O-C-N       | 5.43  | 127.82      | 121.96   |
| 2   | B     | 515  | ASP  | CA-CB-CG    | 5.43  | 118.03      | 112.60   |
| 3   | C     | 199  | LEU  | N-CA-C      | -5.43 | 105.26      | 111.07   |
| 6   | G     | 396  | VAL  | CA-CB-CG1   | 5.43  | 119.62      | 110.40   |
| 6   | G     | 387  | SER  | CA-C-N      | 5.42  | 125.96      | 120.38   |
| 6   | G     | 387  | SER  | C-N-CA      | 5.42  | 125.96      | 120.38   |
| 4   | E     | 522  | PHE  | N-CA-C      | -5.42 | 103.23      | 110.55   |
| 5   | F     | 166  | GLN  | CB-CG-CD    | -5.41 | 103.40      | 112.60   |
| 4   | E     | 427  | GLU  | CA-C-N      | 5.41  | 127.79      | 120.38   |
| 4   | E     | 427  | GLU  | C-N-CA      | 5.41  | 127.79      | 120.38   |
| 5   | F     | 310  | ARG  | CB-CG-CD    | -5.40 | 98.88       | 111.30   |
| 6   | G     | 349  | ILE  | CA-C-N      | 5.40  | 128.29      | 120.79   |
| 6   | G     | 349  | ILE  | C-N-CA      | 5.40  | 128.29      | 120.79   |
| 11  | U     | 1092 | ALA  | CA-C-O      | -5.40 | 115.14      | 120.70   |
| 2   | B     | 400  | VAL  | CB-CA-C     | 5.39  | 118.88      | 111.97   |
| 3   | C     | 359  | ILE  | CB-CA-C     | 5.39  | 114.61      | 109.33   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 6   | G     | 461  | GLN  | CA-C-N      | 5.39  | 128.28      | 120.79   |
| 6   | G     | 461  | GLN  | C-N-CA      | 5.39  | 128.28      | 120.79   |
| 10  | X     | 7    | LEU  | CA-C-N      | 5.39  | 127.45      | 120.44   |
| 10  | X     | 7    | LEU  | C-N-CA      | 5.39  | 127.45      | 120.44   |
| 7   | L     | 321  | ASP  | CA-C-N      | 5.39  | 128.42      | 120.82   |
| 7   | L     | 321  | ASP  | C-N-CA      | 5.39  | 128.42      | 120.82   |
| 5   | F     | 201  | PHE  | CA-CB-CG    | 5.39  | 119.19      | 113.80   |
| 6   | H     | 518  | ILE  | O-C-N       | 5.39  | 127.19      | 121.91   |
| 7   | L     | 133  | PHE  | CA-CB-CG    | -5.39 | 108.41      | 113.80   |
| 6   | G     | 520  | ARG  | CA-C-O      | -5.38 | 115.15      | 120.70   |
| 12  | V     | 301  | LEU  | O-C-N       | 5.38  | 127.62      | 122.07   |
| 3   | C     | 219  | PHE  | CA-C-O      | -5.38 | 115.17      | 120.82   |
| 11  | U     | 437  | ARG  | CA-C-N      | 5.38  | 127.76      | 120.44   |
| 11  | U     | 437  | ARG  | C-N-CA      | 5.38  | 127.76      | 120.44   |
| 7   | L     | 253  | PHE  | CA-CB-CG    | 5.38  | 119.18      | 113.80   |
| 7   | M     | 66   | TYR  | CA-C-N      | 5.38  | 127.44      | 120.44   |
| 7   | M     | 66   | TYR  | C-N-CA      | 5.38  | 127.44      | 120.44   |
| 13  | Y     | 5    | DC   | C2'-C3'-O3' | 5.38  | 119.57      | 111.50   |
| 2   | B     | 142  | ILE  | CB-CA-C     | -5.38 | 104.45      | 110.96   |
| 6   | H     | 378  | SER  | CA-C-N      | 5.38  | 125.80      | 119.83   |
| 6   | H     | 378  | SER  | C-N-CA      | 5.38  | 125.80      | 119.83   |
| 11  | U     | 680  | ASN  | CB-CA-C     | 5.38  | 119.73      | 110.86   |
| 2   | O     | 599  | LEU  | CA-C-O      | -5.38 | 114.57      | 120.70   |
| 3   | C     | 315  | ILE  | CB-CA-C     | -5.38 | 104.88      | 112.14   |
| 11  | U     | 1217 | GLN  | CA-C-N      | 5.37  | 127.48      | 120.28   |
| 11  | U     | 1217 | GLN  | C-N-CA      | 5.37  | 127.48      | 120.28   |
| 2   | B     | 299  | PHE  | CA-C-O      | 5.37  | 126.13      | 120.33   |
| 2   | B     | 703  | THR  | N-CA-CB     | -5.37 | 101.72      | 109.83   |
| 4   | E     | 165  | GLN  | CA-C-N      | 5.37  | 128.01      | 120.28   |
| 4   | E     | 165  | GLN  | C-N-CA      | 5.37  | 128.01      | 120.28   |
| 6   | H     | 331  | PRO  | CB-CA-C     | 5.37  | 116.22      | 111.17   |
| 4   | E     | 26   | ALA  | N-CA-C      | -5.37 | 104.67      | 111.11   |
| 11  | U     | 480  | LYS  | CA-C-O      | -5.37 | 114.84      | 120.63   |
| 2   | B     | 850  | ASP  | CA-CB-CG    | 5.36  | 117.96      | 112.60   |
| 1   | A     | 169  | GLU  | CB-CG-CD    | 5.36  | 121.71      | 112.60   |
| 12  | V     | 670  | VAL  | CA-C-N      | 5.36  | 126.45      | 122.59   |
| 12  | V     | 670  | VAL  | C-N-CA      | 5.36  | 126.45      | 122.59   |
| 7   | M     | 267  | LEU  | CA-C-O      | -5.36 | 115.17      | 120.90   |
| 2   | B     | 230  | PRO  | CB-CA-C     | -5.35 | 106.36      | 111.39   |
| 3   | C     | 206  | CYS  | CB-CA-C     | 5.35  | 121.07      | 110.42   |
| 7   | L     | 7    | SER  | CA-C-N      | 5.35  | 127.40      | 120.44   |
| 7   | L     | 7    | SER  | C-N-CA      | 5.35  | 127.40      | 120.44   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 1209 | CYS  | CB-CA-C  | -5.35 | 102.25      | 110.81   |
| 12  | V     | 1206 | VAL  | CA-C-N   | 5.35  | 126.88      | 120.13   |
| 12  | V     | 1206 | VAL  | C-N-CA   | 5.35  | 126.88      | 120.13   |
| 6   | H     | 369  | ASP  | CB-CA-C  | -5.35 | 99.46       | 110.38   |
| 1   | A     | 328  | LEU  | CA-C-N   | 5.35  | 127.40      | 120.44   |
| 1   | A     | 328  | LEU  | C-N-CA   | 5.35  | 127.40      | 120.44   |
| 6   | G     | 595  | SER  | O-C-N    | 5.35  | 127.87      | 122.09   |
| 12  | V     | 467  | THR  | CA-C-O   | -5.35 | 114.88      | 120.55   |
| 3   | C     | 373  | GLU  | CB-CG-CD | 5.35  | 121.69      | 112.60   |
| 2   | B     | 724  | GLN  | CB-CG-CD | 5.34  | 121.68      | 112.60   |
| 1   | S     | 990  | ASP  | CA-CB-CG | 5.34  | 117.94      | 112.60   |
| 3   | C     | 277  | LYS  | CA-C-O   | -5.34 | 114.76      | 120.42   |
| 11  | U     | 678  | TYR  | CA-C-O   | -5.34 | 114.76      | 120.42   |
| 3   | C     | 305  | THR  | CA-C-O   | -5.34 | 114.60      | 120.69   |
| 2   | B     | 157  | THR  | CB-CA-C  | 5.34  | 119.18      | 110.96   |
| 6   | H     | 519  | SER  | N-CA-C   | -5.34 | 104.51      | 111.02   |
| 11  | U     | 1029 | MET  | CA-C-O   | -5.34 | 115.40      | 121.00   |
| 3   | C     | 400  | PHE  | CA-C-N   | 5.33  | 125.41      | 120.34   |
| 3   | C     | 400  | PHE  | C-N-CA   | 5.33  | 125.41      | 120.34   |
| 8   | Q     | 757  | VAL  | CA-C-O   | -5.33 | 114.12      | 120.78   |
| 6   | H     | 208  | LEU  | N-CA-C   | -5.33 | 105.37      | 111.07   |
| 1   | S     | 928  | THR  | N-CA-CB  | 5.33  | 117.88      | 110.26   |
| 11  | U     | 396  | LYS  | CA-C-N   | 5.33  | 127.73      | 120.54   |
| 11  | U     | 396  | LYS  | C-N-CA   | 5.33  | 127.73      | 120.54   |
| 11  | U     | 870  | ILE  | N-CA-C   | -5.33 | 105.31      | 110.42   |
| 1   | S     | 952  | GLN  | CB-CA-C  | -5.33 | 101.95      | 110.79   |
| 3   | C     | 392  | GLU  | CB-CA-C  | 5.32  | 119.90      | 110.85   |
| 2   | B     | 717  | LEU  | N-CA-C   | -5.32 | 101.61      | 110.17   |
| 4   | E     | 429  | LEU  | CA-C-N   | 5.32  | 129.37      | 120.86   |
| 4   | E     | 429  | LEU  | C-N-CA   | 5.32  | 129.37      | 120.86   |
| 8   | Q     | 648  | ASP  | CA-CB-CG | 5.32  | 117.92      | 112.60   |
| 12  | V     | 922  | HIS  | CA-CB-CG | 5.31  | 119.11      | 113.80   |
| 1   | A     | 966  | GLU  | CB-CG-CD | 5.31  | 121.63      | 112.60   |
| 3   | C     | 325  | ALA  | CA-C-N   | 5.31  | 128.16      | 120.79   |
| 3   | C     | 325  | ALA  | C-N-CA   | 5.31  | 128.16      | 120.79   |
| 8   | P     | 828  | GLN  | CA-C-N   | 5.31  | 129.63      | 121.19   |
| 8   | P     | 828  | GLN  | C-N-CA   | 5.31  | 129.63      | 121.19   |
| 2   | O     | 763  | LEU  | CA-C-O   | -5.30 | 115.24      | 120.70   |
| 8   | P     | 384  | GLU  | N-CA-C   | 5.30  | 116.75      | 110.97   |
| 11  | U     | 809  | PHE  | CA-CB-CG | 5.30  | 119.10      | 113.80   |
| 2   | B     | 576  | GLN  | CB-CA-C  | -5.30 | 101.37      | 110.22   |
| 4   | E     | 31   | GLN  | N-CA-CB  | 5.30  | 117.91      | 110.12   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 8   | P     | 77   | TYR  | CA-C-O   | -5.29 | 114.66      | 120.43   |
| 12  | V     | 966  | LEU  | CA-C-N   | 5.29  | 128.15      | 120.79   |
| 12  | V     | 966  | LEU  | C-N-CA   | 5.29  | 128.15      | 120.79   |
| 4   | E     | 82   | GLU  | CB-CG-CD | 5.29  | 121.60      | 112.60   |
| 8   | Q     | 788  | GLN  | CB-CG-CD | 5.29  | 121.60      | 112.60   |
| 2   | B     | 196  | CYS  | CB-CA-C  | 5.29  | 120.95      | 110.42   |
| 8   | P     | 513  | THR  | CB-CA-C  | -5.29 | 102.90      | 110.62   |
| 11  | U     | 583  | PHE  | CA-C-N   | 5.29  | 127.80      | 120.29   |
| 11  | U     | 583  | PHE  | C-N-CA   | 5.29  | 127.80      | 120.29   |
| 8   | P     | 256  | LYS  | CA-C-O   | -5.29 | 114.94      | 120.55   |
| 2   | B     | 690  | GLU  | N-CA-CB  | -5.29 | 102.84      | 110.56   |
| 5   | F     | 103  | LEU  | CA-C-N   | 5.29  | 125.12      | 120.10   |
| 5   | F     | 103  | LEU  | C-N-CA   | 5.29  | 125.12      | 120.10   |
| 11  | U     | 703  | ASP  | CA-CB-CG | 5.28  | 117.88      | 112.60   |
| 5   | F     | 156  | ASN  | CA-C-O   | -5.28 | 116.02      | 122.41   |
| 8   | Q     | 678  | THR  | O-C-N    | 5.28  | 127.58      | 122.09   |
| 12  | V     | 276  | GLU  | CB-CG-CD | 5.28  | 121.58      | 112.60   |
| 5   | F     | 204  | VAL  | N-CA-C   | -5.28 | 104.74      | 110.23   |
| 6   | H     | 78   | ILE  | N-CA-C   | -5.28 | 104.60      | 110.62   |
| 6   | G     | 481  | GLU  | CB-CA-C  | 5.28  | 119.82      | 110.85   |
| 8   | P     | 800  | ALA  | CA-C-N   | 5.27  | 127.61      | 120.38   |
| 8   | P     | 800  | ALA  | C-N-CA   | 5.27  | 127.61      | 120.38   |
| 2   | B     | 703  | THR  | CA-C-O   | -5.27 | 115.39      | 121.19   |
| 7   | L     | 269  | ARG  | CB-CA-C  | -5.27 | 102.61      | 110.88   |
| 12  | V     | 1340 | HIS  | CA-CB-CG | 5.27  | 119.07      | 113.80   |
| 6   | G     | 444  | GLU  | CB-CG-CD | 5.27  | 121.55      | 112.60   |
| 1   | A     | 376  | GLN  | CA-C-N   | 5.26  | 127.28      | 120.44   |
| 1   | A     | 376  | GLN  | C-N-CA   | 5.26  | 127.28      | 120.44   |
| 1   | S     | 670  | ARG  | CB-CA-C  | 5.26  | 120.89      | 110.42   |
| 7   | M     | 39   | ARG  | CG-CD-NE | 5.26  | 123.58      | 112.00   |
| 10  | X     | 11   | LEU  | CA-C-N   | 5.26  | 127.28      | 120.44   |
| 10  | X     | 11   | LEU  | C-N-CA   | 5.26  | 127.28      | 120.44   |
| 11  | U     | 78   | SER  | CA-C-N   | 5.26  | 125.34      | 120.34   |
| 11  | U     | 78   | SER  | C-N-CA   | 5.26  | 125.34      | 120.34   |
| 5   | F     | 197  | PRO  | N-CA-C   | 5.26  | 119.47      | 110.95   |
| 1   | S     | 1128 | GLN  | CA-C-N   | 5.26  | 128.10      | 120.79   |
| 1   | S     | 1128 | GLN  | C-N-CA   | 5.26  | 128.10      | 120.79   |
| 1   | S     | 1126 | LEU  | CA-C-N   | 5.25  | 128.93      | 121.42   |
| 1   | S     | 1126 | LEU  | C-N-CA   | 5.25  | 128.93      | 121.42   |
| 4   | E     | 355  | LEU  | CA-C-N   | 5.25  | 129.13      | 121.31   |
| 4   | E     | 355  | LEU  | C-N-CA   | 5.25  | 129.13      | 121.31   |
| 1   | S     | 29   | ARG  | CA-C-N   | 5.25  | 127.53      | 120.50   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | S     | 29   | ARG  | C-N-CA    | 5.25  | 127.53      | 120.50   |
| 12  | V     | 381  | ASP  | CA-C-N    | 5.25  | 127.58      | 120.65   |
| 12  | V     | 381  | ASP  | C-N-CA    | 5.25  | 127.58      | 120.65   |
| 2   | B     | 10   | ASN  | CA-CB-CG  | 5.24  | 117.84      | 112.60   |
| 2   | B     | 317  | GLN  | CA-C-N    | -5.24 | 113.32      | 121.18   |
| 2   | B     | 317  | GLN  | C-N-CA    | -5.24 | 113.32      | 121.18   |
| 12  | V     | 1193 | THR  | CA-C-N    | 5.24  | 127.25      | 120.44   |
| 12  | V     | 1193 | THR  | C-N-CA    | 5.24  | 127.25      | 120.44   |
| 3   | C     | 157  | LEU  | O-C-N     | 5.24  | 127.75      | 122.09   |
| 2   | B     | 368  | SER  | CA-C-O    | -5.23 | 115.50      | 120.94   |
| 6   | G     | 559  | LYS  | CA-C-N    | 5.23  | 127.24      | 120.44   |
| 6   | G     | 559  | LYS  | C-N-CA    | 5.23  | 127.24      | 120.44   |
| 8   | Q     | 50   | GLU  | N-CA-CB   | 5.23  | 119.33      | 110.49   |
| 8   | Q     | 542  | THR  | N-CA-CB   | -5.23 | 102.48      | 111.21   |
| 12  | V     | 88   | SER  | CA-C-N    | 5.23  | 126.26      | 119.78   |
| 12  | V     | 88   | SER  | C-N-CA    | 5.23  | 126.26      | 119.78   |
| 2   | B     | 62   | THR  | CA-C-N    | 5.23  | 126.42      | 121.46   |
| 2   | B     | 62   | THR  | C-N-CA    | 5.23  | 126.42      | 121.46   |
| 3   | C     | 192  | THR  | CA-CB-OG1 | 5.23  | 117.44      | 109.60   |
| 7   | L     | 245  | PRO  | CA-C-N    | 5.23  | 128.01      | 120.38   |
| 7   | L     | 245  | PRO  | C-N-CA    | 5.23  | 128.01      | 120.38   |
| 2   | O     | 146  | HIS  | CA-C-N    | 5.23  | 131.38      | 121.97   |
| 2   | O     | 146  | HIS  | C-N-CA    | 5.23  | 131.38      | 121.97   |
| 8   | P     | 158  | PRO  | CA-C-N    | 5.23  | 126.62      | 120.09   |
| 8   | P     | 158  | PRO  | C-N-CA    | 5.23  | 126.62      | 120.09   |
| 5   | F     | 251  | PHE  | CA-CB-CG  | 5.22  | 119.02      | 113.80   |
| 11  | U     | 970  | LEU  | CA-C-O    | -5.22 | 115.52      | 120.90   |
| 12  | V     | 383  | VAL  | CA-C-N    | 5.22  | 127.23      | 120.44   |
| 12  | V     | 383  | VAL  | C-N-CA    | 5.22  | 127.23      | 120.44   |
| 2   | B     | 145  | ARG  | CB-CG-CD  | 5.22  | 123.31      | 111.30   |
| 2   | B     | 19   | ASN  | CB-CA-C   | 5.22  | 118.85      | 111.86   |
| 8   | P     | 221  | GLU  | CB-CG-CD  | 5.21  | 121.47      | 112.60   |
| 11  | U     | 180  | MET  | CA-C-N    | 5.21  | 127.99      | 120.38   |
| 11  | U     | 180  | MET  | C-N-CA    | 5.21  | 127.99      | 120.38   |
| 3   | C     | 390  | PRO  | CA-C-N    | 5.21  | 127.52      | 120.38   |
| 3   | C     | 390  | PRO  | C-N-CA    | 5.21  | 127.52      | 120.38   |
| 4   | E     | 26   | ALA  | O-C-N     | 5.21  | 127.51      | 122.09   |
| 7   | L     | 4    | THR  | CA-C-N    | 5.21  | 129.41      | 120.71   |
| 7   | L     | 4    | THR  | C-N-CA    | 5.21  | 129.41      | 120.71   |
| 7   | L     | 103  | ALA  | CA-C-N    | -5.21 | 112.70      | 121.76   |
| 7   | L     | 103  | ALA  | C-N-CA    | -5.21 | 112.70      | 121.76   |
| 8   | P     | 593  | ASP  | CA-CB-CG  | 5.21  | 117.81      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 283  | TYR  | CA-C-N   | 5.21  | 127.21      | 120.44   |
| 11  | U     | 283  | TYR  | C-N-CA   | 5.21  | 127.21      | 120.44   |
| 11  | U     | 495  | THR  | CA-C-N   | 5.21  | 127.12      | 120.56   |
| 11  | U     | 495  | THR  | C-N-CA   | 5.21  | 127.12      | 120.56   |
| 11  | U     | 655  | GLY  | CA-C-N   | 5.21  | 129.51      | 122.07   |
| 11  | U     | 655  | GLY  | C-N-CA   | 5.21  | 129.51      | 122.07   |
| 12  | V     | 1331 | PHE  | CA-C-O   | -5.20 | 115.03      | 120.55   |
| 2   | B     | 230  | PRO  | N-CA-C   | 5.20  | 115.46      | 110.47   |
| 3   | C     | 315  | ILE  | N-CA-CB  | 5.20  | 117.61      | 110.54   |
| 3   | C     | 407  | VAL  | CA-C-N   | 5.20  | 128.02      | 120.79   |
| 3   | C     | 407  | VAL  | C-N-CA   | 5.20  | 128.02      | 120.79   |
| 7   | L     | 232  | ASN  | CA-C-N   | 5.20  | 129.73      | 122.08   |
| 7   | L     | 232  | ASN  | C-N-CA   | 5.20  | 129.73      | 122.08   |
| 12  | V     | 389  | TYR  | CA-C-N   | 5.20  | 127.20      | 120.44   |
| 12  | V     | 389  | TYR  | C-N-CA   | 5.20  | 127.20      | 120.44   |
| 8   | Q     | 598  | VAL  | N-CA-CB  | 5.20  | 116.39      | 110.72   |
| 11  | U     | 1084 | VAL  | CA-C-N   | 5.20  | 128.02      | 120.79   |
| 11  | U     | 1084 | VAL  | C-N-CA   | 5.20  | 128.02      | 120.79   |
| 3   | C     | 178  | GLU  | CB-CG-CD | 5.20  | 121.43      | 112.60   |
| 12  | V     | 1271 | ALA  | CA-C-O   | -5.20 | 114.91      | 120.42   |
| 2   | O     | 482  | VAL  | N-CA-CB  | -5.19 | 104.30      | 111.99   |
| 1   | S     | 815  | PRO  | CA-C-N   | 5.19  | 127.24      | 120.28   |
| 1   | S     | 815  | PRO  | C-N-CA   | 5.19  | 127.24      | 120.28   |
| 8   | Q     | 50   | GLU  | CB-CG-CD | 5.19  | 121.43      | 112.60   |
| 11  | U     | 1138 | LEU  | CA-C-N   | 5.19  | 125.71      | 120.00   |
| 11  | U     | 1138 | LEU  | C-N-CA   | 5.19  | 125.71      | 120.00   |
| 3   | C     | 366  | GLN  | O-C-N    | 5.19  | 127.63      | 122.08   |
| 4   | E     | 528  | LYS  | CA-C-O   | -5.19 | 114.92      | 120.42   |
| 1   | A     | 1372 | ASP  | CA-CB-CG | 5.19  | 117.79      | 112.60   |
| 4   | E     | 133  | LEU  | N-CA-C   | -5.19 | 105.31      | 110.97   |
| 2   | B     | 138  | ASN  | CA-CB-CG | -5.19 | 107.41      | 112.60   |
| 8   | Q     | 329  | ASP  | CA-CB-CG | 5.19  | 117.79      | 112.60   |
| 7   | M     | 110  | PHE  | CA-C-N   | 5.18  | 127.54      | 120.54   |
| 7   | M     | 110  | PHE  | C-N-CA   | 5.18  | 127.54      | 120.54   |
| 10  | X     | 2    | GLN  | CB-CA-C  | 5.18  | 119.40      | 110.79   |
| 6   | G     | 481  | GLU  | CB-CG-CD | 5.18  | 121.41      | 112.60   |
| 8   | P     | 348  | LEU  | N-CA-CB  | -5.18 | 102.82      | 111.06   |
| 8   | Q     | 283  | ILE  | O-C-N    | 5.18  | 125.97      | 121.98   |
| 11  | U     | 1093 | GLU  | CA-C-N   | 5.18  | 127.49      | 120.65   |
| 11  | U     | 1093 | GLU  | C-N-CA   | 5.18  | 127.49      | 120.65   |
| 3   | C     | 344  | THR  | CA-C-N   | 5.18  | 128.24      | 120.83   |
| 3   | C     | 344  | THR  | C-N-CA   | 5.18  | 128.24      | 120.83   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 518  | PHE  | CB-CA-C  | -5.18 | 102.87      | 111.41   |
| 3   | C     | 144  | ASP  | CA-CB-CG | 5.18  | 117.78      | 112.60   |
| 5   | F     | 348  | THR  | CB-CA-C  | -5.18 | 102.75      | 110.88   |
| 6   | G     | 590  | PRO  | N-CD-CG  | -5.18 | 95.43       | 103.20   |
| 8   | P     | 337  | GLU  | CB-CG-CD | 5.18  | 121.40      | 112.60   |
| 12  | V     | 625  | PRO  | CA-C-N   | 5.18  | 127.17      | 120.44   |
| 12  | V     | 625  | PRO  | C-N-CA   | 5.18  | 127.17      | 120.44   |
| 12  | V     | 1227 | THR  | CA-C-N   | 5.18  | 127.22      | 120.28   |
| 12  | V     | 1227 | THR  | C-N-CA   | 5.18  | 127.22      | 120.28   |
| 7   | M     | 335  | GLN  | CB-CG-CD | 5.17  | 121.40      | 112.60   |
| 11  | U     | 982  | ALA  | CA-C-N   | 5.17  | 127.52      | 120.54   |
| 11  | U     | 982  | ALA  | C-N-CA   | 5.17  | 127.52      | 120.54   |
| 11  | U     | 1059 | ASP  | CA-CB-CG | 5.17  | 117.77      | 112.60   |
| 2   | O     | 47   | ARG  | CB-CA-C  | 5.17  | 119.05      | 110.78   |
| 11  | U     | 461  | ASP  | CB-CA-C  | 5.17  | 120.92      | 110.38   |
| 5   | F     | 88   | HIS  | CA-C-N   | 5.17  | 127.16      | 120.44   |
| 5   | F     | 88   | HIS  | C-N-CA   | 5.17  | 127.16      | 120.44   |
| 4   | E     | 474  | GLU  | CA-C-N   | 5.16  | 127.15      | 120.44   |
| 4   | E     | 474  | GLU  | C-N-CA   | 5.16  | 127.15      | 120.44   |
| 6   | G     | 487  | THR  | CB-CA-C  | 5.16  | 115.86      | 108.68   |
| 7   | L     | 170  | PRO  | N-CA-C   | 5.16  | 121.36      | 114.18   |
| 12  | V     | 1343 | GLY  | CA-C-N   | 5.16  | 127.19      | 120.28   |
| 12  | V     | 1343 | GLY  | C-N-CA   | 5.16  | 127.19      | 120.28   |
| 3   | C     | 398  | ILE  | O-C-N    | 5.16  | 127.25      | 121.94   |
| 4   | E     | 283  | ALA  | CA-C-O   | -5.16 | 115.06      | 120.63   |
| 4   | E     | 110  | PRO  | CA-C-N   | 5.15  | 127.19      | 120.28   |
| 4   | E     | 110  | PRO  | C-N-CA   | 5.15  | 127.19      | 120.28   |
| 11  | U     | 597  | GLN  | CA-C-N   | 5.15  | 131.38      | 121.54   |
| 11  | U     | 597  | GLN  | C-N-CA   | 5.15  | 131.38      | 121.54   |
| 11  | U     | 679  | LYS  | CB-CA-C  | -5.15 | 102.79      | 110.88   |
| 8   | P     | 385  | GLU  | CB-CA-C  | -5.15 | 100.17      | 110.42   |
| 1   | S     | 1020 | ARG  | N-CA-CB  | 5.15  | 117.78      | 110.16   |
| 2   | B     | 70   | GLU  | CB-CG-CD | 5.15  | 121.35      | 112.60   |
| 2   | B     | 328  | VAL  | CA-C-O   | -5.15 | 115.39      | 120.90   |
| 1   | S     | 1052 | PHE  | CA-CB-CG | 5.15  | 118.95      | 113.80   |
| 11  | U     | 335  | VAL  | O-C-N    | 5.15  | 127.25      | 121.90   |
| 11  | U     | 724  | ASP  | CA-CB-CG | 5.15  | 117.75      | 112.60   |
| 12  | V     | 95   | GLU  | CA-C-N   | 5.15  | 127.94      | 120.79   |
| 12  | V     | 95   | GLU  | C-N-CA   | 5.15  | 127.94      | 120.79   |
| 8   | P     | 46   | VAL  | CA-C-O   | -5.15 | 115.07      | 120.27   |
| 8   | P     | 723  | HIS  | CA-C-N   | 5.15  | 127.60      | 120.29   |
| 8   | P     | 723  | HIS  | C-N-CA   | 5.15  | 127.60      | 120.29   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 11  | U     | 770  | ASP  | N-CA-CB  | 5.15  | 117.61      | 109.94   |
| 1   | A     | 89   | HIS  | CA-C-N   | 5.14  | 128.07      | 120.82   |
| 1   | A     | 89   | HIS  | C-N-CA   | 5.14  | 128.07      | 120.82   |
| 12  | V     | 1243 | GLU  | CA-C-N   | 5.14  | 127.13      | 120.44   |
| 12  | V     | 1243 | GLU  | C-N-CA   | 5.14  | 127.13      | 120.44   |
| 6   | H     | 565  | ASP  | CA-CB-CG | 5.14  | 117.74      | 112.60   |
| 1   | S     | 903  | TRP  | CA-CB-CG | -5.14 | 103.84      | 113.60   |
| 11  | U     | 501  | LYS  | CA-C-N   | 5.14  | 127.43      | 120.65   |
| 11  | U     | 501  | LYS  | C-N-CA   | 5.14  | 127.43      | 120.65   |
| 3   | C     | 31   | GLN  | CA-C-O   | -5.13 | 115.61      | 120.90   |
| 3   | C     | 284  | ALA  | O-C-N    | 5.13  | 127.56      | 122.12   |
| 12  | V     | 211  | ILE  | O-C-N    | 5.13  | 126.94      | 121.91   |
| 12  | V     | 166  | ASN  | CA-CB-CG | 5.13  | 117.73      | 112.60   |
| 1   | S     | 669  | GLN  | N-CA-CB  | 5.13  | 117.70      | 110.36   |
| 3   | C     | 306  | ASP  | CA-CB-CG | 5.13  | 117.73      | 112.60   |
| 6   | H     | 189  | GLU  | CB-CG-CD | 5.13  | 121.32      | 112.60   |
| 2   | B     | 638  | LYS  | N-CA-C   | -5.13 | 106.36      | 113.18   |
| 8   | P     | 856  | GLU  | CB-CG-CD | 5.13  | 121.32      | 112.60   |
| 7   | M     | 11   | GLN  | CA-C-O   | -5.13 | 113.62      | 119.41   |
| 8   | P     | 281  | PRO  | N-CA-CB  | 5.12  | 108.20      | 103.39   |
| 8   | P     | 308  | HIS  | CB-CA-C  | 5.12  | 120.23      | 111.68   |
| 1   | A     | 1368 | PHE  | CA-C-N   | 5.12  | 127.11      | 120.56   |
| 1   | A     | 1368 | PHE  | C-N-CA   | 5.12  | 127.11      | 120.56   |
| 1   | S     | 938  | GLU  | CB-CG-CD | 5.12  | 121.30      | 112.60   |
| 10  | X     | 57   | ILE  | CA-C-O   | 5.12  | 122.17      | 119.15   |
| 1   | S     | 820  | SER  | CA-C-N   | 5.12  | 127.90      | 120.79   |
| 1   | S     | 820  | SER  | C-N-CA   | 5.12  | 127.90      | 120.79   |
| 8   | P     | 170  | ILE  | O-C-N    | 5.11  | 128.59      | 121.84   |
| 1   | S     | 109  | VAL  | CA-C-N   | 5.11  | 125.77      | 119.99   |
| 1   | S     | 109  | VAL  | C-N-CA   | 5.11  | 125.77      | 119.99   |
| 7   | M     | 89   | MET  | CA-C-N   | 5.11  | 127.39      | 120.44   |
| 7   | M     | 89   | MET  | C-N-CA   | 5.11  | 127.39      | 120.44   |
| 12  | V     | 247  | ASP  | CA-CB-CG | 5.11  | 117.71      | 112.60   |
| 12  | V     | 1161 | GLN  | CB-CA-C  | -5.11 | 102.63      | 110.81   |
| 2   | O     | 626  | ASP  | CA-CB-CG | 5.11  | 117.71      | 112.60   |
| 1   | A     | 92   | SER  | CA-C-N   | 5.11  | 127.08      | 120.44   |
| 1   | A     | 92   | SER  | C-N-CA   | 5.11  | 127.08      | 120.44   |
| 1   | S     | 552  | GLU  | CB-CA-C  | -5.11 | 102.80      | 110.92   |
| 1   | A     | 222  | GLU  | CA-C-N   | 5.11  | 127.54      | 120.29   |
| 1   | A     | 222  | GLU  | C-N-CA   | 5.11  | 127.54      | 120.29   |
| 2   | O     | 758  | ASN  | CA-C-N   | 5.11  | 127.43      | 120.54   |
| 2   | O     | 758  | ASN  | C-N-CA   | 5.11  | 127.43      | 120.54   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | O     | 849  | SER  | CA-C-N     | 5.11  | 127.08      | 120.44   |
| 2   | O     | 849  | SER  | C-N-CA     | 5.11  | 127.08      | 120.44   |
| 10  | X     | 127  | ASP  | CA-CB-CG   | 5.11  | 117.70      | 112.60   |
| 5   | F     | 276  | GLY  | CA-C-O     | -5.10 | 115.79      | 121.05   |
| 5   | F     | 238  | VAL  | CA-C-O     | -5.10 | 115.64      | 120.95   |
| 1   | S     | 924  | ASP  | CA-C-N     | 5.10  | 127.80      | 122.14   |
| 1   | S     | 924  | ASP  | C-N-CA     | 5.10  | 127.80      | 122.14   |
| 1   | S     | 1065 | VAL  | CA-C-O     | -5.10 | 115.11      | 120.57   |
| 6   | G     | 475  | GLU  | CB-CA-C    | 5.10  | 120.78      | 110.38   |
| 11  | U     | 421  | LEU  | CA-C-O     | -5.10 | 115.64      | 121.00   |
| 11  | U     | 1205 | LEU  | CA-C-O     | -5.10 | 115.10      | 120.71   |
| 11  | U     | 362  | THR  | CA-C-O     | -5.10 | 115.15      | 120.55   |
| 6   | H     | 351  | ALA  | CA-C-N     | 5.09  | 127.37      | 120.65   |
| 6   | H     | 351  | ALA  | C-N-CA     | 5.09  | 127.37      | 120.65   |
| 2   | B     | 171  | GLN  | CB-CG-CD   | 5.09  | 121.25      | 112.60   |
| 6   | H     | 553  | HIS  | O-C-N      | 5.09  | 127.31      | 122.07   |
| 7   | M     | 350  | GLN  | CB-CA-C    | 5.09  | 118.53      | 110.19   |
| 12  | V     | 1061 | CYS  | CA-C-N     | 5.09  | 127.05      | 120.44   |
| 12  | V     | 1061 | CYS  | C-N-CA     | 5.09  | 127.05      | 120.44   |
| 5   | F     | 168  | GLU  | CA-C-O     | -5.08 | 114.35      | 120.10   |
| 8   | Q     | 726  | VAL  | CB-CA-C    | 5.08  | 116.53      | 110.68   |
| 11  | U     | 760  | ILE  | O-C-N      | 5.08  | 127.18      | 121.94   |
| 13  | Y     | 26   | DG   | N9-C1'-C2' | 5.08  | 121.13      | 113.50   |
| 6   | G     | 509  | LEU  | CA-C-O     | -5.08 | 115.66      | 121.00   |
| 12  | V     | 430  | ASP  | CB-CA-C    | -5.08 | 102.67      | 110.81   |
| 8   | P     | 363  | PRO  | CA-C-N     | 5.08  | 127.54      | 120.63   |
| 8   | P     | 363  | PRO  | C-N-CA     | 5.08  | 127.54      | 120.63   |
| 12  | V     | 529  | ILE  | CA-C-O     | -5.08 | 115.47      | 120.85   |
| 1   | A     | 151  | PHE  | CA-CB-CG   | -5.08 | 108.72      | 113.80   |
| 3   | C     | 248  | PRO  | N-CA-CB    | -5.08 | 98.40       | 103.48   |
| 4   | E     | 486  | SER  | CA-C-N     | 5.08  | 127.04      | 120.44   |
| 4   | E     | 486  | SER  | C-N-CA     | 5.08  | 127.04      | 120.44   |
| 5   | F     | 309  | ASN  | CA-CB-CG   | -5.07 | 107.53      | 112.60   |
| 8   | P     | 79   | LEU  | CA-C-N     | 5.07  | 128.91      | 120.94   |
| 8   | P     | 79   | LEU  | C-N-CA     | 5.07  | 128.91      | 120.94   |
| 8   | P     | 280  | GLU  | CB-CA-C    | 5.07  | 117.83      | 109.97   |
| 11  | U     | 587  | ILE  | CA-C-O     | -5.07 | 115.67      | 120.95   |
| 8   | P     | 232  | ASP  | CA-CB-CG   | 5.07  | 117.67      | 112.60   |
| 3   | C     | 6    | VAL  | CA-C-O     | -5.07 | 115.30      | 121.18   |
| 3   | C     | 144  | ASP  | CB-CA-C    | 5.07  | 119.14      | 110.01   |
| 3   | C     | 374  | LEU  | CA-C-O     | -5.07 | 115.18      | 120.55   |
| 11  | U     | 863  | ASP  | CA-CB-CG   | 5.07  | 117.67      | 112.60   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 7   | L     | 61   | THR  | N-CA-CB   | 5.07  | 117.66      | 110.06   |
| 11  | U     | 1261 | GLU  | CB-CG-CD  | 5.07  | 121.22      | 112.60   |
| 2   | B     | 656  | HIS  | CA-CB-CG  | -5.07 | 108.73      | 113.80   |
| 4   | E     | 337  | SER  | CA-C-N    | 5.07  | 127.02      | 120.44   |
| 4   | E     | 337  | SER  | C-N-CA    | 5.07  | 127.02      | 120.44   |
| 5   | F     | 9    | ASP  | CA-CB-CG  | 5.07  | 117.67      | 112.60   |
| 4   | E     | 108  | SER  | CA-C-O    | -5.06 | 116.31      | 122.64   |
| 8   | Q     | 306  | ASP  | CA-CB-CG  | 5.06  | 117.66      | 112.60   |
| 8   | Q     | 327  | SER  | CA-C-N    | 5.06  | 129.31      | 122.07   |
| 8   | Q     | 327  | SER  | C-N-CA    | 5.06  | 129.31      | 122.07   |
| 1   | A     | 281  | LEU  | CA-C-N    | 5.06  | 127.02      | 120.44   |
| 1   | A     | 281  | LEU  | C-N-CA    | 5.06  | 127.02      | 120.44   |
| 6   | G     | 396  | VAL  | CA-C-O    | -5.06 | 115.88      | 121.29   |
| 7   | L     | 346  | LEU  | CA-C-N    | 5.06  | 127.06      | 120.28   |
| 7   | L     | 346  | LEU  | C-N-CA    | 5.06  | 127.06      | 120.28   |
| 12  | V     | 929  | ASP  | CA-CB-CG  | 5.06  | 117.66      | 112.60   |
| 3   | C     | 339  | THR  | CA-CB-OG1 | -5.06 | 102.02      | 109.60   |
| 11  | U     | 919  | VAL  | N-CA-C    | -5.06 | 105.05      | 110.36   |
| 8   | P     | 600  | CYS  | CA-C-O    | -5.05 | 115.19      | 120.80   |
| 11  | U     | 599  | ALA  | CA-C-N    | 5.05  | 127.01      | 120.44   |
| 11  | U     | 599  | ALA  | C-N-CA    | 5.05  | 127.01      | 120.44   |
| 2   | B     | 11   | GLU  | CB-CG-CD  | 5.05  | 121.18      | 112.60   |
| 1   | A     | 1158 | LYS  | CB-CA-C   | -5.05 | 102.41      | 110.79   |
| 6   | G     | 501  | GLN  | CA-C-N    | 5.05  | 125.69      | 119.99   |
| 6   | G     | 501  | GLN  | C-N-CA    | 5.05  | 125.69      | 119.99   |
| 8   | P     | 234  | THR  | O-C-N     | 5.05  | 127.54      | 122.09   |
| 12  | V     | 1322 | GLU  | CA-C-N    | 5.05  | 127.35      | 120.54   |
| 12  | V     | 1322 | GLU  | C-N-CA    | 5.05  | 127.35      | 120.54   |
| 8   | Q     | 842  | ARG  | CB-CA-C   | -5.04 | 102.96      | 110.88   |
| 1   | A     | 1376 | VAL  | CB-CA-C   | 5.04  | 116.98      | 111.08   |
| 2   | B     | 743  | PHE  | N-CA-CB   | -5.04 | 103.76      | 110.57   |
| 1   | S     | 1024 | MET  | N-CA-C    | -5.04 | 106.64      | 112.89   |
| 8   | P     | 842  | ARG  | CB-CA-C   | 5.04  | 119.42      | 110.85   |
| 5   | F     | 172  | GLU  | CB-CG-CD  | 5.04  | 121.17      | 112.60   |
| 6   | G     | 392  | CYS  | CA-C-O    | -5.04 | 116.25      | 121.99   |
| 8   | P     | 546  | GLN  | CB-CA-C   | 5.03  | 118.46      | 109.65   |
| 4   | E     | 128  | ASP  | CA-CB-CG  | 5.03  | 117.63      | 112.60   |
| 3   | C     | 204  | LEU  | N-CA-C    | -5.03 | 107.12      | 113.20   |
| 2   | O     | 745  | LYS  | CA-C-N    | 5.03  | 128.69      | 121.50   |
| 2   | O     | 745  | LYS  | C-N-CA    | 5.03  | 128.69      | 121.50   |
| 1   | A     | 781  | VAL  | CA-C-O    | -5.02 | 115.53      | 120.85   |
| 6   | H     | 78   | ILE  | O-C-N     | 5.02  | 126.81      | 121.89   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | U     | 607 | GLU  | CB-CG-CD | 5.02  | 121.14      | 112.60   |
| 8   | Q     | 490 | MET  | N-CA-C   | -5.02 | 105.89      | 111.36   |
| 12  | V     | 386 | PHE  | N-CA-C   | -5.02 | 105.09      | 111.11   |
| 7   | L     | 347 | THR  | CB-CA-C  | -5.02 | 102.46      | 110.79   |
| 2   | O     | 410 | GLN  | CA-C-N   | 5.02  | 127.31      | 120.54   |
| 2   | O     | 410 | GLN  | C-N-CA   | 5.02  | 127.31      | 120.54   |
| 8   | P     | 471 | PHE  | CA-CB-CG | -5.02 | 108.78      | 113.80   |
| 11  | U     | 325 | GLN  | CA-C-N   | 5.02  | 126.88      | 120.56   |
| 11  | U     | 325 | GLN  | C-N-CA   | 5.02  | 126.88      | 120.56   |
| 3   | C     | 292 | ARG  | O-C-N    | 5.01  | 127.87      | 122.15   |
| 3   | C     | 493 | ASN  | CA-CB-CG | 5.01  | 117.61      | 112.60   |
| 5   | F     | 140 | ARG  | CG-CD-NE | -5.01 | 100.97      | 112.00   |
| 4   | E     | 368 | PHE  | CB-CA-C  | -5.01 | 102.01      | 110.88   |
| 4   | E     | 384 | THR  | N-CA-CB  | 5.01  | 117.43      | 109.82   |
| 6   | G     | 516 | ALA  | CA-C-O   | -5.01 | 115.22      | 120.63   |
| 8   | P     | 559 | ALA  | CA-C-N   | 5.01  | 129.44      | 121.72   |
| 8   | P     | 559 | ALA  | C-N-CA   | 5.01  | 129.44      | 121.72   |
| 11  | U     | 758 | PHE  | CA-C-N   | 5.01  | 126.95      | 120.44   |
| 11  | U     | 758 | PHE  | C-N-CA   | 5.01  | 126.95      | 120.44   |
| 6   | H     | 205 | ASP  | CB-CA-C  | 5.01  | 120.28      | 110.67   |
| 1   | S     | 904 | GLN  | CB-CA-C  | 5.00  | 118.67      | 110.96   |
| 6   | H     | 484 | PHE  | CA-CB-CG | 5.00  | 118.80      | 113.80   |

There are no chirality outliers.

All (152) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1013 | GLY  | Peptide |
| 1   | A     | 1121 | SER  | Peptide |
| 1   | A     | 1220 | PRO  | Peptide |
| 1   | A     | 1350 | GLU  | Peptide |
| 1   | A     | 1375 | THR  | Peptide |
| 1   | A     | 138  | THR  | Peptide |
| 1   | A     | 1428 | CYS  | Peptide |
| 1   | A     | 284  | GLY  | Peptide |
| 1   | A     | 484  | GLU  | Peptide |
| 1   | A     | 824  | CYS  | Peptide |
| 1   | A     | 897  | HIS  | Peptide |
| 1   | A     | 922  | GLU  | Peptide |
| 1   | A     | 923  | GLU  | Peptide |
| 2   | B     | 132  | ASP  | Peptide |
| 2   | B     | 139  | GLY  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | B     | 140 | PRO  | Peptide   |
| 2   | B     | 145 | ARG  | Peptide   |
| 2   | B     | 191 | LEU  | Peptide   |
| 2   | B     | 225 | ASP  | Peptide   |
| 2   | B     | 258 | ALA  | Peptide   |
| 2   | B     | 324 | LYS  | Peptide   |
| 2   | B     | 335 | GLY  | Peptide   |
| 2   | B     | 345 | PHE  | Peptide   |
| 2   | B     | 367 | TYR  | Sidechain |
| 2   | B     | 608 | ASN  | Peptide   |
| 2   | B     | 636 | PHE  | Peptide   |
| 2   | B     | 637 | PRO  | Peptide   |
| 2   | B     | 668 | ALA  | Peptide   |
| 2   | B     | 711 | THR  | Peptide   |
| 2   | B     | 748 | LYS  | Peptide   |
| 2   | B     | 857 | SER  | Peptide   |
| 3   | C     | 208 | GLY  | Peptide   |
| 3   | C     | 278 | ASP  | Peptide   |
| 3   | C     | 539 | GLU  | Peptide   |
| 3   | C     | 79  | PHE  | Sidechain |
| 4   | E     | 108 | SER  | Peptide   |
| 4   | E     | 126 | ALA  | Peptide   |
| 4   | E     | 147 | GLY  | Peptide   |
| 4   | E     | 151 | GLU  | Peptide   |
| 4   | E     | 464 | MET  | Peptide   |
| 4   | E     | 500 | TYR  | Peptide   |
| 4   | E     | 76  | GLY  | Peptide   |
| 5   | F     | 285 | LEU  | Peptide   |
| 6   | G     | 132 | LEU  | Peptide   |
| 6   | G     | 276 | GLY  | Peptide   |
| 6   | G     | 388 | PRO  | Peptide   |
| 6   | G     | 427 | LEU  | Peptide   |
| 6   | G     | 430 | LYS  | Peptide   |
| 6   | G     | 500 | GLU  | Peptide   |
| 6   | G     | 563 | ARG  | Peptide   |
| 6   | G     | 61  | PRO  | Peptide   |
| 6   | H     | 132 | LEU  | Peptide   |
| 6   | H     | 186 | PRO  | Peptide   |
| 6   | H     | 276 | GLY  | Peptide   |
| 6   | H     | 279 | TRP  | Peptide   |
| 6   | H     | 33  | SER  | Peptide   |
| 6   | H     | 563 | ARG  | Peptide   |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 7   | L     | 103 | ALA  | Peptide |
| 7   | L     | 109 | GLN  | Peptide |
| 7   | L     | 252 | PHE  | Peptide |
| 7   | L     | 55  | CYS  | Peptide |
| 7   | M     | 215 | GLU  | Peptide |
| 7   | M     | 350 | GLN  | Peptide |
| 7   | M     | 55  | CYS  | Peptide |
| 2   | O     | 154 | SER  | Peptide |
| 2   | O     | 247 | ILE  | Peptide |
| 2   | O     | 316 | PHE  | Peptide |
| 2   | O     | 483 | ILE  | Peptide |
| 2   | O     | 485 | ASP  | Peptide |
| 2   | O     | 525 | ASN  | Peptide |
| 2   | O     | 578 | ILE  | Peptide |
| 2   | O     | 581 | VAL  | Peptide |
| 2   | O     | 593 | PHE  | Peptide |
| 2   | O     | 635 | THR  | Peptide |
| 2   | O     | 636 | PHE  | Peptide |
| 2   | O     | 637 | PRO  | Peptide |
| 2   | O     | 857 | SER  | Peptide |
| 8   | P     | 131 | CYS  | Peptide |
| 8   | P     | 146 | GLY  | Peptide |
| 8   | P     | 170 | ILE  | Peptide |
| 8   | P     | 23  | ALA  | Peptide |
| 8   | P     | 24  | GLY  | Peptide |
| 8   | P     | 270 | ALA  | Peptide |
| 8   | P     | 283 | ILE  | Peptide |
| 8   | P     | 292 | PRO  | Peptide |
| 8   | P     | 319 | GLY  | Peptide |
| 8   | P     | 331 | SER  | Peptide |
| 8   | P     | 344 | PRO  | Peptide |
| 8   | P     | 345 | GLY  | Peptide |
| 8   | P     | 36  | PHE  | Peptide |
| 8   | P     | 361 | SER  | Peptide |
| 8   | P     | 382 | GLN  | Peptide |
| 8   | P     | 383 | PRO  | Peptide |
| 8   | P     | 389 | GLY  | Peptide |
| 8   | P     | 391 | PRO  | Peptide |
| 8   | P     | 397 | ALA  | Peptide |
| 8   | P     | 398 | SER  | Peptide |
| 8   | P     | 450 | SER  | Peptide |
| 8   | P     | 519 | THR  | Peptide |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 8   | P     | 556  | LEU  | Peptide           |
| 8   | P     | 582  | LEU  | Peptide           |
| 8   | P     | 584  | LEU  | Peptide           |
| 8   | P     | 589  | ASN  | Peptide           |
| 8   | P     | 594  | LEU  | Mainchain,Peptide |
| 8   | P     | 62   | ASP  | Peptide           |
| 8   | P     | 635  | GLN  | Peptide           |
| 8   | P     | 636  | GLU  | Peptide           |
| 8   | P     | 679  | PHE  | Sidechain         |
| 8   | P     | 722  | GLY  | Peptide           |
| 8   | P     | 724  | SER  | Peptide           |
| 8   | P     | 725  | GLY  | Peptide           |
| 8   | P     | 755  | GLN  | Peptide           |
| 8   | P     | 781  | PRO  | Peptide           |
| 8   | P     | 856  | GLU  | Peptide           |
| 8   | Q     | 315  | PHE  | Peptide           |
| 8   | Q     | 338  | LEU  | Peptide           |
| 8   | Q     | 389  | GLY  | Peptide           |
| 8   | Q     | 538  | ASP  | Peptide           |
| 8   | Q     | 549  | THR  | Peptide           |
| 8   | Q     | 584  | LEU  | Peptide           |
| 8   | Q     | 594  | LEU  | Peptide           |
| 8   | Q     | 647  | VAL  | Peptide           |
| 8   | Q     | 720  | LYS  | Peptide           |
| 8   | Q     | 724  | SER  | Peptide           |
| 1   | S     | 1121 | SER  | Peptide           |
| 1   | S     | 1350 | GLU  | Peptide           |
| 1   | S     | 284  | GLY  | Peptide           |
| 1   | S     | 31   | LYS  | Peptide           |
| 1   | S     | 484  | GLU  | Peptide           |
| 1   | S     | 495  | HIS  | Peptide           |
| 1   | S     | 561  | THR  | Peptide           |
| 1   | S     | 736  | VAL  | Peptide           |
| 1   | S     | 822  | LEU  | Peptide           |
| 1   | S     | 898  | LEU  | Peptide           |
| 1   | S     | 923  | GLU  | Peptide           |
| 1   | S     | 960  | HIS  | Peptide           |
| 11  | U     | 1154 | PRO  | Peptide           |
| 11  | U     | 415  | ASN  | Peptide           |
| 11  | U     | 547  | PHE  | Peptide           |
| 11  | U     | 640  | ASP  | Peptide           |
| 11  | U     | 933  | ALA  | Peptide           |

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| Mol | Chain | Res  | Type | Group             |
|-----|-------|------|------|-------------------|
| 12  | V     | 1224 | PRO  | Peptide           |
| 12  | V     | 204  | PRO  | Peptide           |
| 12  | V     | 377  | HIS  | Peptide           |
| 12  | V     | 411  | CYS  | Peptide           |
| 12  | V     | 541  | PHE  | Peptide           |
| 10  | X     | 152  | ARG  | Peptide           |
| 10  | X     | 61   | TYR  | Mainchain,Peptide |
| 10  | X     | 93   | PRO  | Mainchain,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     | 247     | 0            |
| 1   | S     | 9933  | 10028    | 9969     | 199     | 0            |
| 2   | B     | 5605  | 5790     | 5768     | 212     | 0            |
| 2   | O     | 5594  | 5759     | 5740     | 128     | 0            |
| 3   | C     | 4396  | 4442     | 4427     | 117     | 0            |
| 4   | E     | 3224  | 3390     | 3384     | 121     | 0            |
| 5   | F     | 2726  | 2740     | 2729     | 62      | 0            |
| 6   | G     | 4483  | 4537     | 4523     | 148     | 0            |
| 6   | H     | 4216  | 4288     | 4273     | 100     | 0            |
| 7   | L     | 2974  | 2977     | 2971     | 91      | 0            |
| 7   | M     | 2974  | 2977     | 2972     | 117     | 0            |
| 8   | P     | 5598  | 5681     | 5652     | 251     | 0            |
| 8   | Q     | 5631  | 5724     | 5694     | 116     | 0            |
| 9   | W     | 271   | 242      | 195      | 8       | 0            |
| 10  | X     | 1233  | 1251     | 1248     | 54      | 0            |
| 11  | U     | 9484  | 9883     | 9852     | 189     | 0            |
| 12  | V     | 9289  | 9518     | 9465     | 155     | 0            |
| 13  | Y     | 597   | 326      | 326      | 1       | 0            |
| 14  | Z     | 592   | 325      | 325      | 6       | 0            |
| 15  | G     | 1     | 0        | 0        | 0       | 0            |
| 15  | L     | 2     | 0        | 0        | 0       | 0            |
| 15  | M     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 88227 | 89365    | 88944    | 2112    | 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 12.

All (2112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 7:M:311:TYR:CD2  | 10:X:6:ARG:HD2   | 1.47                     | 1.49              |
| 7:M:311:TYR:CD2  | 10:X:6:ARG:CD    | 2.05                     | 1.38              |
| 7:M:361:TYR:CE1  | 10:X:101:SER:HA  | 1.69                     | 1.26              |
| 7:M:311:TYR:HD2  | 10:X:6:ARG:CD    | 1.43                     | 1.13              |
| 1:A:30:VAL:HG21  | 6:H:372:ALA:HB1  | 1.26                     | 1.09              |
| 5:F:311:PHE:O    | 5:F:315:CYS:SG   | 2.09                     | 1.09              |
| 7:M:311:TYR:CE2  | 10:X:6:ARG:CD    | 2.36                     | 1.09              |
| 7:M:311:TYR:CD2  | 10:X:6:ARG:HD3   | 1.89                     | 1.05              |
| 7:M:312:ALA:HB2  | 10:X:5:SER:HB2   | 1.36                     | 1.04              |
| 7:M:215:GLU:OE1  | 7:M:313:TYR:OH   | 1.74                     | 1.02              |
| 7:M:361:TYR:CD1  | 10:X:101:SER:HB3 | 1.95                     | 1.02              |
| 1:A:900:SER:HG   | 1:A:903:TRP:CD1  | 1.78                     | 1.00              |
| 7:M:311:TYR:HE2  | 10:X:6:ARG:NH1   | 1.59                     | 1.00              |
| 4:E:391:CYS:SG   | 4:E:398:VAL:HG11 | 2.02                     | 0.99              |
| 7:M:311:TYR:CE2  | 10:X:6:ARG:HD3   | 1.98                     | 0.98              |
| 3:C:286:CYS:O    | 3:C:340:TYR:OH   | 1.81                     | 0.95              |
| 6:G:393:MET:HG2  | 8:P:236:LEU:HD21 | 1.47                     | 0.95              |
| 3:C:224:ASN:ND2  | 3:C:249:SER:HB3  | 1.80                     | 0.94              |
| 7:M:361:TYR:CE1  | 10:X:101:SER:CA  | 2.49                     | 0.94              |
| 7:M:312:ALA:HB2  | 10:X:5:SER:CB    | 1.99                     | 0.92              |
| 8:P:154:LEU:HD22 | 8:P:258:LEU:HD23 | 1.49                     | 0.91              |
| 10:X:44:THR:HG21 | 10:X:116:SER:HA  | 1.53                     | 0.91              |
| 1:A:30:VAL:HG21  | 6:H:372:ALA:CB   | 1.99                     | 0.91              |
| 4:E:391:CYS:SG   | 4:E:423:LEU:HD21 | 2.11                     | 0.90              |
| 12:V:263:ARG:NH2 | 12:V:293:ASP:OD2 | 2.05                     | 0.90              |
| 8:P:679:PHE:C    | 8:P:679:PHE:CD2  | 2.50                     | 0.89              |
| 3:C:224:ASN:HD21 | 3:C:249:SER:HB3  | 1.38                     | 0.89              |
| 6:G:214:ARG:NH1  | 6:G:328:LEU:O    | 2.05                     | 0.88              |
| 7:L:313:TYR:CE1  | 7:L:319:ILE:HG23 | 2.07                     | 0.88              |
| 7:L:354:ILE:CG1  | 7:L:369:LYS:HG2  | 2.03                     | 0.88              |
| 3:C:241:CYS:SG   | 4:E:37:PRO:HD3   | 2.13                     | 0.88              |
| 1:A:78:ILE:HG23  | 1:A:123:GLN:HE22 | 1.38                     | 0.88              |
| 12:V:352:SER:O   | 12:V:356:TYR:HB2 | 1.75                     | 0.87              |
| 7:L:354:ILE:HG12 | 7:L:369:LYS:HG2  | 1.56                     | 0.87              |
| 1:S:494:LEU:HD11 | 1:S:518:LEU:HD11 | 1.57                     | 0.87              |
| 1:A:30:VAL:CG2   | 6:H:372:ALA:HB1  | 2.04                     | 0.86              |
| 7:M:73:ARG:HD3   | 7:M:86:GLU:OE1   | 1.75                     | 0.86              |
| 1:A:300:GLY:O    | 1:A:303:SER:OG   | 1.94                     | 0.85              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 5:F:289:LEU:HD12 | 6:G:539:LEU:HD21  | 1.57                     | 0.85              |
| 5:F:289:LEU:HD12 | 6:G:539:LEU:CD2   | 2.07                     | 0.85              |
| 7:M:311:TYR:HD2  | 10:X:6:ARG:HD2    | 0.91                     | 0.85              |
| 7:L:357:GLY:O    | 7:L:366:ILE:HG22  | 1.77                     | 0.84              |
| 1:S:288:GLU:HB3  | 1:S:292:HIS:HB2   | 1.59                     | 0.84              |
| 7:M:311:TYR:HE2  | 10:X:6:ARG:CZ     | 1.89                     | 0.84              |
| 3:C:224:ASN:ND2  | 3:C:249:SER:CB    | 2.39                     | 0.84              |
| 1:A:30:VAL:CG2   | 6:H:372:ALA:CB    | 2.54                     | 0.84              |
| 7:M:311:TYR:CE2  | 10:X:6:ARG:NH1    | 2.47                     | 0.82              |
| 7:L:339:TYR:OH   | 7:L:343:ARG:NH1   | 2.11                     | 0.81              |
| 1:S:868:PHE:CZ   | 1:S:910:LEU:HD22  | 2.16                     | 0.81              |
| 2:B:138:ASN:ND2  | 8:P:15:CYS:SG     | 2.54                     | 0.80              |
| 11:U:511:MET:SD  | 11:U:514:ARG:NH1  | 2.55                     | 0.80              |
| 8:P:402:CYS:SG   | 8:P:421:LEU:HB2   | 2.22                     | 0.80              |
| 7:M:361:TYR:CD1  | 10:X:101:SER:CB   | 2.64                     | 0.80              |
| 8:P:198:CYS:N    | 8:P:242:LEU:O     | 2.14                     | 0.79              |
| 11:U:525:MET:SD  | 11:U:594:CYS:SG   | 2.80                     | 0.79              |
| 7:L:356:PHE:CD1  | 7:L:367:THR:HG23  | 2.18                     | 0.79              |
| 6:G:303:LEU:O    | 6:G:306:LEU:HB3   | 1.82                     | 0.79              |
| 7:M:197:LEU:HD13 | 7:M:201:TRP:CZ2   | 2.19                     | 0.78              |
| 12:V:364:TRP:CH2 | 12:V:384:MET:HE3  | 2.17                     | 0.78              |
| 12:V:586:ALA:HB1 | 12:V:644:LEU:HD13 | 1.64                     | 0.78              |
| 1:A:919:VAL:O    | 1:A:923:GLU:OE2   | 2.01                     | 0.78              |
| 6:G:333:ASP:OD1  | 6:G:336:SER:N     | 2.17                     | 0.78              |
| 7:L:313:TYR:CD2  | 7:L:314:GLN:HG2   | 2.19                     | 0.78              |
| 8:Q:531:ASN:ND2  | 8:Q:573:GLY:O     | 2.16                     | 0.78              |
| 7:M:311:TYR:HE2  | 10:X:6:ARG:HH11   | 1.28                     | 0.78              |
| 2:B:259:LEU:HD12 | 2:B:284:PRO:HB2   | 1.66                     | 0.78              |
| 8:Q:510:THR:OG1  | 8:Q:645:HIS:ND1   | 2.17                     | 0.77              |
| 1:A:286:GLN:C    | 1:A:288:GLU:H     | 1.92                     | 0.77              |
| 6:G:547:ASN:HD22 | 6:G:550:THR:HG23  | 1.49                     | 0.77              |
| 2:O:480:TYR:HE2  | 2:O:622:LEU:HD13  | 1.49                     | 0.77              |
| 11:U:606:TYR:OH  | 11:U:662:GLU:OE2  | 2.02                     | 0.77              |
| 7:M:338:LEU:HD23 | 7:M:368:LEU:HD13  | 1.66                     | 0.77              |
| 11:U:1149:VAL:O  | 11:U:1212:PHE:HD2 | 1.68                     | 0.77              |
| 2:O:257:ILE:HD12 | 2:O:299:PHE:CE2   | 2.21                     | 0.76              |
| 4:E:455:GLN:NE2  | 4:E:459:GLU:OE1   | 2.18                     | 0.76              |
| 2:O:155:SER:O    | 2:O:156:GLN:HB3   | 1.84                     | 0.76              |
| 1:S:1033:ASP:OD2 | 1:S:1093:SER:HB2  | 1.85                     | 0.76              |
| 5:F:18:SER:O     | 5:F:100:ASN:ND2   | 2.19                     | 0.75              |
| 6:G:60:LEU:O     | 6:G:102:ARG:NH1   | 2.20                     | 0.75              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:H:103:VAL:O    | 6:H:106:THR:OG1   | 2.04                     | 0.75              |
| 1:S:974:ASP:O    | 1:S:976:ASP:N     | 2.20                     | 0.75              |
| 1:S:57:LEU:HB2   | 1:S:116:MET:HE1   | 1.67                     | 0.75              |
| 1:S:288:GLU:CB   | 1:S:292:HIS:HB2   | 2.15                     | 0.75              |
| 1:A:1113:ASN:O   | 1:A:1117:ARG:NE   | 2.20                     | 0.74              |
| 7:M:197:LEU:CD1  | 7:M:201:TRP:CZ2   | 2.69                     | 0.74              |
| 5:F:255:LEU:HD12 | 5:F:260:LEU:HD21  | 1.70                     | 0.74              |
| 8:P:366:LEU:HD22 | 8:P:393:MET:SD    | 2.27                     | 0.74              |
| 7:M:311:TYR:CE2  | 10:X:6:ARG:CZ     | 2.70                     | 0.74              |
| 3:C:55:MET:SD    | 3:C:60:VAL:HG21   | 2.27                     | 0.74              |
| 6:G:406:GLN:HE21 | 6:G:599:TRP:HB2   | 1.52                     | 0.74              |
| 8:P:11:LEU:HD13  | 8:P:429:LEU:HD23  | 1.67                     | 0.74              |
| 11:U:322:PHE:O   | 11:U:326:VAL:HG23 | 1.87                     | 0.73              |
| 1:S:1045:GLU:OE2 | 1:S:1104:ARG:N    | 2.21                     | 0.73              |
| 2:B:242:ILE:O    | 2:B:243:CYS:SG    | 2.46                     | 0.73              |
| 5:F:289:LEU:O    | 6:G:485:ARG:NH1   | 2.14                     | 0.73              |
| 7:L:342:LEU:HD21 | 7:L:358:GLU:O     | 1.87                     | 0.73              |
| 8:Q:11:LEU:HD11  | 8:Q:429:LEU:HD22  | 1.69                     | 0.73              |
| 8:P:347:VAL:C    | 8:P:348:LEU:HD12  | 2.14                     | 0.73              |
| 8:Q:486:LEU:HD23 | 8:Q:490:MET:HE3   | 1.70                     | 0.73              |
| 1:A:944:ASP:OD1  | 1:A:951:ARG:NH1   | 2.21                     | 0.72              |
| 8:P:527:CYS:SG   | 8:P:580:VAL:HB    | 2.29                     | 0.72              |
| 1:A:35:TYR:HE2   | 6:H:311:ASN:CB    | 2.01                     | 0.72              |
| 11:U:751:GLU:CD  | 11:U:841:TYR:OH   | 2.32                     | 0.72              |
| 8:P:11:LEU:HD22  | 8:P:429:LEU:HD22  | 1.71                     | 0.72              |
| 8:P:674:ASP:OD2  | 8:P:677:ALA:N     | 2.22                     | 0.72              |
| 2:O:601:ILE:HD12 | 2:O:613:ARG:O     | 1.90                     | 0.71              |
| 8:P:362:THR:HB   | 8:P:363:PRO:HD2   | 1.72                     | 0.71              |
| 1:S:1410:CYS:SG  | 1:S:1414:SER:OG   | 2.48                     | 0.71              |
| 2:O:423:TYR:CE1  | 8:Q:606:LEU:HD12  | 2.23                     | 0.71              |
| 5:F:282:GLY:HA3  | 5:F:347:TRP:CH2   | 2.25                     | 0.71              |
| 6:G:425:SER:HA   | 6:G:428:LEU:HD12  | 1.72                     | 0.71              |
| 8:P:65:TRP:O     | 8:P:66:HIS:HB2    | 1.91                     | 0.71              |
| 8:P:603:PHE:HD1  | 8:P:639:CYS:HG    | 1.38                     | 0.71              |
| 3:C:118:LEU:HA   | 3:C:121:ILE:HD12  | 1.72                     | 0.71              |
| 7:L:315:LEU:CD2  | 7:L:336:ILE:HD13  | 2.20                     | 0.71              |
| 3:C:397:PHE:CZ   | 3:C:404:ALA:HA    | 2.26                     | 0.71              |
| 1:S:940:GLN:HE21 | 1:S:1011:ARG:HD2  | 1.54                     | 0.71              |
| 1:S:993:GLN:HE22 | 1:S:1074:GLU:HB2  | 1.56                     | 0.71              |
| 1:A:394:SER:HB2  | 1:A:436:GLN:HE21  | 1.56                     | 0.70              |
| 13:Y:9:DT:C6     | 13:Y:10:DT:H72    | 2.26                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:U:711:ASN:HA   | 11:U:714:ILE:HD12 | 1.73                     | 0.70              |
| 2:B:682:CYS:HB3   | 2:B:692:TYR:HB3   | 1.73                     | 0.70              |
| 1:A:185:LEU:HD12  | 1:A:191:VAL:HG22  | 1.74                     | 0.70              |
| 5:F:139:ARG:O     | 5:F:142:ALA:HB3   | 1.91                     | 0.70              |
| 3:C:82:ALA:HB3    | 3:C:189:PRO:HB3   | 1.72                     | 0.70              |
| 1:S:830:LEU:HD22  | 1:S:871:LEU:HD21  | 1.72                     | 0.70              |
| 7:L:204:MET:SD    | 7:L:226:ARG:NH1   | 2.64                     | 0.70              |
| 1:A:992:HIS:HB3   | 1:A:1077:MET:HE1  | 1.73                     | 0.70              |
| 6:G:480:LEU:HD11  | 6:G:517:LEU:HD23  | 1.74                     | 0.70              |
| 1:A:35:TYR:CE2    | 6:H:311:ASN:CB    | 2.75                     | 0.69              |
| 5:F:283:GLN:NE2   | 5:F:332:CYS:SG    | 2.65                     | 0.69              |
| 8:P:11:LEU:HD13   | 8:P:429:LEU:CD2   | 2.22                     | 0.69              |
| 1:S:988:LEU:HD21  | 1:S:1077:MET:HE2  | 1.74                     | 0.69              |
| 11:U:647:LEU:HD13 | 11:U:721:PHE:CE1  | 2.28                     | 0.69              |
| 1:A:34:LYS:H      | 1:A:34:LYS:HE2    | 1.56                     | 0.69              |
| 6:G:159:LEU:HD23  | 6:G:177:LEU:HD12  | 1.74                     | 0.69              |
| 6:G:393:MET:HG2   | 8:P:236:LEU:CD2   | 2.23                     | 0.69              |
| 8:P:11:LEU:HD11   | 8:P:431:THR:HG23  | 1.74                     | 0.69              |
| 8:P:446:MET:CE    | 8:P:451:ALA:HB2   | 2.23                     | 0.69              |
| 1:S:57:LEU:CB     | 1:S:116:MET:HE1   | 2.23                     | 0.69              |
| 6:H:342:THR:HB    | 6:H:384:PRO:HG3   | 1.74                     | 0.68              |
| 2:O:581:VAL:C     | 2:O:582:THR:OG1   | 2.32                     | 0.68              |
| 8:P:735:TRP:O     | 8:P:807:ARG:NH1   | 2.26                     | 0.68              |
| 8:P:367:CYS:HA    | 8:P:392:PRO:HA    | 1.74                     | 0.68              |
| 1:S:428:VAL:HG22  | 1:S:476:PHE:CE1   | 2.28                     | 0.68              |
| 7:M:197:LEU:HD13  | 7:M:201:TRP:CH2   | 2.28                     | 0.68              |
| 12:V:435:ILE:HG22 | 12:V:436:LEU:HD23 | 1.74                     | 0.68              |
| 1:A:1045:GLU:OE2  | 1:A:1104:ARG:N    | 2.26                     | 0.68              |
| 2:O:602:MET:HE2   | 8:Q:548:LEU:HD11  | 1.75                     | 0.68              |
| 1:A:30:VAL:CG2    | 6:H:372:ALA:HB3   | 2.24                     | 0.68              |
| 2:B:240:VAL:CG1   | 2:B:256:LEU:HD11  | 2.24                     | 0.68              |
| 2:O:707:TRP:CH2   | 2:O:715:GLY:HA3   | 2.29                     | 0.68              |
| 7:M:311:TYR:CE2   | 10:X:6:ARG:NE     | 2.62                     | 0.68              |
| 1:S:751:ARG:HA    | 1:S:754:CYS:SG    | 2.33                     | 0.68              |
| 1:S:880:ARG:HB2   | 1:S:881:GLN:OE1   | 1.93                     | 0.68              |
| 1:A:656:ALA:HB3   | 1:A:683:ARG:NH2   | 2.09                     | 0.68              |
| 7:M:198:LYS:HD3   | 7:M:198:LYS:C     | 2.19                     | 0.68              |
| 6:G:412:ASP:O     | 6:G:415:THR:N     | 2.28                     | 0.67              |
| 2:B:15:LEU:O      | 2:B:79:CYS:SG     | 2.53                     | 0.67              |
| 8:Q:538:ASP:O     | 8:Q:570:ASP:O     | 2.13                     | 0.67              |
| 7:M:208:ASP:O     | 7:M:295:ARG:NH2   | 2.27                     | 0.67              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:H:83:SER:O     | 6:H:86:GLN:NE2    | 2.27                     | 0.67              |
| 2:B:298:PHE:CE1  | 2:B:312:TRP:CD1   | 2.82                     | 0.67              |
| 3:C:142:PRO:HA   | 3:C:145:TYR:HE1   | 1.60                     | 0.67              |
| 1:A:139:VAL:O    | 1:A:141:GLN:N     | 2.27                     | 0.67              |
| 3:C:227:ILE:HD11 | 3:C:239:VAL:HG12  | 1.77                     | 0.67              |
| 11:U:746:VAL:O   | 11:U:750:CYS:SG   | 2.53                     | 0.67              |
| 2:B:259:LEU:CD1  | 2:B:284:PRO:HB2   | 2.24                     | 0.67              |
| 2:B:664:SER:HB2  | 2:B:742:CYS:SG    | 2.35                     | 0.67              |
| 5:F:160:ASP:O    | 5:F:164:LYS:HB2   | 1.95                     | 0.67              |
| 2:B:298:PHE:CE1  | 2:B:312:TRP:HD1   | 2.13                     | 0.67              |
| 2:B:330:ILE:HG22 | 2:B:339:GLU:CD    | 2.20                     | 0.67              |
| 6:G:346:THR:O    | 6:G:349:ILE:N     | 2.27                     | 0.67              |
| 2:O:602:MET:N    | 2:O:602:MET:SD    | 2.67                     | 0.67              |
| 1:A:1224:TRP:CZ3 | 1:A:1225:LEU:HD13 | 2.30                     | 0.66              |
| 7:M:8:LEU:HD21   | 7:M:25:TYR:HE2    | 1.60                     | 0.66              |
| 2:B:707:TRP:CH2  | 2:B:715:GLY:HA3   | 2.31                     | 0.66              |
| 6:G:483:LEU:O    | 6:G:513:ARG:NH2   | 2.25                     | 0.66              |
| 8:P:84:GLY:HA3   | 8:P:126:PRO:HA    | 1.77                     | 0.66              |
| 8:P:510:THR:HA   | 8:P:526:THR:O     | 1.95                     | 0.66              |
| 7:M:361:TYR:CZ   | 10:X:101:SER:HA   | 2.29                     | 0.66              |
| 1:A:868:PHE:CZ   | 1:A:910:LEU:HD23  | 2.31                     | 0.66              |
| 1:A:900:SER:OG   | 1:A:903:TRP:CD1   | 2.49                     | 0.66              |
| 1:A:159:SER:OG   | 8:P:848:ARG:NH1   | 2.28                     | 0.66              |
| 7:L:338:LEU:HD11 | 7:L:342:LEU:HD11  | 1.77                     | 0.66              |
| 1:S:780:HIS:NE2  | 9:W:88:THR:O      | 2.25                     | 0.66              |
| 1:S:1419:ALA:HB2 | 1:S:1440:GLN:HE22 | 1.59                     | 0.66              |
| 11:U:371:SER:HA  | 11:U:375:TRP:CD1  | 2.31                     | 0.66              |
| 4:E:495:THR:HG22 | 12:V:162:PHE:CZ   | 2.31                     | 0.66              |
| 6:G:284:LEU:O    | 6:G:287:SER:OG    | 2.11                     | 0.66              |
| 4:E:446:TRP:CD1  | 4:E:450:THR:HG21  | 2.31                     | 0.66              |
| 7:L:354:ILE:HG12 | 7:L:369:LYS:CG    | 2.26                     | 0.66              |
| 4:E:22:LEU:O     | 4:E:27:ARG:NH2    | 2.29                     | 0.66              |
| 8:P:861:ALA:O    | 8:P:865:ARG:HB2   | 1.96                     | 0.66              |
| 11:U:341:LEU:C   | 11:U:345:GLN:HE22 | 2.02                     | 0.66              |
| 11:U:341:LEU:O   | 11:U:345:GLN:NE2  | 2.28                     | 0.66              |
| 7:L:322:GLN:OE1  | 7:L:335:GLN:NE2   | 2.29                     | 0.66              |
| 1:A:833:CYS:O    | 1:A:837:CYS:SG    | 2.50                     | 0.66              |
| 7:L:41:VAL:HB    | 7:L:52:ARG:HB2    | 1.78                     | 0.66              |
| 3:C:87:GLN:CD    | 3:C:87:GLN:H      | 2.03                     | 0.65              |
| 8:Q:48:ASP:O     | 8:Q:51:GLY:O      | 2.13                     | 0.65              |
| 4:E:73:VAL:HG23  | 4:E:82:GLU:HG3    | 1.77                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:145:ARG:HG3    | 2:O:150:PHE:CE1    | 2.31                     | 0.65              |
| 2:B:17:CYS:O       | 2:B:17:CYS:SG      | 2.49                     | 0.65              |
| 2:B:723:ASN:ND2    | 2:O:484:ASP:OD1    | 2.30                     | 0.65              |
| 8:P:399:LEU:O      | 8:P:423:LEU:O      | 2.15                     | 0.65              |
| 2:B:484:ASP:OD1    | 2:B:484:ASP:N      | 2.29                     | 0.65              |
| 1:S:424:LEU:HD21   | 1:S:472:PHE:HB3    | 1.79                     | 0.65              |
| 7:M:215:GLU:CD     | 7:M:313:TYR:OH     | 2.40                     | 0.65              |
| 1:A:835:LYS:HE2    | 1:A:903:TRP:CZ2    | 2.31                     | 0.65              |
| 3:C:254:MET:HB3    | 3:C:297:MET:HE1    | 1.78                     | 0.65              |
| 6:G:336:SER:OG     | 6:G:338:LEU:N      | 2.22                     | 0.65              |
| 2:O:522:LYS:C      | 2:O:523:CYS:SG     | 2.80                     | 0.65              |
| 1:S:1330:LEU:O     | 1:S:1333:PHE:HB3   | 1.97                     | 0.65              |
| 1:S:927:LEU:CD2    | 1:S:932:TRP:HB2    | 2.28                     | 0.65              |
| 6:G:249:TYR:HA     | 6:G:252:LEU:HD12   | 1.78                     | 0.64              |
| 12:V:366:LYS:O     | 12:V:370:ASN:ND2   | 2.31                     | 0.64              |
| 3:C:142:PRO:HA     | 3:C:145:TYR:CE1    | 2.32                     | 0.64              |
| 5:F:196:LEU:HD21   | 5:F:201:PHE:CD1    | 2.32                     | 0.64              |
| 6:G:212:ALA:O      | 6:G:231:SER:OG     | 2.15                     | 0.64              |
| 11:U:843:VAL:O     | 11:U:846:ALA:HB3   | 1.97                     | 0.64              |
| 11:U:1149:VAL:O    | 11:U:1212:PHE:CD2  | 2.49                     | 0.64              |
| 2:B:298:PHE:HE1    | 2:B:312:TRP:CD1    | 2.15                     | 0.64              |
| 6:H:73:VAL:HA      | 6:H:76:ASN:HD22    | 1.63                     | 0.64              |
| 8:P:602:LEU:O      | 8:P:640:LEU:N      | 2.26                     | 0.64              |
| 1:A:818:PHE:HZ     | 1:A:861:SER:HB2    | 1.61                     | 0.64              |
| 4:E:473:MET:CE     | 4:E:496:VAL:HG11   | 2.27                     | 0.64              |
| 4:E:495:THR:HG22   | 12:V:162:PHE:HZ    | 1.62                     | 0.64              |
| 5:F:189:LEU:HA     | 5:F:192:LEU:HD12   | 1.78                     | 0.64              |
| 5:F:207:VAL:HA     | 5:F:210:LEU:HD12   | 1.80                     | 0.64              |
| 3:C:224:ASN:HD22   | 3:C:249:SER:CB     | 2.10                     | 0.64              |
| 6:G:454:ALA:O      | 6:G:455:THR:C      | 2.39                     | 0.64              |
| 11:U:777:CYS:SG    | 11:U:778:TYR:N     | 2.71                     | 0.64              |
| 11:U:1025:CYS:SG   | 11:U:1074:ILE:HG23 | 2.38                     | 0.64              |
| 2:O:257:ILE:HD12   | 2:O:299:PHE:CD2    | 2.33                     | 0.64              |
| 3:C:267:ASN:O      | 3:C:555:ARG:NH2    | 2.31                     | 0.64              |
| 8:Q:603:PHE:HA     | 8:Q:638:VAL:O      | 1.98                     | 0.64              |
| 4:E:418:GLU:OE2    | 12:V:237:GLU:O     | 2.16                     | 0.63              |
| 2:O:248:ILE:O      | 2:O:249:LYS:O      | 2.15                     | 0.63              |
| 1:S:959:ILE:HG22   | 1:S:960:HIS:CE1    | 2.33                     | 0.63              |
| 1:A:1393:VAL:HG21  | 6:H:570:LEU:HD21   | 1.80                     | 0.63              |
| 11:U:445:LEU:HD21  | 11:U:463:LEU:HD13  | 1.79                     | 0.63              |
| 12:V:1013:VAL:HG21 | 12:V:1075:TRP:CD2  | 2.33                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:P:655:PHE:CE2    | 8:P:754:ILE:HD12   | 2.33                     | 0.63              |
| 7:M:198:LYS:HD3    | 7:M:198:LYS:O      | 1.98                     | 0.63              |
| 1:A:27:ALA:HB3     | 6:H:372:ALA:CB     | 2.28                     | 0.63              |
| 7:M:361:TYR:CD1    | 10:X:101:SER:CA    | 2.81                     | 0.63              |
| 6:H:461:GLN:OE1    | 6:H:465:GLN:NE2    | 2.31                     | 0.63              |
| 1:S:1161:THR:O     | 1:S:1321:ARG:NH2   | 2.31                     | 0.63              |
| 1:A:818:PHE:HA     | 1:A:821:LEU:HB3    | 1.81                     | 0.63              |
| 6:G:374:LEU:HD13   | 6:G:393:MET:HE1    | 1.81                     | 0.63              |
| 8:P:154:LEU:CD2    | 8:P:258:LEU:HD23   | 2.27                     | 0.63              |
| 6:G:414:LEU:HD21   | 6:G:462:ALA:HB3    | 1.80                     | 0.62              |
| 7:L:357:GLY:O      | 7:L:366:ILE:CG2    | 2.44                     | 0.62              |
| 1:A:845:LEU:HD23   | 1:A:856:LEU:HD11   | 1.81                     | 0.62              |
| 2:B:299:PHE:HZ     | 2:B:313:LYS:HD2    | 1.63                     | 0.62              |
| 12:V:364:TRP:CZ2   | 12:V:384:MET:HE3   | 2.34                     | 0.62              |
| 1:A:35:TYR:CE2     | 6:H:311:ASN:HB2    | 2.35                     | 0.62              |
| 7:L:356:PHE:CE1    | 7:L:367:THR:CG2    | 2.81                     | 0.62              |
| 3:C:60:VAL:O       | 3:C:64:PHE:CD2     | 2.53                     | 0.62              |
| 4:E:518:PRO:HB2    | 4:E:521:THR:HG23   | 1.79                     | 0.62              |
| 2:O:426:LEU:HD12   | 8:Q:490:MET:HE1    | 1.81                     | 0.62              |
| 1:S:1368:PHE:CZ    | 1:S:1392:PRO:HB2   | 2.35                     | 0.62              |
| 11:U:620:ALA:O     | 11:U:624:MET:HG2   | 2.00                     | 0.62              |
| 7:L:275:ASP:O      | 7:L:283:ASN:ND2    | 2.32                     | 0.62              |
| 1:S:874:ARG:O      | 1:S:946:LEU:HD11   | 2.00                     | 0.62              |
| 11:U:1060:ILE:HD11 | 11:U:1212:PHE:CD2  | 2.33                     | 0.62              |
| 1:A:1330:LEU:C     | 1:A:1332:PRO:HD2   | 2.24                     | 0.62              |
| 1:S:351:THR:HG21   | 1:S:391:SER:HB2    | 1.80                     | 0.62              |
| 1:S:1336:TYR:OH    | 1:S:1357:ALA:O     | 2.18                     | 0.62              |
| 2:B:47:ARG:NH2     | 2:B:112:LEU:HD21   | 2.15                     | 0.61              |
| 1:A:35:TYR:HE2     | 6:H:311:ASN:HB2    | 1.64                     | 0.61              |
| 3:C:254:MET:HE3    | 3:C:294:VAL:HG22   | 1.81                     | 0.61              |
| 7:L:212:TRP:CZ3    | 7:L:296:ALA:HB3    | 2.36                     | 0.61              |
| 11:U:1047:ARG:HG2  | 11:U:1051:GLN:HE21 | 1.64                     | 0.61              |
| 1:A:815:PRO:HA     | 1:A:818:PHE:CE2    | 2.35                     | 0.61              |
| 11:U:599:ALA:HB2   | 11:U:661:GLN:HA    | 1.82                     | 0.61              |
| 8:P:253:VAL:HG23   | 8:P:272:VAL:HA     | 1.81                     | 0.61              |
| 7:M:95:LEU:HD22    | 7:M:102:TYR:OH     | 2.01                     | 0.61              |
| 1:S:182:VAL:HA     | 1:S:185:LEU:HG     | 1.83                     | 0.61              |
| 4:E:70:GLU:CB      | 4:E:83:LEU:HD22    | 2.31                     | 0.61              |
| 4:E:424:VAL:HA     | 4:E:429:LEU:HD22   | 1.82                     | 0.61              |
| 5:F:275:LEU:HD22   | 5:F:325:VAL:HG23   | 1.82                     | 0.61              |
| 6:G:367:TYR:O      | 6:G:370:LEU:HB3    | 2.00                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:M:361:TYR:CD1   | 10:X:101:SER:HA   | 2.29                     | 0.61              |
| 1:A:327:ILE:O     | 1:A:388:ARG:NH1   | 2.34                     | 0.61              |
| 1:A:428:VAL:HG22  | 1:A:476:PHE:CE1   | 2.36                     | 0.61              |
| 7:M:309:ILE:HG12  | 7:M:333:PHE:HD1   | 1.66                     | 0.61              |
| 2:B:851:PHE:HA    | 2:B:854:GLN:HE21  | 1.65                     | 0.61              |
| 4:E:429:LEU:O     | 4:E:460:ARG:NH2   | 2.33                     | 0.61              |
| 8:P:241:VAL:O     | 8:P:253:VAL:N     | 2.33                     | 0.61              |
| 8:P:284:PHE:CG    | 8:P:350:ALA:HB3   | 2.36                     | 0.61              |
| 12:V:479:THR:O    | 12:V:483:SER:OG   | 2.12                     | 0.61              |
| 6:G:569:ALA:O     | 6:G:573:ARG:HG3   | 2.01                     | 0.60              |
| 2:O:181:MET:HG3   | 2:O:217:LEU:HD22  | 1.83                     | 0.60              |
| 7:M:322:GLN:OE1   | 7:M:335:GLN:NE2   | 2.34                     | 0.60              |
| 1:A:474:PHE:CD2   | 1:A:510:TYR:CD2   | 2.88                     | 0.60              |
| 11:U:474:LEU:HG   | 11:U:506:LEU:HD11 | 1.82                     | 0.60              |
| 1:A:494:LEU:HD13  | 1:A:518:LEU:HD22  | 1.82                     | 0.60              |
| 3:C:162:ARG:HB3   | 3:C:162:ARG:HH11  | 1.66                     | 0.60              |
| 7:M:361:TYR:HD1   | 10:X:101:SER:HB3  | 1.62                     | 0.60              |
| 1:A:137:LEU:HD13  | 1:A:141:GLN:HB3   | 1.84                     | 0.60              |
| 2:B:287:VAL:HG23  | 2:B:288:GLN:O     | 2.01                     | 0.60              |
| 6:G:397:PHE:O     | 6:G:400:ALA:HB3   | 2.00                     | 0.60              |
| 8:P:366:LEU:CD2   | 8:P:393:MET:SD    | 2.88                     | 0.60              |
| 1:S:927:LEU:HD21  | 1:S:932:TRP:HB2   | 1.82                     | 0.60              |
| 4:E:391:CYS:SG    | 4:E:398:VAL:CG1   | 2.86                     | 0.60              |
| 8:P:74:ARG:HD2    | 8:P:90:LEU:HB2    | 1.83                     | 0.60              |
| 11:U:450:THR:HG21 | 12:V:356:TYR:CD2  | 2.37                     | 0.60              |
| 4:E:156:LEU:HB2   | 4:E:161:GLN:HE22  | 1.66                     | 0.60              |
| 8:Q:487:ASN:ND2   | 7:M:15:LEU:O      | 2.33                     | 0.60              |
| 1:S:1045:GLU:HA   | 1:S:1104:ARG:HD3  | 1.82                     | 0.60              |
| 2:B:667:TYR:O     | 2:B:713:PHE:CD1   | 2.55                     | 0.60              |
| 6:H:72:THR:O      | 6:H:76:ASN:ND2    | 2.34                     | 0.60              |
| 3:C:191:ILE:HG13  | 3:C:232:ILE:HD12  | 1.84                     | 0.60              |
| 4:E:361:THR:HG23  | 4:E:401:ALA:HB2   | 1.84                     | 0.60              |
| 2:O:584:LEU:C     | 2:O:586:PRO:HD2   | 2.27                     | 0.60              |
| 8:P:390:LEU:HG    | 8:P:390:LEU:O     | 2.02                     | 0.60              |
| 3:C:315:ILE:HG22  | 3:C:399:HIS:HA    | 1.83                     | 0.60              |
| 1:S:1368:PHE:CZ   | 1:S:1392:PRO:CB   | 2.84                     | 0.60              |
| 1:A:167:CYS:SG    | 1:A:196:LEU:HD23  | 2.42                     | 0.60              |
| 3:C:114:ILE:O     | 3:C:117:VAL:HG12  | 2.00                     | 0.60              |
| 4:E:284:ILE:O     | 4:E:288:LEU:N     | 2.35                     | 0.60              |
| 6:G:137:SER:OG    | 6:G:190:GLU:OE1   | 2.17                     | 0.60              |
| 6:G:147:ALA:HA    | 6:G:159:LEU:CD1   | 2.32                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:L:105:PRO:O     | 7:L:107:PRO:HD3   | 2.02                     | 0.59              |
| 2:O:522:LYS:HG3   | 2:O:523:CYS:H     | 1.67                     | 0.59              |
| 12:V:979:MET:HE2  | 12:V:1009:ALA:HB2 | 1.83                     | 0.59              |
| 4:E:298:LEU:HD21  | 4:E:347:TRP:CZ2   | 2.37                     | 0.59              |
| 6:G:147:ALA:HA    | 6:G:159:LEU:HD11  | 1.83                     | 0.59              |
| 6:G:336:SER:HG    | 6:G:338:LEU:H     | 1.45                     | 0.59              |
| 2:O:480:TYR:CE2   | 2:O:622:LEU:HD13  | 2.34                     | 0.59              |
| 7:M:228:ILE:HD12  | 7:M:238:ILE:HD12  | 1.84                     | 0.59              |
| 12:V:417:LEU:HD11 | 12:V:453:PHE:CE1  | 2.38                     | 0.59              |
| 6:G:128:ALA:HA    | 6:G:131:LEU:HD12  | 1.84                     | 0.59              |
| 1:A:900:SER:HG    | 1:A:903:TRP:CG    | 2.18                     | 0.59              |
| 4:E:522:PHE:C     | 4:E:523:LEU:HG    | 2.27                     | 0.59              |
| 8:P:133:PHE:CD1   | 8:P:133:PHE:C     | 2.80                     | 0.59              |
| 8:P:198:CYS:O     | 8:P:241:VAL:HA    | 2.02                     | 0.59              |
| 1:A:29:ARG:NH2    | 6:H:365:GLU:HG3   | 2.17                     | 0.59              |
| 1:S:424:LEU:O     | 1:S:428:VAL:HG23  | 2.03                     | 0.59              |
| 7:M:361:TYR:HA    | 10:X:101:SER:HB3  | 1.84                     | 0.59              |
| 8:P:360:HIS:CE1   | 8:P:367:CYS:HB2   | 2.38                     | 0.59              |
| 1:A:29:ARG:HH22   | 6:H:365:GLU:HG3   | 1.67                     | 0.59              |
| 3:C:490:LEU:HA    | 3:C:493:ASN:HD22  | 1.68                     | 0.59              |
| 4:E:291:LEU:O     | 4:E:295:LEU:HG    | 2.03                     | 0.59              |
| 4:E:368:PHE:HD1   | 4:E:383:LEU:HD11  | 1.67                     | 0.59              |
| 6:G:475:GLU:OE1   | 6:G:475:GLU:HA    | 2.03                     | 0.59              |
| 2:O:586:PRO:HB2   | 2:O:587:LEU:HD23  | 1.85                     | 0.59              |
| 11:U:331:LYS:O    | 11:U:334:VAL:HB   | 2.02                     | 0.59              |
| 6:H:67:LEU:HD11   | 6:H:106:THR:HG21  | 1.85                     | 0.59              |
| 1:S:547:ALA:HB1   | 1:S:582:HIS:HA    | 1.85                     | 0.59              |
| 11:U:548:LYS:O    | 11:U:616:ASN:ND2  | 2.36                     | 0.59              |
| 11:U:874:LEU:HA   | 11:U:877:LEU:HD12 | 1.85                     | 0.59              |
| 1:A:21:ALA:HA     | 6:H:415:THR:HB    | 1.85                     | 0.58              |
| 1:A:30:VAL:HG22   | 6:H:372:ALA:HB3   | 1.85                     | 0.58              |
| 1:A:135:VAL:HA    | 1:A:178:LEU:HD12  | 1.84                     | 0.58              |
| 2:B:130:MET:HG3   | 2:B:144:TRP:CD1   | 2.38                     | 0.58              |
| 7:L:79:ASP:OD1    | 7:L:81:MET:N      | 2.30                     | 0.58              |
| 8:P:328:TRP:HB3   | 8:P:334:LEU:HD13  | 1.85                     | 0.58              |
| 1:S:415:MET:HE2   | 1:S:419:PHE:HZ    | 1.68                     | 0.58              |
| 2:B:519:ARG:NH1   | 2:B:520:LEU:O     | 2.35                     | 0.58              |
| 7:L:356:PHE:CE1   | 7:L:367:THR:HG23  | 2.37                     | 0.58              |
| 1:S:1020:ARG:O    | 1:S:1023:GLU:HB2  | 2.02                     | 0.58              |
| 3:C:134:PHE:CE2   | 5:F:166:GLN:HB3   | 2.38                     | 0.58              |
| 8:P:202:PRO:HB3   | 8:P:225:PHE:CD2   | 2.38                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:P:349:CYS:SG     | 8:P:399:LEU:HA     | 2.43                     | 0.58              |
| 6:G:346:THR:O      | 6:G:347:LYS:C      | 2.47                     | 0.58              |
| 8:Q:606:LEU:O      | 8:Q:609:VAL:N      | 2.36                     | 0.58              |
| 1:S:554:ALA:O      | 1:S:565:PRO:HG2    | 2.03                     | 0.58              |
| 11:U:1215:TYR:O    | 11:U:1219:LYS:HB2  | 2.03                     | 0.58              |
| 1:A:351:THR:HG21   | 1:A:391:SER:CB     | 2.32                     | 0.58              |
| 1:A:415:MET:HE2    | 1:A:451:TRP:CZ2    | 2.38                     | 0.58              |
| 2:B:684:ILE:HG12   | 2:B:692:TYR:CD2    | 2.39                     | 0.58              |
| 4:E:473:MET:HE1    | 4:E:496:VAL:HG11   | 1.84                     | 0.58              |
| 7:L:304:THR:HG22   | 7:L:306:ASP:HB2    | 1.85                     | 0.58              |
| 7:M:311:TYR:O      | 10:X:9:ARG:NE      | 2.37                     | 0.58              |
| 11:U:518:ILE:HG12  | 11:U:587:ILE:HD11  | 1.84                     | 0.58              |
| 2:B:231:PRO:O      | 2:B:234:SER:OG     | 2.15                     | 0.58              |
| 2:B:485:ASP:OD1    | 2:O:725:THR:HG23   | 2.03                     | 0.58              |
| 6:G:249:TYR:O      | 6:G:252:LEU:HB2    | 2.03                     | 0.58              |
| 2:O:523:CYS:HA     | 2:O:581:VAL:O      | 2.03                     | 0.58              |
| 8:P:339:ARG:NH1    | 8:P:385:GLU:O      | 2.37                     | 0.58              |
| 1:A:1410:CYS:SG    | 1:A:1414:SER:OG    | 2.61                     | 0.58              |
| 4:E:424:VAL:HG12   | 4:E:437:MET:HE3    | 1.84                     | 0.58              |
| 12:V:1119:GLN:HE21 | 12:V:1158:LEU:HD13 | 1.68                     | 0.58              |
| 2:B:122:LEU:HD21   | 2:B:155:SER:HA     | 1.86                     | 0.58              |
| 8:P:402:CYS:HG     | 8:P:421:LEU:HB2    | 1.68                     | 0.58              |
| 8:Q:339:ARG:NE     | 7:M:101:LEU:HD21   | 2.19                     | 0.58              |
| 7:M:105:PRO:O      | 7:M:107:PRO:HD3    | 2.03                     | 0.58              |
| 5:F:309:ASN:O      | 5:F:312:GLN:HB3    | 2.03                     | 0.58              |
| 1:S:992:HIS:CE1    | 1:S:1077:MET:HE1   | 2.39                     | 0.58              |
| 1:A:1336:TYR:OH    | 1:A:1357:ALA:O     | 2.19                     | 0.58              |
| 2:B:346:LYS:O      | 2:B:349:LEU:HD12   | 2.03                     | 0.58              |
| 6:G:246:VAL:O      | 6:G:250:THR:OG1    | 2.22                     | 0.58              |
| 8:Q:141:VAL:HG21   | 8:Q:241:VAL:HG21   | 1.86                     | 0.58              |
| 8:Q:173:VAL:HG22   | 8:Q:258:LEU:HD13   | 1.86                     | 0.58              |
| 7:M:311:TYR:HB3    | 10:X:9:ARG:HD3     | 1.86                     | 0.58              |
| 6:G:268:TYR:CE1    | 1:S:93:PHE:CE2     | 2.91                     | 0.57              |
| 8:P:760:ASP:OD1    | 8:P:796:ASP:OD2    | 2.22                     | 0.57              |
| 1:S:346:TRP:CE2    | 1:S:387:GLN:HG2    | 2.38                     | 0.57              |
| 7:M:345:LEU:HD11   | 10:X:93:PRO:HG2    | 1.84                     | 0.57              |
| 2:B:387:ARG:NH2    | 7:L:123:TRP:CD1    | 2.72                     | 0.57              |
| 2:B:684:ILE:HG12   | 2:B:692:TYR:CE2    | 2.39                     | 0.57              |
| 3:C:364:TRP:HB2    | 3:C:410:GLN:NE2    | 2.19                     | 0.57              |
| 4:E:70:GLU:HB2     | 4:E:83:LEU:HD22    | 1.86                     | 0.57              |
| 8:Q:508:CYS:O      | 8:Q:643:SER:CB     | 2.52                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:G:416:LEU:HD22   | 1:S:22:TRP:HZ3     | 1.68                     | 0.57              |
| 1:S:52:ARG:HA      | 1:S:55:GLN:HB2     | 1.86                     | 0.57              |
| 12:V:275:LEU:HA    | 12:V:278:LEU:HG    | 1.86                     | 0.57              |
| 2:B:402:PHE:CD2    | 8:P:465:ILE:HD11   | 2.39                     | 0.57              |
| 2:B:512:GLN:NE2    | 8:P:570:ASP:OD1    | 2.36                     | 0.57              |
| 6:H:229:LEU:HD23   | 6:H:252:LEU:HD23   | 1.85                     | 0.57              |
| 8:Q:232:ASP:O      | 8:Q:236:LEU:HG     | 2.04                     | 0.57              |
| 12:V:1279:ILE:HG22 | 12:V:1337:LEU:HD23 | 1.87                     | 0.57              |
| 2:B:332:ASP:OD2    | 2:B:337:GLY:N      | 2.31                     | 0.57              |
| 8:Q:716:ARG:O      | 8:Q:720:LYS:HG3    | 2.04                     | 0.57              |
| 11:U:668:LEU:CD1   | 11:U:749:VAL:HG13  | 2.34                     | 0.57              |
| 1:A:53:SER:HA      | 1:A:168:GLN:NE2    | 2.19                     | 0.57              |
| 2:B:61:SER:OG      | 2:B:116:ASN:ND2    | 2.30                     | 0.57              |
| 10:X:53:LEU:HD23   | 10:X:68:ILE:HG22   | 1.85                     | 0.57              |
| 1:S:818:PHE:HA     | 1:S:821:LEU:HB2    | 1.86                     | 0.57              |
| 7:M:322:GLN:CD     | 7:M:335:GLN:NE2    | 2.62                     | 0.57              |
| 12:V:193:THR:O     | 12:V:196:ILE:HG22  | 2.04                     | 0.57              |
| 6:H:97:GLN:O       | 6:H:101:GLU:HG3    | 2.05                     | 0.57              |
| 2:B:298:PHE:HE2    | 2:B:362:LEU:HB2    | 1.70                     | 0.57              |
| 4:E:357:LEU:HB2    | 7:M:89:MET:HE1     | 1.87                     | 0.57              |
| 8:Q:517:LEU:O      | 8:Q:519:THR:N      | 2.38                     | 0.57              |
| 3:C:61:ILE:HG13    | 3:C:65:PRO:HD3     | 1.87                     | 0.57              |
| 3:C:114:ILE:HA     | 3:C:117:VAL:HG12   | 1.87                     | 0.57              |
| 11:U:297:GLN:OE1   | 11:U:1104:THR:O    | 2.22                     | 0.57              |
| 4:E:444:LEU:O      | 4:E:475:LYS:NZ     | 2.37                     | 0.56              |
| 6:G:252:LEU:HD13   | 6:G:268:TYR:CE1    | 2.40                     | 0.56              |
| 8:P:676:VAL:O      | 8:P:679:PHE:HB3    | 2.05                     | 0.56              |
| 7:M:98:ARG:HD2     | 7:M:101:LEU:HD11   | 1.86                     | 0.56              |
| 11:U:171:GLN:NE2   | 11:U:172:GLN:OE1   | 2.38                     | 0.56              |
| 2:B:393:PRO:HA     | 7:L:131:THR:O      | 2.06                     | 0.56              |
| 2:O:13:GLU:HB3     | 2:O:26:GLN:HG2     | 1.87                     | 0.56              |
| 8:P:29:LEU:O       | 8:P:36:PHE:N       | 2.34                     | 0.56              |
| 8:P:480:ASN:HA     | 8:P:483:LEU:HD12   | 1.87                     | 0.56              |
| 12:V:307:LEU:HA    | 12:V:310:CYS:SG    | 2.46                     | 0.56              |
| 1:A:715:GLU:O      | 1:A:719:VAL:HG12   | 2.05                     | 0.56              |
| 1:A:1331:LEU:N     | 1:A:1332:PRO:CD    | 2.68                     | 0.56              |
| 2:B:480:TYR:CE2    | 2:B:622:LEU:HD11   | 2.40                     | 0.56              |
| 2:B:522:LYS:C      | 2:B:523:CYS:SG     | 2.89                     | 0.56              |
| 3:C:192:THR:OG1    | 5:F:138:ARG:NH2    | 2.38                     | 0.56              |
| 6:G:510:GLN:OE1    | 6:G:510:GLN:HA     | 2.04                     | 0.56              |
| 6:H:138:ALA:O      | 6:H:141:ARG:HB3    | 2.05                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:L:20:ARG:O       | 8:P:494:CYS:SG    | 2.64                     | 0.56              |
| 2:O:488:VAL:HG11   | 2:O:650:ALA:HA    | 1.87                     | 0.56              |
| 7:M:58:GLN:O       | 7:M:61:THR:OG1    | 2.17                     | 0.56              |
| 7:M:197:LEU:HD12   | 7:M:201:TRP:HZ2   | 1.70                     | 0.56              |
| 12:V:443:LEU:HD22  | 12:V:491:THR:HG21 | 1.86                     | 0.56              |
| 3:C:99:ASN:ND2     | 3:C:107:GLN:OE1   | 2.39                     | 0.56              |
| 1:S:558:PHE:C      | 1:S:558:PHE:CD2   | 2.83                     | 0.56              |
| 1:A:393:VAL:HG13   | 1:A:407:LEU:HD11  | 1.87                     | 0.56              |
| 1:A:1425:ARG:CZ    | 1:A:1425:ARG:HA   | 2.35                     | 0.56              |
| 6:G:406:GLN:HG2    | 6:G:599:TRP:CE3   | 2.40                     | 0.56              |
| 2:O:256:LEU:HD23   | 2:O:268:PHE:HB2   | 1.88                     | 0.56              |
| 8:Q:27:ARG:C       | 8:Q:400:ASN:HD21  | 2.12                     | 0.56              |
| 7:M:212:TRP:CZ3    | 7:M:296:ALA:HB3   | 2.40                     | 0.56              |
| 1:A:746:ALA:O      | 1:A:750:VAL:HG23  | 2.06                     | 0.56              |
| 7:L:313:TYR:CE2    | 7:L:314:GLN:HG2   | 2.40                     | 0.56              |
| 11:U:506:LEU:HD22  | 11:U:513:MET:HE1  | 1.87                     | 0.56              |
| 11:U:1277:GLN:HE21 | 11:U:1278:HIS:CE1 | 2.23                     | 0.56              |
| 4:E:441:ILE:HD12   | 4:E:457:LEU:HD22  | 1.87                     | 0.56              |
| 4:E:476:LEU:HD11   | 4:E:493:MET:HG2   | 1.88                     | 0.56              |
| 8:Q:43:LEU:HB3     | 8:Q:45:TYR:CE1    | 2.39                     | 0.56              |
| 8:Q:563:ILE:HG22   | 8:Q:564:THR:N     | 2.20                     | 0.56              |
| 1:S:665:THR:HA     | 9:W:80:VAL:HG22   | 1.85                     | 0.56              |
| 1:A:1176:SER:HA    | 1:S:964:LEU:HD13  | 1.87                     | 0.56              |
| 2:O:522:LYS:HG3    | 2:O:523:CYS:N     | 2.19                     | 0.56              |
| 2:B:423:TYR:CZ     | 8:P:606:LEU:HB3   | 2.40                     | 0.56              |
| 3:C:458:ARG:HA     | 3:C:458:ARG:CZ    | 2.36                     | 0.56              |
| 5:F:290:GLN:O      | 6:G:485:ARG:NH2   | 2.39                     | 0.56              |
| 6:G:393:MET:HE2    | 8:P:236:LEU:HD21  | 1.88                     | 0.56              |
| 1:A:1326:GLN:OE1   | 1:A:1326:GLN:N    | 2.38                     | 0.56              |
| 2:B:398:LEU:HG     | 2:B:399:LYS:N     | 2.20                     | 0.56              |
| 2:B:593:PHE:C      | 2:B:593:PHE:CD1   | 2.84                     | 0.56              |
| 6:G:491:LYS:HD3    | 6:G:498:ASN:HD22  | 1.70                     | 0.56              |
| 8:P:711:SER:HA     | 8:P:782:ILE:HG21  | 1.88                     | 0.56              |
| 2:B:523:CYS:HA     | 2:B:581:VAL:O     | 2.05                     | 0.55              |
| 2:B:759:MET:O      | 2:B:762:THR:OG1   | 2.25                     | 0.55              |
| 3:C:169:PHE:CE2    | 4:E:17:ALA:HB2    | 2.41                     | 0.55              |
| 4:E:406:VAL:HG11   | 4:E:420:LEU:HD11  | 1.87                     | 0.55              |
| 6:G:450:LEU:HD13   | 6:G:512:LEU:HD22  | 1.88                     | 0.55              |
| 11:U:912:LEU:HA    | 11:U:915:ILE:HD12 | 1.88                     | 0.55              |
| 2:B:84:ASP:HA      | 2:B:140:PRO:HD3   | 1.88                     | 0.55              |
| 7:L:101:LEU:HB2    | 7:L:102:TYR:CE2   | 2.41                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:P:66:HIS:CD2    | 8:P:67:LEU:N       | 2.75                     | 0.55              |
| 8:P:526:THR:HG22  | 8:P:581:THR:HG22   | 1.88                     | 0.55              |
| 12:V:794:ARG:NH2  | 12:V:926:ARG:O     | 2.37                     | 0.55              |
| 12:V:1351:THR:HA  | 12:V:1354:THR:HG22 | 1.88                     | 0.55              |
| 1:A:29:ARG:O      | 1:A:29:ARG:HG3     | 2.06                     | 0.55              |
| 1:A:375:LEU:HD21  | 1:A:392:PHE:CE1    | 2.40                     | 0.55              |
| 6:G:449:PRO:O     | 6:G:450:LEU:C      | 2.45                     | 0.55              |
| 2:O:318:VAL:HG11  | 2:O:321:LYS:HE2    | 1.89                     | 0.55              |
| 11:U:430:PHE:O    | 11:U:437:ARG:NE    | 2.40                     | 0.55              |
| 3:C:247:LEU:HB3   | 3:C:248:PRO:HD3    | 1.87                     | 0.55              |
| 3:C:312:ILE:HG23  | 3:C:398:ILE:HG23   | 1.87                     | 0.55              |
| 8:P:529:LEU:N     | 8:P:578:ARG:O      | 2.36                     | 0.55              |
| 7:M:185:SER:O     | 7:M:189:GLN:HG3    | 2.06                     | 0.55              |
| 2:B:16:LEU:HD23   | 2:B:17:CYS:N       | 2.21                     | 0.55              |
| 2:B:339:GLU:O     | 2:B:340:GLN:NE2    | 2.40                     | 0.55              |
| 6:G:360:ALA:O     | 6:G:363:ALA:HB3    | 2.07                     | 0.55              |
| 2:O:505:THR:HG21  | 8:Q:546:GLN:HB2    | 1.89                     | 0.55              |
| 2:O:585:SER:N     | 2:O:586:PRO:CD     | 2.69                     | 0.55              |
| 1:S:737:ALA:HB1   | 1:S:738:PRO:HD2    | 1.89                     | 0.55              |
| 11:U:441:LEU:HD13 | 11:U:466:ILE:HG21  | 1.89                     | 0.55              |
| 11:U:832:LEU:O    | 11:U:835:SER:O     | 2.23                     | 0.55              |
| 1:A:1335:PHE:CE1  | 1:A:1339:LEU:HD12  | 2.41                     | 0.55              |
| 8:Q:511:SER:OG    | 8:Q:526:THR:OG1    | 2.24                     | 0.55              |
| 11:U:951:VAL:HG11 | 11:U:995:LEU:HD11  | 1.87                     | 0.55              |
| 1:A:351:THR:HG21  | 1:A:391:SER:HB2    | 1.89                     | 0.55              |
| 3:C:306:ASP:O     | 4:E:176:ARG:HB2    | 2.07                     | 0.55              |
| 6:G:447:TYR:CD1   | 6:G:490:GLU:HB2    | 2.42                     | 0.55              |
| 6:H:229:LEU:HD23  | 6:H:252:LEU:CD2    | 2.37                     | 0.55              |
| 7:L:356:PHE:CD1   | 7:L:367:THR:CG2    | 2.89                     | 0.55              |
| 2:O:503:ASP:OD1   | 2:O:604:ARG:NH2    | 2.37                     | 0.55              |
| 8:P:546:GLN:HB3   | 8:P:564:THR:HG22   | 1.88                     | 0.55              |
| 8:Q:28:VAL:HG23   | 8:Q:400:ASN:HD21   | 1.71                     | 0.55              |
| 8:Q:505:PRO:HB3   | 8:Q:533:SER:HB3    | 1.88                     | 0.55              |
| 7:M:265:ILE:HG23  | 7:M:269:ARG:HH12   | 1.71                     | 0.55              |
| 11:U:341:LEU:HG   | 11:U:345:GLN:HE22  | 1.72                     | 0.55              |
| 11:U:595:LEU:O    | 11:U:630:GLN:NE2   | 2.40                     | 0.55              |
| 12:V:364:TRP:CE2  | 12:V:384:MET:HG2   | 2.41                     | 0.55              |
| 2:B:299:PHE:CZ    | 2:B:313:LYS:HD2    | 2.41                     | 0.55              |
| 1:S:1046:HIS:HB2  | 1:S:1104:ARG:HD2   | 1.89                     | 0.55              |
| 12:V:193:THR:HA   | 12:V:196:ILE:HG22  | 1.88                     | 0.55              |
| 2:B:483:ILE:HG13  | 2:B:488:VAL:HG21   | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:773:LEU:HA    | 2:B:838:ILE:HG21  | 1.89                     | 0.55              |
| 3:C:254:MET:HE1   | 3:C:281:LEU:HD22  | 1.88                     | 0.55              |
| 2:O:710:ARG:HD2   | 2:O:711:THR:HG23  | 1.89                     | 0.55              |
| 8:P:65:TRP:O      | 8:P:66:HIS:CB     | 2.55                     | 0.55              |
| 1:S:1081:ILE:O    | 1:S:1085:LEU:HG   | 2.06                     | 0.55              |
| 11:U:867:PRO:HA   | 11:U:870:ILE:HD12 | 1.89                     | 0.55              |
| 2:B:834:LEU:O     | 2:B:837:GLU:HB2   | 2.07                     | 0.55              |
| 7:L:354:ILE:HG13  | 7:L:369:LYS:HG2   | 1.86                     | 0.55              |
| 12:V:221:ASP:HA   | 12:V:224:HIS:NE2  | 2.22                     | 0.55              |
| 2:B:83:SER:HB2    | 8:P:15:CYS:HB2    | 1.89                     | 0.54              |
| 2:B:851:PHE:O     | 2:B:854:GLN:HG2   | 2.07                     | 0.54              |
| 3:C:124:ALA:O     | 5:F:140:ARG:NH1   | 2.40                     | 0.54              |
| 1:S:1224:TRP:CZ3  | 1:S:1225:LEU:HD13 | 2.42                     | 0.54              |
| 6:G:497:PHE:CD2   | 8:P:254:ILE:HD11  | 2.42                     | 0.54              |
| 11:U:668:LEU:HD12 | 11:U:749:VAL:HG22 | 1.89                     | 0.54              |
| 1:A:385:HIS:ND1   | 1:A:388:ARG:CZ    | 2.71                     | 0.54              |
| 2:B:700:PHE:O     | 2:B:703:THR:OG1   | 2.20                     | 0.54              |
| 5:F:345:SER:O     | 5:F:348:THR:OG1   | 2.15                     | 0.54              |
| 8:P:11:LEU:HD11   | 8:P:431:THR:CG2   | 2.37                     | 0.54              |
| 8:P:25:LYS:HB2    | 8:P:26:PRO:HD3    | 1.90                     | 0.54              |
| 8:P:36:PHE:CE1    | 8:P:46:VAL:HG22   | 2.43                     | 0.54              |
| 1:S:715:GLU:O     | 1:S:719:VAL:HG13  | 2.06                     | 0.54              |
| 1:S:990:ASP:O     | 1:S:994:SER:HB2   | 2.07                     | 0.54              |
| 1:S:1368:PHE:CE2  | 1:S:1396:ILE:HD11 | 2.43                     | 0.54              |
| 2:B:723:ASN:HD22  | 2:O:484:ASP:CG    | 2.16                     | 0.54              |
| 3:C:330:SER:HB2   | 3:C:334:ARG:HB3   | 1.90                     | 0.54              |
| 6:H:179:LEU:O     | 6:H:183:THR:OG1   | 2.23                     | 0.54              |
| 8:P:123:CYS:SG    | 8:P:126:PRO:HD3   | 2.48                     | 0.54              |
| 1:A:942:GLU:OE1   | 1:A:1012:THR:HG23 | 2.07                     | 0.54              |
| 2:O:682:CYS:SG    | 2:O:692:TYR:HB3   | 2.47                     | 0.54              |
| 8:P:69:LEU:HD12   | 8:P:76:LEU:HD12   | 1.89                     | 0.54              |
| 1:A:32:ARG:HB3    | 6:H:311:ASN:HD21  | 1.72                     | 0.54              |
| 1:A:818:PHE:CE1   | 1:A:864:LEU:HG    | 2.41                     | 0.54              |
| 2:B:240:VAL:HG12  | 2:B:241:HIS:N     | 2.23                     | 0.54              |
| 2:B:308:ALA:HB3   | 2:B:325:LEU:CD1   | 2.38                     | 0.54              |
| 4:E:420:LEU:HA    | 4:E:423:LEU:HD12  | 1.89                     | 0.54              |
| 5:F:346:ILE:O     | 5:F:349:ASP:HB2   | 2.06                     | 0.54              |
| 8:P:465:ILE:HG22  | 8:P:466:SER:N     | 2.23                     | 0.54              |
| 8:P:875:HIS:HB3   | 8:P:876:PRO:HD3   | 1.90                     | 0.54              |
| 12:V:801:CYS:SG   | 12:V:802:GLN:NE2  | 2.80                     | 0.54              |
| 1:A:659:GLU:HG2   | 1:A:676:GLN:HE21  | 1.73                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:335:GLY:HA3   | 8:P:8:VAL:O       | 2.08                     | 0.54              |
| 2:B:763:LEU:O     | 2:B:764:GLU:C     | 2.50                     | 0.54              |
| 6:H:290:TYR:O     | 6:H:295:ASP:N     | 2.41                     | 0.54              |
| 12:V:278:LEU:N    | 12:V:279:PRO:CD   | 2.71                     | 0.54              |
| 12:V:404:ARG:HA   | 12:V:407:ILE:HG22 | 1.88                     | 0.54              |
| 1:A:684:LEU:HD11  | 1:A:722:LEU:HD21  | 1.89                     | 0.54              |
| 2:B:322:TRP:HB3   | 2:B:325:LEU:HD21  | 1.90                     | 0.54              |
| 3:C:197:ASP:N     | 3:C:198:PRO:HD2   | 2.22                     | 0.54              |
| 8:P:170:ILE:HG23  | 8:P:259:VAL:HG13  | 1.90                     | 0.54              |
| 8:P:586:PRO:HD3   | 8:P:592:LEU:HD12  | 1.88                     | 0.54              |
| 12:V:178:SER:HA   | 12:V:181:LYS:HG3  | 1.90                     | 0.54              |
| 6:G:81:ARG:HG3    | 6:G:92:GLN:HE21   | 1.71                     | 0.54              |
| 2:O:146:HIS:O     | 2:O:148:LYS:N     | 2.41                     | 0.54              |
| 2:O:487:LEU:HB2   | 2:O:584:LEU:CD2   | 2.38                     | 0.54              |
| 1:S:346:TRP:NE1   | 1:S:387:GLN:HE21  | 2.06                     | 0.54              |
| 1:S:940:GLN:HE21  | 1:S:1011:ARG:CD   | 2.19                     | 0.54              |
| 1:S:1018:ILE:HG22 | 1:S:1084:ARG:HD2  | 1.90                     | 0.54              |
| 7:M:133:PHE:O     | 7:M:154:LEU:HD12  | 2.08                     | 0.54              |
| 11:U:275:ILE:HD12 | 11:U:312:LEU:HD11 | 1.89                     | 0.54              |
| 11:U:430:PHE:CD2  | 11:U:437:ARG:HB2  | 2.43                     | 0.54              |
| 2:B:61:SER:CB     | 2:B:116:ASN:HD21  | 2.20                     | 0.53              |
| 4:E:338:ASP:HB3   | 4:E:382:LEU:HD12  | 1.89                     | 0.53              |
| 4:E:504:ILE:HG21  | 4:E:534:LEU:HD13  | 1.91                     | 0.53              |
| 6:G:266:LEU:O     | 6:G:270:VAL:HG23  | 2.08                     | 0.53              |
| 6:G:497:PHE:CE2   | 8:P:254:ILE:HD11  | 2.42                     | 0.53              |
| 2:O:277:CYS:HB2   | 2:O:316:PHE:HB3   | 1.91                     | 0.53              |
| 8:Q:482:ALA:O     | 8:Q:486:LEU:HB2   | 2.08                     | 0.53              |
| 7:M:31:ALA:O      | 7:M:34:ARG:HB2    | 2.08                     | 0.53              |
| 7:M:354:ILE:HG12  | 7:M:369:LYS:HG2   | 1.89                     | 0.53              |
| 1:A:928:THR:HG23  | 1:A:971:GLY:HA3   | 1.89                     | 0.53              |
| 2:B:100:LYS:HB3   | 2:B:102:ASN:HB2   | 1.90                     | 0.53              |
| 2:B:256:LEU:HG    | 2:B:257:ILE:N     | 2.23                     | 0.53              |
| 2:B:631:LYS:O     | 2:B:631:LYS:HD2   | 2.07                     | 0.53              |
| 6:G:483:LEU:HD12  | 6:G:513:ARG:HA    | 1.90                     | 0.53              |
| 7:L:356:PHE:CE1   | 7:L:367:THR:HG21  | 2.42                     | 0.53              |
| 8:P:730:CYS:SG    | 8:P:752:SER:N     | 2.82                     | 0.53              |
| 11:U:221:SER:OG   | 11:U:226:ARG:HA   | 2.08                     | 0.53              |
| 2:B:276:VAL:HG12  | 2:B:277:CYS:O     | 2.08                     | 0.53              |
| 2:B:731:LEU:HD13  | 8:P:680:LEU:HD21  | 1.89                     | 0.53              |
| 3:C:71:LEU:O      | 3:C:75:CYS:SG     | 2.63                     | 0.53              |
| 4:E:27:ARG:O      | 4:E:31:GLN:HB2    | 2.08                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:E:434:GLN:NE2  | 4:E:460:ARG:CZ    | 2.72                     | 0.53              |
| 6:H:246:VAL:HG21 | 6:H:276:GLY:HA2   | 1.91                     | 0.53              |
| 8:P:66:HIS:CD2   | 8:P:66:HIS:C      | 2.87                     | 0.53              |
| 8:P:471:PHE:CD1  | 8:P:471:PHE:C     | 2.86                     | 0.53              |
| 8:Q:491:ASN:HB3  | 8:Q:535:PHE:CE1   | 2.43                     | 0.53              |
| 8:Q:542:THR:HG22 | 8:Q:603:PHE:O     | 2.09                     | 0.53              |
| 8:Q:580:VAL:HG12 | 8:Q:582:LEU:CD2   | 2.38                     | 0.53              |
| 1:S:815:PRO:HA   | 1:S:818:PHE:CE2   | 2.43                     | 0.53              |
| 11:U:66:ARG:NH1  | 11:U:70:THR:OG1   | 2.41                     | 0.53              |
| 1:A:481:VAL:O    | 1:A:485:SER:OG    | 2.14                     | 0.53              |
| 6:G:399:GLU:CD   | 6:G:591:LEU:HB2   | 2.33                     | 0.53              |
| 6:H:62:ALA:HA    | 6:H:102:ARG:HD2   | 1.89                     | 0.53              |
| 8:P:249:GLN:HG2  | 8:P:277:HIS:CD2   | 2.44                     | 0.53              |
| 1:S:415:MET:HE2  | 1:S:419:PHE:CZ    | 2.43                     | 0.53              |
| 11:U:221:SER:CB  | 11:U:229:VAL:HG21 | 2.37                     | 0.53              |
| 3:C:247:LEU:N    | 3:C:248:PRO:CD    | 2.71                     | 0.53              |
| 2:O:580:ALA:C    | 2:O:581:VAL:HG23  | 2.33                     | 0.53              |
| 8:P:517:LEU:O    | 8:P:519:THR:N     | 2.42                     | 0.53              |
| 8:P:518:GLN:N    | 8:Q:581:THR:O     | 2.42                     | 0.53              |
| 1:A:992:HIS:O    | 1:A:1073:ARG:NH2  | 2.41                     | 0.53              |
| 4:E:434:GLN:OE1  | 4:E:462:VAL:HG12  | 2.08                     | 0.53              |
| 7:L:16:LEU:HD11  | 8:P:483:LEU:CD2   | 2.38                     | 0.53              |
| 7:L:315:LEU:HB3  | 7:L:334:HIS:ND1   | 2.24                     | 0.53              |
| 7:L:354:ILE:HA   | 7:L:368:LEU:O     | 2.08                     | 0.53              |
| 8:P:508:CYS:HA   | 8:P:528:VAL:O     | 2.08                     | 0.53              |
| 1:S:197:LEU:HD22 | 1:S:206:VAL:CG1   | 2.39                     | 0.53              |
| 7:M:197:LEU:HD12 | 7:M:201:TRP:CZ2   | 2.43                     | 0.53              |
| 1:A:35:TYR:HE2   | 6:H:311:ASN:CG    | 2.16                     | 0.53              |
| 1:A:1020:ARG:O   | 1:A:1023:GLU:HB3  | 2.09                     | 0.53              |
| 6:H:40:GLN:HB3   | 6:H:44:GLN:HE22   | 1.73                     | 0.53              |
| 1:S:415:MET:HE3  | 1:S:451:TRP:CZ2   | 2.44                     | 0.53              |
| 7:M:311:TYR:OH   | 10:X:100:PRO:O    | 2.24                     | 0.53              |
| 7:M:341:TRP:CH2  | 10:X:100:PRO:HD3  | 2.43                     | 0.53              |
| 11:U:364:ILE:O   | 11:U:367:VAL:HB   | 2.09                     | 0.53              |
| 1:A:182:VAL:O    | 1:A:185:LEU:HB2   | 2.09                     | 0.53              |
| 4:E:391:CYS:SG   | 4:E:423:LEU:CD2   | 2.92                     | 0.53              |
| 6:H:58:GLN:HE22  | 6:H:98:ARG:HG2    | 1.72                     | 0.53              |
| 8:P:27:ARG:O     | 8:P:38:SER:N      | 2.35                     | 0.53              |
| 1:S:844:SER:OG   | 1:S:856:LEU:HD21  | 2.09                     | 0.53              |
| 1:A:348:PHE:CZ   | 1:A:356:THR:HG23  | 2.43                     | 0.53              |
| 3:C:28:LEU:HD23  | 3:C:28:LEU:C      | 2.34                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:F:285:LEU:HD13  | 5:F:346:ILE:CD1    | 2.39                     | 0.53              |
| 8:P:247:ASP:OD1   | 8:P:247:ASP:N      | 2.35                     | 0.53              |
| 8:Q:604:TYR:O     | 8:Q:638:VAL:HG23   | 2.08                     | 0.53              |
| 6:G:262:PRO:O     | 6:G:265:ALA:HB3    | 2.09                     | 0.53              |
| 6:H:239:LEU:CD1   | 6:H:241:PRO:HD3    | 2.39                     | 0.53              |
| 8:P:599:SER:HB2   | 8:P:644:ARG:HG2    | 1.90                     | 0.53              |
| 11:U:592:ARG:NH2  | 11:U:626:THR:OG1   | 2.42                     | 0.53              |
| 11:U:751:GLU:OE2  | 11:U:841:TYR:OH    | 2.26                     | 0.53              |
| 1:A:27:ALA:HB3    | 6:H:372:ALA:HB2    | 1.90                     | 0.52              |
| 2:O:164:SER:OG    | 2:O:215:TYR:OH     | 2.27                     | 0.52              |
| 2:O:503:ASP:CG    | 2:O:604:ARG:HE     | 2.17                     | 0.52              |
| 8:Q:484:THR:OG1   | 8:Q:485:SER:N      | 2.39                     | 0.52              |
| 12:V:1186:LEU:HB3 | 12:V:1237:VAL:HG11 | 1.91                     | 0.52              |
| 2:B:254:ILE:HG13  | 2:B:254:ILE:O      | 2.09                     | 0.52              |
| 3:C:60:VAL:HG23   | 3:C:64:PHE:CZ      | 2.45                     | 0.52              |
| 3:C:350:MET:SD    | 7:L:250:GLU:HA     | 2.49                     | 0.52              |
| 7:L:62:ILE:HA     | 7:L:98:ARG:NH2     | 2.24                     | 0.52              |
| 7:M:16:LEU:O      | 7:M:18:GLN:OE1     | 2.28                     | 0.52              |
| 7:M:155:LYS:NZ    | 7:M:164:ASP:OD1    | 2.40                     | 0.52              |
| 1:A:286:GLN:C     | 1:A:288:GLU:N      | 2.63                     | 0.52              |
| 7:L:230:LEU:HA    | 7:L:293:PRO:CD     | 2.40                     | 0.52              |
| 12:V:979:MET:HG3  | 12:V:980:LEU:HD23  | 1.89                     | 0.52              |
| 1:A:845:LEU:HD23  | 1:A:856:LEU:CD1    | 2.39                     | 0.52              |
| 4:E:384:THR:O     | 4:E:388:THR:HG23   | 2.10                     | 0.52              |
| 5:F:192:LEU:HB3   | 5:F:201:PHE:CZ     | 2.44                     | 0.52              |
| 6:H:270:VAL:O     | 6:H:273:LEU:HB2    | 2.09                     | 0.52              |
| 6:H:531:THR:OG1   | 6:H:532:LYS:N      | 2.42                     | 0.52              |
| 8:P:37:LEU:CD2    | 8:P:39:THR:HG23    | 2.39                     | 0.52              |
| 1:S:765:LEU:HD11  | 1:S:787:LEU:HD21   | 1.91                     | 0.52              |
| 12:V:273:ILE:HG21 | 12:V:281:ILE:CD1   | 2.39                     | 0.52              |
| 2:B:91:LEU:HD13   | 2:B:111:ILE:CG2    | 2.39                     | 0.52              |
| 3:C:288:PRO:HA    | 3:C:340:TYR:CE1    | 2.44                     | 0.52              |
| 10:X:44:THR:HG21  | 10:X:116:SER:CA    | 2.33                     | 0.52              |
| 11:U:218:LEU:CD2  | 11:U:229:VAL:HG11  | 2.39                     | 0.52              |
| 11:U:485:PHE:HD1  | 11:U:488:LEU:HD13  | 1.73                     | 0.52              |
| 11:U:503:VAL:HG13 | 11:U:506:LEU:HD12  | 1.92                     | 0.52              |
| 1:A:482:PRO:HD3   | 1:A:517:ARG:HD3    | 1.91                     | 0.52              |
| 1:A:1161:THR:O    | 1:A:1321:ARG:NH2   | 2.41                     | 0.52              |
| 2:B:191:LEU:HD23  | 2:B:197:THR:HG23   | 1.92                     | 0.52              |
| 2:B:584:LEU:C     | 2:B:586:PRO:HD2    | 2.35                     | 0.52              |
| 6:G:54:LEU:HD23   | 6:G:58:GLN:HG3     | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:766:GLU:OE1   | 8:Q:874:ARG:NH2   | 2.41                     | 0.52              |
| 1:S:1118:ASN:HB2  | 1:S:1119:PHE:CD1  | 2.44                     | 0.52              |
| 12:V:458:TYR:CD2  | 12:V:477:LEU:HD21 | 2.45                     | 0.52              |
| 1:A:288:GLU:HA    | 1:A:292:HIS:HB3   | 1.91                     | 0.52              |
| 1:A:1249:LEU:HD12 | 1:A:1252:GLU:HB2  | 1.92                     | 0.52              |
| 6:H:241:PRO:O     | 6:H:242:ARG:HB3   | 2.08                     | 0.52              |
| 8:P:763:ASN:O     | 8:P:791:SER:OG    | 2.18                     | 0.52              |
| 7:M:295:ARG:O     | 7:M:297:ILE:N     | 2.43                     | 0.52              |
| 12:V:432:CYS:SG   | 12:V:469:CYS:SG   | 3.06                     | 0.52              |
| 14:Z:42:DT:H2"    | 14:Z:43:DG:C8     | 2.45                     | 0.52              |
| 6:G:20:ASN:HD21   | 6:G:72:THR:HG22   | 1.73                     | 0.52              |
| 6:G:21:ASP:OD1    | 6:G:195:LEU:HD12  | 2.09                     | 0.52              |
| 2:O:840:LEU:HD21  | 8:Q:812:VAL:CG1   | 2.39                     | 0.52              |
| 8:Q:173:VAL:CG2   | 8:Q:258:LEU:HD13  | 2.40                     | 0.52              |
| 7:M:354:ILE:CG1   | 7:M:369:LYS:HG2   | 2.39                     | 0.52              |
| 12:V:518:LEU:HD23 | 12:V:521:LEU:HD21 | 1.92                     | 0.52              |
| 1:A:240:GLN:OE1   | 1:A:310:VAL:HG11  | 2.09                     | 0.52              |
| 1:A:874:ARG:NH1   | 1:A:939:ILE:HD13  | 2.24                     | 0.52              |
| 5:F:187:ARG:O     | 5:F:190:SER:OG    | 2.23                     | 0.52              |
| 6:G:513:ARG:HD3   | 6:G:543:MET:SD    | 2.50                     | 0.52              |
| 6:H:225:PRO:O     | 6:H:259:MET:SD    | 2.67                     | 0.52              |
| 1:S:448:TYR:CD2   | 1:S:489:LEU:HD22  | 2.44                     | 0.52              |
| 12:V:586:ALA:O    | 12:V:644:LEU:HB2  | 2.09                     | 0.52              |
| 2:O:170:ILE:O     | 2:O:170:ILE:HG22  | 2.10                     | 0.52              |
| 8:P:399:LEU:HD23  | 8:P:399:LEU:H     | 1.74                     | 0.52              |
| 1:S:1183:CYS:SG   | 1:S:1184:ARG:N    | 2.82                     | 0.52              |
| 11:U:962:PHE:CE2  | 11:U:992:LEU:HD11 | 2.45                     | 0.52              |
| 12:V:415:GLN:N    | 12:V:415:GLN:OE1  | 2.41                     | 0.52              |
| 2:B:242:ILE:C     | 2:B:243:CYS:SG    | 2.92                     | 0.51              |
| 2:B:510:MET:HE2   | 2:B:515:ASP:HB2   | 1.93                     | 0.51              |
| 3:C:183:LEU:O     | 3:C:186:VAL:N     | 2.42                     | 0.51              |
| 6:G:483:LEU:HD13  | 6:G:513:ARG:HG3   | 1.91                     | 0.51              |
| 1:A:273:MET:HB3   | 1:A:298:TRP:CE2   | 2.45                     | 0.51              |
| 1:A:313:THR:HG22  | 1:A:317:LYS:HG3   | 1.93                     | 0.51              |
| 1:A:874:ARG:O     | 1:A:946:LEU:HD11  | 2.10                     | 0.51              |
| 1:A:1305:LEU:C    | 1:A:1308:LEU:HD21 | 2.35                     | 0.51              |
| 2:B:290:MET:HA    | 2:B:339:GLU:OE1   | 2.11                     | 0.51              |
| 4:E:391:CYS:O     | 4:E:395:THR:OG1   | 2.13                     | 0.51              |
| 6:G:379:GLU:HB2   | 6:G:380:PRO:HD3   | 1.92                     | 0.51              |
| 2:O:228:ILE:HG22  | 2:O:229:ILE:H     | 1.76                     | 0.51              |
| 2:O:609:CYS:SG    | 8:Q:644:ARG:NH1   | 2.84                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:P:875:HIS:HB3    | 8:P:876:PRO:CD    | 2.40                     | 0.51              |
| 8:Q:143:LEU:HD12   | 8:Q:197:LEU:HD21  | 1.92                     | 0.51              |
| 1:S:736:VAL:HG12   | 1:S:737:ALA:HB2   | 1.92                     | 0.51              |
| 11:U:1142:LEU:HD11 | 11:U:1205:LEU:HB2 | 1.92                     | 0.51              |
| 1:A:407:LEU:HD21   | 1:A:433:VAL:CG1   | 2.41                     | 0.51              |
| 2:B:711:THR:O      | 2:B:713:PHE:N     | 2.43                     | 0.51              |
| 2:O:16:LEU:HD12    | 2:O:79:CYS:SG     | 2.49                     | 0.51              |
| 8:Q:23:ALA:HB2     | 8:Q:348:LEU:HD23  | 1.91                     | 0.51              |
| 1:S:1143:LEU:HD11  | 1:S:1185:TRP:HA   | 1.91                     | 0.51              |
| 11:U:628:LEU:HD22  | 11:U:702:LEU:HD11 | 1.93                     | 0.51              |
| 11:U:806:SER:O     | 11:U:810:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:296:ARG:HG2    | 1:A:354:LEU:HD11  | 1.91                     | 0.51              |
| 1:A:474:PHE:CE2    | 1:A:510:TYR:CD2   | 2.97                     | 0.51              |
| 7:L:66:TYR:O       | 7:L:69:ILE:HB     | 2.09                     | 0.51              |
| 8:P:599:SER:CB     | 8:P:644:ARG:HG2   | 2.40                     | 0.51              |
| 12:V:230:GLU:HA    | 12:V:233:ASP:HB3  | 1.93                     | 0.51              |
| 12:V:1125:ILE:HG23 | 12:V:1130:CYS:HB2 | 1.93                     | 0.51              |
| 1:A:465:CYS:SG     | 1:A:466:SER:N     | 2.84                     | 0.51              |
| 1:A:1227:ALA:HB2   | 1:A:1256:LEU:HD12 | 1.93                     | 0.51              |
| 3:C:87:GLN:CD      | 3:C:87:GLN:N      | 2.69                     | 0.51              |
| 3:C:247:LEU:HD12   | 3:C:247:LEU:O     | 2.10                     | 0.51              |
| 6:G:282:PRO:O      | 6:G:285:GLU:N     | 2.43                     | 0.51              |
| 7:L:11:GLN:O       | 7:L:88:LYS:NZ     | 2.44                     | 0.51              |
| 1:S:1249:LEU:HD12  | 1:S:1252:GLU:HB2  | 1.92                     | 0.51              |
| 7:M:356:PHE:HZ     | 11:U:435:MET:HE2  | 1.76                     | 0.51              |
| 11:U:1076:ASN:H    | 11:U:1079:THR:HB  | 1.75                     | 0.51              |
| 1:A:34:LYS:H       | 1:A:34:LYS:CE     | 2.24                     | 0.51              |
| 1:A:768:LEU:O      | 1:A:772:GLN:C     | 2.54                     | 0.51              |
| 3:C:207:HIS:CG     | 4:E:93:ILE:HG13   | 2.46                     | 0.51              |
| 4:E:117:VAL:HA     | 4:E:120:ILE:HD12  | 1.93                     | 0.51              |
| 5:F:317:ALA:HB1    | 5:F:318:PRO:CD    | 2.40                     | 0.51              |
| 8:P:25:LYS:O       | 8:P:27:ARG:NH1    | 2.44                     | 0.51              |
| 8:P:361:SER:OG     | 8:P:398:SER:O     | 2.19                     | 0.51              |
| 1:S:1076:LEU:N     | 1:S:1076:LEU:HD23 | 2.26                     | 0.51              |
| 7:M:275:ASP:O      | 7:M:283:ASN:ND2   | 2.43                     | 0.51              |
| 11:U:450:THR:HG21  | 12:V:356:TYR:CG   | 2.45                     | 0.51              |
| 11:U:466:ILE:HG22  | 11:U:467:VAL:N    | 2.25                     | 0.51              |
| 1:A:463:HIS:NE2    | 1:A:473:LEU:HD22  | 2.26                     | 0.51              |
| 1:A:653:LEU:O      | 1:A:657:LEU:HD13  | 2.11                     | 0.51              |
| 1:A:1252:GLU:O     | 1:A:1298:ARG:NH2  | 2.43                     | 0.51              |
| 6:G:476:PHE:CZ     | 6:G:519:SER:HB2   | 2.45                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:L:155:LYS:NZ     | 7:L:164:ASP:OD1   | 2.32                     | 0.51              |
| 2:O:406:ARG:NH1    | 8:Q:318:HIS:O     | 2.44                     | 0.51              |
| 8:P:341:TYR:O      | 8:P:342:CYS:SG    | 2.65                     | 0.51              |
| 8:P:515:SER:OG     | 8:P:516:ARG:N     | 2.43                     | 0.51              |
| 10:X:69:ARG:NH2    | 10:X:82:ALA:O     | 2.44                     | 0.51              |
| 12:V:364:TRP:CZ2   | 12:V:384:MET:HG2  | 2.46                     | 0.51              |
| 12:V:1246:VAL:HG11 | 12:V:1301:PHE:CD1 | 2.45                     | 0.51              |
| 6:G:146:GLN:NE2    | 6:G:150:TRP:CZ2   | 2.79                     | 0.51              |
| 6:G:592:TYR:CD1    | 6:G:592:TYR:C     | 2.88                     | 0.51              |
| 2:O:672:MET:HG3    | 2:O:707:TRP:CZ2   | 2.46                     | 0.51              |
| 8:Q:284:PHE:HB3    | 8:Q:315:PHE:HD2   | 1.75                     | 0.51              |
| 7:M:38:LEU:HD21    | 7:M:84:MET:HE1    | 1.92                     | 0.51              |
| 1:A:929:TYR:CE1    | 1:A:933:LEU:HD11  | 2.46                     | 0.51              |
| 2:B:308:ALA:HB3    | 2:B:325:LEU:HD13  | 1.92                     | 0.51              |
| 3:C:60:VAL:CG2     | 3:C:64:PHE:CZ     | 2.94                     | 0.51              |
| 3:C:304:GLU:CD     | 4:E:165:GLN:HG2   | 2.36                     | 0.51              |
| 2:O:281:PHE:CZ     | 2:O:321:LYS:HB3   | 2.46                     | 0.51              |
| 8:Q:537:LEU:HD22   | 8:Q:541:TRP:CE2   | 2.46                     | 0.51              |
| 12:V:374:VAL:HG22  | 12:V:376:GLU:H    | 1.76                     | 0.51              |
| 2:B:401:CYS:HB2    | 8:P:465:ILE:HG21  | 1.92                     | 0.51              |
| 3:C:57:SER:C       | 3:C:59:THR:H      | 2.17                     | 0.51              |
| 3:C:82:ALA:O       | 5:F:138:ARG:NH1   | 2.44                     | 0.51              |
| 3:C:162:ARG:HB3    | 3:C:162:ARG:NH1   | 2.25                     | 0.51              |
| 7:L:146:ARG:NH1    | 7:L:205:ASP:OD2   | 2.41                     | 0.51              |
| 2:O:85:PHE:CZ      | 2:O:156:GLN:HB2   | 2.46                     | 0.51              |
| 8:Q:563:ILE:HG21   | 8:Q:565:TYR:CE1   | 2.46                     | 0.51              |
| 9:W:81:GLY:O       | 9:W:83:LYS:N      | 2.44                     | 0.51              |
| 12:V:211:ILE:O     | 12:V:215:LEU:HG   | 2.11                     | 0.51              |
| 1:A:137:LEU:HB2    | 1:A:141:GLN:HG3   | 1.92                     | 0.50              |
| 7:L:155:LYS:NZ     | 7:L:162:SER:O     | 2.40                     | 0.50              |
| 2:O:257:ILE:CD1    | 2:O:299:PHE:CE2   | 2.93                     | 0.50              |
| 1:S:556:MET:HE3    | 1:S:1010:GLY:HA3  | 1.93                     | 0.50              |
| 4:E:405:PRO:O      | 4:E:409:ALA:N     | 2.44                     | 0.50              |
| 6:G:147:ALA:CB     | 6:G:159:LEU:HD11  | 2.42                     | 0.50              |
| 2:O:430:VAL:HA     | 8:Q:497:LEU:HD11  | 1.93                     | 0.50              |
| 2:O:777:ILE:HG21   | 8:Q:830:LEU:HD13  | 1.93                     | 0.50              |
| 8:Q:367:CYS:HA     | 8:Q:392:PRO:HA    | 1.94                     | 0.50              |
| 1:S:327:ILE:O      | 1:S:388:ARG:NH1   | 2.44                     | 0.50              |
| 1:A:737:ALA:HB3    | 1:A:738:PRO:HD3   | 1.92                     | 0.50              |
| 2:B:365:ILE:HG23   | 2:B:367:TYR:CE2   | 2.46                     | 0.50              |
| 3:C:41:PHE:CE2     | 3:C:45:LEU:HD11   | 2.45                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S:346:TRP:HE1   | 1:S:387:GLN:HE21   | 1.59                     | 0.50              |
| 1:A:78:ILE:CG2    | 1:A:123:GLN:HE22   | 2.19                     | 0.50              |
| 1:A:1368:PHE:HE1  | 1:A:1392:PRO:CG    | 2.24                     | 0.50              |
| 2:B:242:ILE:CG1   | 2:B:243:CYS:N      | 2.74                     | 0.50              |
| 2:B:520:LEU:HD12  | 8:P:567:ILE:HB     | 1.92                     | 0.50              |
| 3:C:539:GLU:OE1   | 3:C:539:GLU:N      | 2.44                     | 0.50              |
| 4:E:439:GLY:O     | 4:E:443:GLU:OE1    | 2.28                     | 0.50              |
| 6:G:453:SER:OG    | 6:G:512:LEU:HD21   | 2.10                     | 0.50              |
| 6:G:457:LEU:HD23  | 6:G:458:LEU:CD2    | 2.41                     | 0.50              |
| 6:H:522:LEU:O     | 6:H:525:VAL:HB     | 2.12                     | 0.50              |
| 8:Q:16:CYS:SG     | 8:Q:426:LYS:O      | 2.68                     | 0.50              |
| 9:W:85:PHE:O      | 9:W:87:TRP:N       | 2.44                     | 0.50              |
| 7:M:311:TYR:HB3   | 10:X:9:ARG:CD      | 2.41                     | 0.50              |
| 1:A:78:ILE:HG23   | 1:A:123:GLN:NE2    | 2.17                     | 0.50              |
| 1:A:163:ARG:O     | 1:A:166:PHE:HB3    | 2.12                     | 0.50              |
| 1:A:1261:PHE:HB2  | 1:A:1291:ILE:HG21  | 1.94                     | 0.50              |
| 1:A:1333:PHE:CD1  | 1:A:1333:PHE:C     | 2.90                     | 0.50              |
| 2:B:277:CYS:HB2   | 2:B:316:PHE:HB3    | 1.93                     | 0.50              |
| 2:B:299:PHE:CE2   | 2:B:313:LYS:HB2    | 2.46                     | 0.50              |
| 3:C:168:GLY:O     | 7:L:344:GLY:O      | 2.30                     | 0.50              |
| 4:E:284:ILE:O     | 4:E:288:LEU:HB2    | 2.11                     | 0.50              |
| 8:P:139:VAL:CG1   | 8:P:154:LEU:HD11   | 2.41                     | 0.50              |
| 1:A:415:MET:HE2   | 1:A:451:TRP:CH2    | 2.47                     | 0.50              |
| 2:B:636:PHE:HZ    | 2:B:651:LEU:HD11   | 1.76                     | 0.50              |
| 3:C:92:TRP:NE1    | 5:F:118:GLY:HA2    | 2.26                     | 0.50              |
| 4:E:333:LEU:N     | 4:E:334:PRO:CD     | 2.74                     | 0.50              |
| 5:F:285:LEU:HD13  | 5:F:346:ILE:HD13   | 1.92                     | 0.50              |
| 6:H:203:LEU:O     | 6:H:206:VAL:N      | 2.44                     | 0.50              |
| 7:L:169:PHE:CZ    | 7:L:193:ALA:HB1    | 2.46                     | 0.50              |
| 8:P:200:VAL:HA    | 8:P:218:PHE:O      | 2.11                     | 0.50              |
| 1:S:959:ILE:HG22  | 1:S:960:HIS:ND1    | 2.27                     | 0.50              |
| 12:V:243:VAL:HG22 | 12:V:244:PRO:HD3   | 1.93                     | 0.50              |
| 1:A:1210:PHE:CZ   | 1:A:1249:LEU:HD13  | 2.46                     | 0.50              |
| 2:B:423:TYR:CG    | 8:P:606:LEU:HD13   | 2.45                     | 0.50              |
| 6:G:146:GLN:NE2   | 6:G:150:TRP:CE2    | 2.80                     | 0.50              |
| 6:G:596:TYR:CD1   | 6:G:596:TYR:C      | 2.89                     | 0.50              |
| 2:O:711:THR:O     | 2:O:713:PHE:N      | 2.45                     | 0.50              |
| 7:M:195:GLU:HA    | 7:M:198:LYS:HB2    | 1.94                     | 0.50              |
| 11:U:1138:LEU:HA  | 11:U:1141:LEU:HD23 | 1.92                     | 0.50              |
| 12:V:223:GLN:O    | 12:V:227:VAL:HG23  | 2.12                     | 0.50              |
| 12:V:282:ILE:HA   | 12:V:285:ILE:HD12  | 1.94                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:A:1075:LEU:CD1   | 1:A:1119:PHE:CD2  | 2.95                     | 0.50              |
| 2:B:239:TYR:CD2    | 2:B:286:ALA:HA    | 2.47                     | 0.50              |
| 5:F:253:ARG:NH2    | 5:F:300:GLN:O     | 2.45                     | 0.50              |
| 6:G:159:LEU:HD23   | 6:G:177:LEU:CD1   | 2.42                     | 0.50              |
| 6:G:364:ALA:O      | 6:G:367:TYR:N     | 2.45                     | 0.50              |
| 6:G:592:TYR:CD1    | 6:G:593:LEU:N     | 2.80                     | 0.50              |
| 8:P:197:LEU:HA     | 8:P:242:LEU:O     | 2.12                     | 0.50              |
| 8:Q:570:ASP:OD1    | 8:Q:570:ASP:N     | 2.39                     | 0.50              |
| 11:U:1003:PHE:C    | 11:U:1003:PHE:CD2 | 2.89                     | 0.50              |
| 6:H:250:THR:HG22   | 6:H:282:PRO:HA    | 1.93                     | 0.50              |
| 6:H:541:VAL:HG21   | 6:H:554:LEU:HD22  | 1.93                     | 0.50              |
| 12:V:413:GLN:OE1   | 12:V:413:GLN:N    | 2.45                     | 0.50              |
| 1:A:874:ARG:NH2    | 1:A:944:ASP:O     | 2.45                     | 0.49              |
| 3:C:533:TRP:O      | 3:C:537:GLY:N     | 2.45                     | 0.49              |
| 4:E:156:LEU:HD13   | 4:E:160:CYS:SG    | 2.52                     | 0.49              |
| 6:G:521:GLY:HA3    | 6:G:537:PHE:CE1   | 2.47                     | 0.49              |
| 8:Q:143:LEU:CD2    | 8:Q:150:TRP:HE3   | 2.25                     | 0.49              |
| 7:M:216:PRO:HG2    | 7:M:226:ARG:HD3   | 1.94                     | 0.49              |
| 11:U:218:LEU:HD21  | 11:U:229:VAL:HG11 | 1.94                     | 0.49              |
| 11:U:647:LEU:HD12  | 11:U:647:LEU:N    | 2.26                     | 0.49              |
| 11:U:909:LEU:HA    | 11:U:912:LEU:HD12 | 1.94                     | 0.49              |
| 1:A:424:LEU:HD23   | 1:A:476:PHE:HB2   | 1.94                     | 0.49              |
| 1:A:663:SER:HB3    | 1:A:676:GLN:HE22  | 1.77                     | 0.49              |
| 2:B:176:ILE:HG22   | 2:B:177:GLU:N     | 2.28                     | 0.49              |
| 4:E:432:ASP:O      | 4:E:436:LEU:HG    | 2.12                     | 0.49              |
| 4:E:497:MET:HG2    | 4:E:512:LEU:HD13  | 1.94                     | 0.49              |
| 5:F:103:LEU:HD23   | 5:F:108:ARG:HD3   | 1.94                     | 0.49              |
| 5:F:275:LEU:CD2    | 5:F:325:VAL:HG23  | 2.42                     | 0.49              |
| 6:G:136:LEU:HD23   | 6:G:136:LEU:H     | 1.76                     | 0.49              |
| 6:G:376:ASP:N      | 6:G:376:ASP:OD1   | 2.46                     | 0.49              |
| 1:S:184:HIS:HA     | 1:S:187:VAL:HG12  | 1.94                     | 0.49              |
| 1:S:548:LEU:O      | 1:S:552:GLU:HG3   | 2.11                     | 0.49              |
| 1:S:1358:VAL:O     | 1:S:1362:LEU:HG   | 2.12                     | 0.49              |
| 11:U:543:LEU:O     | 11:U:547:PHE:HB3  | 2.11                     | 0.49              |
| 12:V:386:PHE:HB2   | 12:V:431:MET:HE1  | 1.94                     | 0.49              |
| 12:V:1013:VAL:HG21 | 12:V:1075:TRP:CE2 | 2.48                     | 0.49              |
| 1:A:264:GLN:O      | 1:A:268:ASP:HB2   | 2.11                     | 0.49              |
| 2:B:401:CYS:O      | 2:B:404:SER:OG    | 2.19                     | 0.49              |
| 3:C:188:VAL:HG22   | 3:C:219:PHE:HA    | 1.94                     | 0.49              |
| 3:C:283:GLN:O      | 3:C:286:CYS:SG    | 2.69                     | 0.49              |
| 4:E:372:ILE:HA     | 4:E:375:LEU:HD12  | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:G:252:LEU:HA    | 6:G:255:CYS:SG    | 2.53                     | 0.49              |
| 7:L:117:GLU:HB3   | 7:L:183:LEU:HD12  | 1.93                     | 0.49              |
| 8:P:242:LEU:HD23  | 8:P:252:CYS:HB3   | 1.93                     | 0.49              |
| 12:V:174:ARG:HA   | 12:V:177:VAL:HG12 | 1.94                     | 0.49              |
| 1:A:750:VAL:HG21  | 1:A:790:HIS:HB3   | 1.94                     | 0.49              |
| 1:A:818:PHE:CD1   | 1:A:864:LEU:HG    | 2.47                     | 0.49              |
| 1:A:1206:PHE:CD1  | 1:A:1206:PHE:C    | 2.89                     | 0.49              |
| 2:B:418:ILE:O     | 2:B:422:SER:OG    | 2.29                     | 0.49              |
| 4:E:509:ARG:HD2   | 4:E:534:LEU:HB2   | 1.92                     | 0.49              |
| 6:G:371:LEU:O     | 6:G:375:LEU:HD12  | 2.11                     | 0.49              |
| 8:Q:505:PRO:CB    | 8:Q:533:SER:HB3   | 2.42                     | 0.49              |
| 1:S:474:PHE:CE1   | 1:S:510:TYR:CE2   | 3.00                     | 0.49              |
| 1:S:1115:GLU:O    | 1:S:1118:ASN:HB2  | 2.12                     | 0.49              |
| 11:U:386:GLY:HA2  | 11:U:425:ILE:HD12 | 1.93                     | 0.49              |
| 12:V:424:HIS:O    | 12:V:428:LEU:HG   | 2.12                     | 0.49              |
| 1:A:818:PHE:HZ    | 1:A:861:SER:CB    | 2.23                     | 0.49              |
| 1:A:1263:PHE:CZ   | 1:A:1322:VAL:HG11 | 2.47                     | 0.49              |
| 2:B:636:PHE:HB3   | 2:B:637:PRO:HD3   | 1.94                     | 0.49              |
| 3:C:145:TYR:C     | 3:C:147:PRO:HD2   | 2.37                     | 0.49              |
| 6:G:280:GLY:N     | 6:G:281:PRO:CD    | 2.76                     | 0.49              |
| 2:O:519:ARG:HG3   | 2:O:520:LEU:O     | 2.13                     | 0.49              |
| 8:P:11:LEU:HD22   | 8:P:429:LEU:CD2   | 2.40                     | 0.49              |
| 8:P:473:LYS:O     | 8:P:476:VAL:HB    | 2.12                     | 0.49              |
| 11:U:770:ASP:O    | 11:U:774:LEU:HD13 | 2.12                     | 0.49              |
| 1:A:379:LEU:HD23  | 1:A:384:VAL:HG21  | 1.94                     | 0.49              |
| 2:B:487:LEU:O     | 2:B:581:VAL:HA    | 2.12                     | 0.49              |
| 2:O:139:GLY:O     | 2:O:141:LEU:N     | 2.45                     | 0.49              |
| 8:P:7:ARG:HG3     | 8:P:8:VAL:HG23    | 1.93                     | 0.49              |
| 8:Q:492:VAL:HG22  | 8:Q:535:PHE:CD2   | 2.48                     | 0.49              |
| 12:V:979:MET:CE   | 12:V:1009:ALA:HB2 | 2.42                     | 0.49              |
| 12:V:1392:ARG:HD3 | 12:V:1396:GLY:HA2 | 1.95                     | 0.49              |
| 1:A:822:LEU:HD23  | 1:A:823:THR:N     | 2.27                     | 0.49              |
| 2:B:254:ILE:O     | 2:B:254:ILE:CG1   | 2.60                     | 0.49              |
| 2:B:364:LYS:HB2   | 2:B:365:ILE:HD12  | 1.95                     | 0.49              |
| 2:B:524:GLN:O     | 2:B:580:ALA:HA    | 2.12                     | 0.49              |
| 4:E:505:THR:HG23  | 4:E:508:GLN:HG3   | 1.95                     | 0.49              |
| 6:H:296:THR:HG21  | 6:H:357:THR:CG2   | 2.42                     | 0.49              |
| 7:L:315:LEU:HB3   | 7:L:334:HIS:CE1   | 2.48                     | 0.49              |
| 2:O:585:SER:N     | 2:O:586:PRO:HD2   | 2.27                     | 0.49              |
| 8:P:773:MET:C     | 8:P:781:PRO:HB3   | 2.38                     | 0.49              |
| 1:S:313:THR:HA    | 1:S:316:LEU:HB3   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:U:807:MET:O     | 11:U:810:VAL:HB   | 2.12                     | 0.49              |
| 12:V:64:SER:O      | 12:V:112:ASN:ND2  | 2.38                     | 0.49              |
| 3:C:82:ALA:HB3     | 3:C:189:PRO:CB    | 2.40                     | 0.49              |
| 3:C:169:PHE:CD2    | 4:E:17:ALA:HB2    | 2.48                     | 0.49              |
| 4:E:97:ASN:O       | 4:E:98:LEU:C      | 2.56                     | 0.49              |
| 5:F:287:TYR:CE2    | 5:F:343:GLY:HA2   | 2.48                     | 0.49              |
| 6:G:371:LEU:O      | 6:G:372:ALA:C     | 2.56                     | 0.49              |
| 6:G:471:VAL:O      | 6:G:474:SER:HB2   | 2.12                     | 0.49              |
| 8:Q:505:PRO:O      | 8:Q:532:SER:N     | 2.43                     | 0.49              |
| 1:S:288:GLU:HB2    | 1:S:292:HIS:HB2   | 1.93                     | 0.49              |
| 1:S:1368:PHE:CZ    | 1:S:1392:PRO:HB3  | 2.48                     | 0.49              |
| 11:U:648:GLU:HA    | 11:U:651:ILE:HD12 | 1.95                     | 0.49              |
| 6:G:491:LYS:HD3    | 6:G:498:ASN:ND2   | 2.27                     | 0.49              |
| 7:L:176:SER:N      | 7:L:189:GLN:HE22  | 2.11                     | 0.49              |
| 8:P:603:PHE:HB2    | 8:P:639:CYS:SG    | 2.53                     | 0.49              |
| 8:Q:604:TYR:HB3    | 8:Q:638:VAL:CG2   | 2.43                     | 0.49              |
| 11:U:302:ASN:HD21  | 11:U:357:ARG:HB2  | 1.78                     | 0.49              |
| 11:U:910:GLU:O     | 11:U:913:GLN:HB3  | 2.13                     | 0.49              |
| 12:V:110:PHE:CZ    | 12:V:114:LEU:HD11 | 2.48                     | 0.49              |
| 1:A:22:TRP:CZ2     | 6:H:423:ARG:NH2   | 2.81                     | 0.49              |
| 2:B:423:TYR:CD1    | 8:P:606:LEU:HD22  | 2.48                     | 0.49              |
| 3:C:319:THR:O      | 3:C:320:GLN:C     | 2.55                     | 0.49              |
| 3:C:508:VAL:CG1    | 3:C:512:MET:HE2   | 2.43                     | 0.49              |
| 7:L:356:PHE:HD1    | 7:L:367:THR:HG1   | 1.61                     | 0.49              |
| 8:P:267:ASP:OD1    | 8:P:269:ASN:N     | 2.40                     | 0.49              |
| 8:P:279:GLU:OE1    | 8:P:279:GLU:HA    | 2.13                     | 0.49              |
| 8:P:502:GLY:O      | 8:P:504:ARG:N     | 2.44                     | 0.49              |
| 1:S:593:LEU:HD11   | 1:S:625:CYS:SG    | 2.53                     | 0.49              |
| 1:S:923:GLU:HG2    | 1:S:926:HIS:HB2   | 1.94                     | 0.49              |
| 1:A:831:PHE:CE1    | 1:A:899:PRO:HD2   | 2.48                     | 0.48              |
| 2:B:292:SER:OG     | 2:B:361:ASP:OD1   | 2.31                     | 0.48              |
| 2:B:423:TYR:O      | 2:B:427:ILE:N     | 2.44                     | 0.48              |
| 5:F:95:LEU:HA      | 5:F:98:LEU:HD12   | 1.95                     | 0.48              |
| 8:P:224:LEU:O      | 8:P:227:LEU:N     | 2.46                     | 0.48              |
| 8:Q:248:GLY:HA2    | 8:Q:282:VAL:HG23  | 1.94                     | 0.48              |
| 1:S:795:ARG:HD2    | 1:S:815:PRO:HD3   | 1.94                     | 0.48              |
| 7:M:169:PHE:CZ     | 7:M:193:ALA:HB1   | 2.48                     | 0.48              |
| 7:M:216:PRO:HB2    | 7:M:219:PRO:HB3   | 1.94                     | 0.48              |
| 11:U:1177:VAL:HG22 | 11:U:1194:MET:HE1 | 1.95                     | 0.48              |
| 4:E:67:LEU:HA      | 4:E:86:LEU:HB3    | 1.95                     | 0.48              |
| 6:H:13:LEU:HA      | 6:H:16:TRP:CE3    | 2.48                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:527:CYS:O     | 8:P:580:VAL:N     | 2.45                     | 0.48              |
| 8:P:705:VAL:HG13  | 8:P:788:GLN:HE21  | 1.79                     | 0.48              |
| 1:S:1063:TRP:CZ3  | 1:S:1329:ARG:NH2  | 2.81                     | 0.48              |
| 10:X:6:ARG:NH2    | 10:X:103:ASN:HA   | 2.28                     | 0.48              |
| 12:V:149:ILE:HA   | 12:V:152:THR:HG22 | 1.95                     | 0.48              |
| 1:A:245:ARG:NH2   | 1:A:263:PRO:HD3   | 2.29                     | 0.48              |
| 2:B:66:THR:O      | 2:B:68:LYS:NZ     | 2.35                     | 0.48              |
| 6:G:476:PHE:HD2   | 6:G:520:ARG:HA    | 1.79                     | 0.48              |
| 7:L:228:ILE:O     | 7:L:235:SER:OG    | 2.27                     | 0.48              |
| 2:O:716:ILE:HD13  | 8:Q:556:LEU:HD21  | 1.95                     | 0.48              |
| 8:P:359:TYR:O     | 8:P:401:ILE:HD13  | 2.13                     | 0.48              |
| 4:E:473:MET:O     | 4:E:477:CYS:SG    | 2.70                     | 0.48              |
| 8:Q:23:ALA:HB2    | 8:Q:348:LEU:CD2   | 2.44                     | 0.48              |
| 10:X:65:PRO:HB3   | 10:X:98:TRP:HB2   | 1.96                     | 0.48              |
| 12:V:157:LEU:HD13 | 12:V:176:ILE:HG21 | 1.94                     | 0.48              |
| 12:V:171:ASN:HD21 | 12:V:173:PRO:HB2  | 1.78                     | 0.48              |
| 12:V:816:LEU:HA   | 12:V:819:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:286:GLN:HB3   | 1:A:288:GLU:HG3   | 1.94                     | 0.48              |
| 2:B:40:THR:HG21   | 2:B:69:GLU:O      | 2.13                     | 0.48              |
| 2:B:308:ALA:N     | 2:B:325:LEU:HD12  | 2.29                     | 0.48              |
| 2:B:430:VAL:HG21  | 8:P:638:VAL:CG1   | 2.43                     | 0.48              |
| 6:G:451:TRP:CZ3   | 6:G:452:VAL:HG22  | 2.48                     | 0.48              |
| 6:H:48:GLU:O      | 6:H:51:ARG:HB2    | 2.14                     | 0.48              |
| 2:O:829:LYS:N     | 8:Q:824:ASP:O     | 2.47                     | 0.48              |
| 8:P:527:CYS:N     | 8:P:580:VAL:O     | 2.40                     | 0.48              |
| 8:Q:709:LYS:HB2   | 8:Q:879:ILE:HG22  | 1.95                     | 0.48              |
| 11:U:528:ASN:HD22 | 12:V:250:SER:HA   | 1.79                     | 0.48              |
| 11:U:543:LEU:O    | 11:U:547:PHE:CB   | 2.61                     | 0.48              |
| 12:V:259:LEU:HA   | 12:V:262:VAL:HG12 | 1.95                     | 0.48              |
| 2:B:710:ARG:O     | 2:B:711:THR:OG1   | 2.31                     | 0.48              |
| 3:C:146:TYR:N     | 3:C:147:PRO:CD    | 2.76                     | 0.48              |
| 3:C:334:ARG:HD3   | 7:L:252:PHE:CE1   | 2.48                     | 0.48              |
| 3:C:352:LEU:HD12  | 3:C:396:LEU:HD23  | 1.96                     | 0.48              |
| 5:F:3:SER:HA      | 5:F:6:GLN:NE2     | 2.29                     | 0.48              |
| 5:F:312:GLN:O     | 5:F:315:CYS:SG    | 2.71                     | 0.48              |
| 6:H:480:LEU:O     | 6:H:483:LEU:HB3   | 2.14                     | 0.48              |
| 2:O:268:PHE:O     | 2:O:269:GLN:HG2   | 2.13                     | 0.48              |
| 1:S:139:VAL:HG12  | 1:S:140:GLU:N     | 2.29                     | 0.48              |
| 1:S:830:LEU:HD22  | 1:S:871:LEU:CD2   | 2.41                     | 0.48              |
| 12:V:180:LEU:HA   | 12:V:183:LEU:HD11 | 1.96                     | 0.48              |
| 12:V:515:LYS:HD3  | 12:V:551:ILE:HG22 | 1.96                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:348:PHE:CZ   | 1:A:356:THR:CG2  | 2.97                     | 0.48              |
| 2:B:172:TRP:CZ3  | 2:B:176:ILE:HD11 | 2.49                     | 0.48              |
| 2:B:364:LYS:HG2  | 2:B:402:PHE:CE2  | 2.49                     | 0.48              |
| 4:E:21:GLN:OE1   | 4:E:21:GLN:N     | 2.46                     | 0.48              |
| 4:E:424:VAL:CG1  | 4:E:437:MET:HE3  | 2.43                     | 0.48              |
| 6:G:203:LEU:O    | 6:G:207:LEU:HD23 | 2.13                     | 0.48              |
| 6:G:430:LYS:NZ   | 8:P:328:TRP:HB2  | 2.28                     | 0.48              |
| 8:P:13:GLY:C     | 8:P:14:PHE:CD1   | 2.92                     | 0.48              |
| 8:P:84:GLY:O     | 8:P:130:LEU:HD21 | 2.14                     | 0.48              |
| 7:M:198:LYS:C    | 7:M:198:LYS:CD   | 2.86                     | 0.48              |
| 3:C:333:LEU:N    | 3:C:333:LEU:HD23 | 2.29                     | 0.48              |
| 6:G:406:GLN:NE2  | 6:G:599:TRP:HB2  | 2.26                     | 0.48              |
| 7:L:356:PHE:HE1  | 7:L:367:THR:HG21 | 1.79                     | 0.48              |
| 1:S:556:MET:SD   | 1:S:998:TYR:CD1  | 3.06                     | 0.48              |
| 12:V:825:ILE:O   | 12:V:828:LYS:HG2 | 2.14                     | 0.48              |
| 1:A:22:TRP:HZ2   | 6:H:423:ARG:NH2  | 2.10                     | 0.48              |
| 1:A:286:GLN:HB2  | 1:A:288:GLU:OE2  | 2.14                     | 0.48              |
| 2:B:87:THR:HB    | 2:B:89:ILE:HD12  | 1.96                     | 0.48              |
| 2:B:423:TYR:O    | 2:B:426:LEU:HB3  | 2.13                     | 0.48              |
| 2:B:667:TYR:O    | 2:B:713:PHE:CE1  | 2.67                     | 0.48              |
| 3:C:302:LEU:HD21 | 3:C:315:ILE:HD11 | 1.95                     | 0.48              |
| 3:C:330:SER:OG   | 3:C:334:ARG:NH1  | 2.47                     | 0.48              |
| 7:M:146:ARG:CZ   | 7:M:201:TRP:HB2  | 2.44                     | 0.48              |
| 7:M:207:ILE:HG23 | 7:M:228:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:230:VAL:HG12 | 1:A:234:MET:CE   | 2.44                     | 0.48              |
| 1:A:1033:ASP:OD1 | 1:A:1093:SER:OG  | 2.31                     | 0.48              |
| 2:B:426:LEU:O    | 2:B:429:LEU:HB3  | 2.14                     | 0.48              |
| 5:F:69:GLU:HA    | 5:F:74:ARG:NH2   | 2.28                     | 0.48              |
| 8:Q:69:LEU:HD12  | 8:Q:76:LEU:HD12  | 1.96                     | 0.48              |
| 8:Q:543:LEU:C    | 8:Q:544:CYS:SG   | 2.97                     | 0.48              |
| 8:Q:654:ARG:NH2  | 8:Q:758:ALA:O    | 2.47                     | 0.48              |
| 1:A:245:ARG:HH22 | 1:A:262:MET:HA   | 1.79                     | 0.47              |
| 5:F:196:LEU:HD21 | 5:F:201:PHE:CE1  | 2.48                     | 0.47              |
| 6:G:424:THR:O    | 6:G:428:LEU:HG   | 2.14                     | 0.47              |
| 6:H:31:GLN:O     | 6:H:39:ARG:NH1   | 2.47                     | 0.47              |
| 8:P:243:CYS:N    | 8:P:251:CYS:O    | 2.37                     | 0.47              |
| 8:P:270:ALA:HB3  | 8:P:271:LEU:HB2  | 1.96                     | 0.47              |
| 8:P:504:ARG:N    | 8:P:505:PRO:CD   | 2.77                     | 0.47              |
| 8:P:771:VAL:O    | 8:P:784:ALA:O    | 2.32                     | 0.47              |
| 1:S:494:LEU:CD1  | 1:S:518:LEU:HD11 | 2.38                     | 0.47              |
| 1:S:948:ASP:O    | 1:S:951:ARG:HB3  | 2.14                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:V:639:ILE:HD13 | 12:V:740:CYS:SG    | 2.54                     | 0.47              |
| 1:A:351:THR:HG21  | 1:A:391:SER:OG     | 2.14                     | 0.47              |
| 4:E:398:VAL:HG12  | 4:E:399:CYS:SG     | 2.54                     | 0.47              |
| 6:H:232:LEU:O     | 6:H:248:VAL:CG1    | 2.62                     | 0.47              |
| 2:O:518:PHE:HB2   | 8:Q:568:PRO:HG2    | 1.96                     | 0.47              |
| 2:O:651:LEU:HD23  | 2:O:655:PHE:CE1    | 2.49                     | 0.47              |
| 8:P:151:LYS:HA    | 8:P:173:VAL:O      | 2.15                     | 0.47              |
| 7:M:73:ARG:CD     | 7:M:86:GLU:OE1     | 2.54                     | 0.47              |
| 11:U:1007:LEU:HA  | 11:U:1035:LEU:HD13 | 1.95                     | 0.47              |
| 12:V:791:ASN:HA   | 12:V:794:ARG:HD3   | 1.95                     | 0.47              |
| 1:A:181:ALA:O     | 1:A:185:LEU:HD23   | 2.15                     | 0.47              |
| 1:A:1330:LEU:O    | 1:A:1333:PHE:HB3   | 2.14                     | 0.47              |
| 2:B:478:ILE:HD11  | 2:B:597:VAL:HG21   | 1.96                     | 0.47              |
| 3:C:123:SER:HA    | 5:F:140:ARG:NH2    | 2.29                     | 0.47              |
| 5:F:200:ASN:O     | 5:F:204:VAL:HG23   | 2.15                     | 0.47              |
| 6:G:296:THR:O     | 6:G:299:GLU:HB3    | 2.14                     | 0.47              |
| 6:G:477:SER:HA    | 6:G:520:ARG:HH21   | 1.78                     | 0.47              |
| 2:O:580:ALA:C     | 2:O:581:VAL:CG2    | 2.86                     | 0.47              |
| 8:P:60:PHE:CD1    | 8:P:60:PHE:N       | 2.82                     | 0.47              |
| 8:P:776:LEU:HD13  | 8:P:881:LEU:HD11   | 1.96                     | 0.47              |
| 7:M:295:ARG:C     | 7:M:297:ILE:N      | 2.71                     | 0.47              |
| 11:U:372:VAL:C    | 11:U:374:SER:N     | 2.71                     | 0.47              |
| 11:U:651:ILE:HD13 | 11:U:738:LYS:HG3   | 1.97                     | 0.47              |
| 12:V:537:SER:HB2  | 12:V:584:ILE:HG21  | 1.96                     | 0.47              |
| 2:B:298:PHE:CE2   | 2:B:362:LEU:HD12   | 2.50                     | 0.47              |
| 3:C:24:GLN:O      | 3:C:25:ALA:C       | 2.57                     | 0.47              |
| 6:G:332:PRO:HD2   | 8:P:262:ARG:O      | 2.13                     | 0.47              |
| 6:G:457:LEU:HD23  | 6:G:458:LEU:HD23   | 1.95                     | 0.47              |
| 6:G:511:GLN:HE22  | 6:G:547:ASN:HB2    | 1.80                     | 0.47              |
| 8:P:572:LEU:HA    | 8:P:578:ARG:NH1    | 2.29                     | 0.47              |
| 1:S:375:LEU:HD11  | 1:S:396:LEU:HD11   | 1.96                     | 0.47              |
| 11:U:330:LEU:O    | 11:U:334:VAL:HG23  | 2.14                     | 0.47              |
| 12:V:413:GLN:HB2  | 12:V:415:GLN:OE1   | 2.14                     | 0.47              |
| 12:V:614:LEU:HA   | 12:V:617:VAL:HG12  | 1.96                     | 0.47              |
| 1:A:664:MET:HE2   | 1:A:733:ALA:HB2    | 1.95                     | 0.47              |
| 2:B:411:HIS:O     | 2:B:414:LEU:HB3    | 2.15                     | 0.47              |
| 8:P:27:ARG:O      | 8:P:37:LEU:HA      | 2.13                     | 0.47              |
| 8:P:113:SER:OG    | 8:P:115:VAL:HG12   | 2.15                     | 0.47              |
| 8:P:527:CYS:SG    | 8:P:527:CYS:O      | 2.71                     | 0.47              |
| 10:X:78:ASN:HD22  | 10:X:86:CYS:HB3    | 1.79                     | 0.47              |
| 12:V:243:VAL:N    | 12:V:244:PRO:CD    | 2.77                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:B:596:THR:HA     | 2:B:619:ARG:HG3    | 1.97                     | 0.47              |
| 2:B:602:MET:N      | 2:B:602:MET:SD     | 2.88                     | 0.47              |
| 3:C:224:ASN:HD21   | 3:C:249:SER:CB     | 2.11                     | 0.47              |
| 4:E:395:THR:HG21   | 4:E:429:LEU:HD12   | 1.97                     | 0.47              |
| 6:G:37:LEU:O       | 6:G:41:GLN:HG3     | 2.15                     | 0.47              |
| 6:G:214:ARG:NH1    | 6:G:330:PRO:HD3    | 2.29                     | 0.47              |
| 7:L:16:LEU:HD11    | 8:P:483:LEU:HD22   | 1.94                     | 0.47              |
| 8:P:843:GLU:OE1    | 8:P:844:VAL:HG23   | 2.14                     | 0.47              |
| 8:Q:28:VAL:HG23    | 8:Q:400:ASN:ND2    | 2.30                     | 0.47              |
| 1:S:989:MET:SD     | 1:S:1077:MET:HG2   | 2.54                     | 0.47              |
| 1:A:263:PRO:O      | 1:A:267:VAL:HG12   | 2.14                     | 0.47              |
| 1:A:818:PHE:CD1    | 1:A:819:ASP:N      | 2.83                     | 0.47              |
| 1:A:821:LEU:HD23   | 1:A:821:LEU:C      | 2.40                     | 0.47              |
| 1:A:1025:VAL:HG21  | 1:A:1085:LEU:HD13  | 1.95                     | 0.47              |
| 3:C:79:PHE:N       | 3:C:79:PHE:CD1     | 2.79                     | 0.47              |
| 3:C:180:VAL:HG11   | 3:C:214:ILE:CD1    | 2.45                     | 0.47              |
| 4:E:283:ALA:O      | 4:E:287:GLN:HG3    | 2.14                     | 0.47              |
| 6:G:480:LEU:CD1    | 6:G:517:LEU:HD23   | 2.44                     | 0.47              |
| 2:O:338:THR:O      | 2:O:340:GLN:NE2    | 2.48                     | 0.47              |
| 2:O:614:TYR:CG     | 8:Q:639:CYS:HB3    | 2.50                     | 0.47              |
| 8:P:75:LEU:C       | 8:P:90:LEU:HD21    | 2.40                     | 0.47              |
| 8:P:154:LEU:HD22   | 8:P:258:LEU:CD2    | 2.34                     | 0.47              |
| 8:P:557:ASP:OD1    | 8:P:557:ASP:N      | 2.48                     | 0.47              |
| 8:Q:398:SER:HA     | 8:Q:424:SER:HA     | 1.97                     | 0.47              |
| 8:Q:491:ASN:HD21   | 7:M:9:LEU:HD21     | 1.78                     | 0.47              |
| 8:Q:733:LEU:HD22   | 8:Q:746:VAL:HG11   | 1.97                     | 0.47              |
| 1:S:379:LEU:HD23   | 1:S:384:VAL:HG21   | 1.95                     | 0.47              |
| 1:S:827:ARG:HA     | 1:S:830:LEU:HD12   | 1.96                     | 0.47              |
| 1:S:862:PRO:HA     | 1:S:865:ILE:HD12   | 1.97                     | 0.47              |
| 1:S:869:GLN:CD     | 1:S:920:LEU:HD21   | 2.40                     | 0.47              |
| 11:U:321:ARG:HD2   | 12:V:444:HIS:CE1   | 2.49                     | 0.47              |
| 11:U:643:PRO:HB3   | 11:U:721:PHE:CE1   | 2.50                     | 0.47              |
| 11:U:807:MET:HE1   | 11:U:870:ILE:HG23  | 1.97                     | 0.47              |
| 11:U:990:THR:O     | 11:U:993:SER:OG    | 2.24                     | 0.47              |
| 11:U:1010:THR:HG22 | 11:U:1032:LEU:HD13 | 1.96                     | 0.47              |
| 12:V:382:LEU:HD12  | 12:V:420:THR:OG1   | 2.14                     | 0.47              |
| 2:B:364:LYS:CG     | 2:B:402:PHE:CE2    | 2.98                     | 0.47              |
| 3:C:227:ILE:HD11   | 3:C:239:VAL:CG1    | 2.43                     | 0.47              |
| 5:F:164:LYS:O      | 5:F:168:GLU:HG2    | 2.15                     | 0.47              |
| 8:P:359:TYR:CD2    | 8:P:420:LEU:HD23   | 2.50                     | 0.47              |
| 8:Q:485:SER:O      | 8:Q:486:LEU:C      | 2.56                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:580:VAL:O      | 1:S:584:LEU:HG     | 2.15                     | 0.47              |
| 1:S:665:THR:CA     | 9:W:80:VAL:HG22    | 2.45                     | 0.47              |
| 7:M:326:ASN:HD22   | 7:M:364:LYS:HG3    | 1.80                     | 0.47              |
| 11:U:1010:THR:HG21 | 11:U:1031:LEU:HG   | 1.95                     | 0.47              |
| 12:V:1139:MET:HE1  | 12:V:1188:ILE:HG12 | 1.96                     | 0.47              |
| 1:A:1305:LEU:C     | 1:A:1308:LEU:CD2   | 2.88                     | 0.47              |
| 4:E:423:LEU:O      | 4:E:429:LEU:HD13   | 2.14                     | 0.47              |
| 6:G:283:LEU:O      | 6:G:286:ALA:HB3    | 2.15                     | 0.47              |
| 1:S:414:LEU:HD12   | 1:S:426:SER:HB2    | 1.97                     | 0.47              |
| 11:U:731:GLN:NE2   | 11:U:792:ALA:HB2   | 2.30                     | 0.47              |
| 2:B:298:PHE:CD1    | 2:B:312:TRP:HD1    | 2.32                     | 0.47              |
| 2:B:402:PHE:HD2    | 8:P:465:ILE:HD11   | 1.80                     | 0.47              |
| 2:B:738:LEU:HD22   | 2:B:742:CYS:SG     | 2.55                     | 0.47              |
| 4:E:473:MET:HE2    | 4:E:473:MET:HA     | 1.97                     | 0.47              |
| 8:Q:794:LEU:HD22   | 8:Q:867:LEU:HD22   | 1.97                     | 0.47              |
| 1:A:923:GLU:OE1    | 1:A:923:GLU:HA     | 2.14                     | 0.46              |
| 2:B:83:SER:OG      | 8:P:15:CYS:SG      | 2.64                     | 0.46              |
| 2:B:281:PHE:N      | 2:B:281:PHE:CD1    | 2.83                     | 0.46              |
| 4:E:388:THR:HB     | 4:E:426:MET:SD     | 2.55                     | 0.46              |
| 2:O:170:ILE:O      | 2:O:171:GLN:C      | 2.56                     | 0.46              |
| 8:P:201:SER:O      | 8:P:219:THR:HA     | 2.15                     | 0.46              |
| 8:P:446:MET:HE1    | 8:P:451:ALA:HB2    | 1.96                     | 0.46              |
| 8:Q:733:LEU:CD2    | 8:Q:746:VAL:HG11   | 2.45                     | 0.46              |
| 7:M:170:PRO:HB3    | 7:M:222:SER:O      | 2.15                     | 0.46              |
| 7:M:341:TRP:CZ2    | 10:X:100:PRO:HD3   | 2.51                     | 0.46              |
| 11:U:221:SER:HB2   | 11:U:229:VAL:HG21  | 1.97                     | 0.46              |
| 12:V:62:GLY:HA2    | 12:V:112:ASN:HD22  | 1.80                     | 0.46              |
| 12:V:1338:LEU:HD23 | 12:V:1341:LEU:HD23 | 1.97                     | 0.46              |
| 1:A:25:LEU:HD11    | 6:H:416:LEU:HD13   | 1.96                     | 0.46              |
| 1:A:1287:VAL:O     | 1:A:1291:ILE:HG12  | 2.15                     | 0.46              |
| 3:C:169:PHE:CE1    | 3:C:209:ARG:HD3    | 2.49                     | 0.46              |
| 4:E:395:THR:O      | 4:E:399:CYS:SG     | 2.73                     | 0.46              |
| 6:G:306:LEU:O      | 6:G:309:ALA:HB3    | 2.14                     | 0.46              |
| 8:P:288:LEU:HG     | 8:P:313:VAL:HG21   | 1.96                     | 0.46              |
| 8:P:516:ARG:O      | 8:P:517:LEU:HD22   | 2.15                     | 0.46              |
| 2:B:132:ASP:OD2    | 2:B:145:ARG:NH1    | 2.45                     | 0.46              |
| 2:B:490:GLY:HA2    | 2:B:579:THR:HA     | 1.96                     | 0.46              |
| 2:B:636:PHE:HB3    | 2:B:637:PRO:CD     | 2.46                     | 0.46              |
| 4:E:70:GLU:HB3     | 4:E:83:LEU:HD22    | 1.96                     | 0.46              |
| 7:L:126:LEU:HD11   | 7:L:128:TYR:O      | 2.15                     | 0.46              |
| 8:P:150:TRP:CZ3    | 8:P:195:PRO:HG3    | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:243:CYS:SG    | 8:P:251:CYS:O     | 2.72                     | 0.46              |
| 1:S:1263:PHE:CZ   | 1:S:1322:VAL:HG11 | 2.51                     | 0.46              |
| 11:U:286:GLY:O    | 11:U:289:LEU:HB3  | 2.15                     | 0.46              |
| 11:U:707:GLU:O    | 11:U:710:THR:HB   | 2.15                     | 0.46              |
| 12:V:98:SER:O     | 12:V:101:GLU:HG2  | 2.16                     | 0.46              |
| 14:Z:40:DC:H2"    | 14:Z:41:DC:C6     | 2.51                     | 0.46              |
| 1:A:174:GLN:NE2   | 1:A:209:TRP:CD1   | 2.84                     | 0.46              |
| 4:E:23:GLU:OE2    | 4:E:25:PRO:HG2    | 2.16                     | 0.46              |
| 5:F:141:SER:O     | 5:F:144:HIS:HB3   | 2.16                     | 0.46              |
| 5:F:158:GLN:HA    | 5:F:207:VAL:HG13  | 1.96                     | 0.46              |
| 5:F:274:TYR:HE2   | 5:F:314:LEU:HD21  | 1.80                     | 0.46              |
| 6:H:58:GLN:NE2    | 6:H:98:ARG:HG2    | 2.30                     | 0.46              |
| 6:H:119:ARG:HD2   | 6:H:161:LEU:HD23  | 1.97                     | 0.46              |
| 6:H:412:ASP:O     | 6:H:415:THR:OG1   | 2.28                     | 0.46              |
| 8:P:159:CYS:SG    | 8:P:160:PRO:HD3   | 2.54                     | 0.46              |
| 8:P:227:LEU:O     | 8:P:227:LEU:HD12  | 2.16                     | 0.46              |
| 8:P:829:TYR:OH    | 8:P:879:ILE:CD1   | 2.64                     | 0.46              |
| 1:S:470:LEU:O     | 1:S:473:LEU:HB2   | 2.14                     | 0.46              |
| 1:S:672:VAL:HG12  | 1:S:676:GLN:HE21  | 1.81                     | 0.46              |
| 12:V:980:LEU:HD22 | 12:V:1075:TRP:CZ3 | 2.50                     | 0.46              |
| 1:A:1266:MET:HE2  | 1:A:1266:MET:HA   | 1.98                     | 0.46              |
| 2:B:40:THR:HG23   | 2:B:70:GLU:HA     | 1.97                     | 0.46              |
| 3:C:458:ARG:HA    | 3:C:458:ARG:NE    | 2.30                     | 0.46              |
| 6:G:365:GLU:HG3   | 1:S:29:ARG:HH22   | 1.81                     | 0.46              |
| 1:S:477:LEU:HD13  | 1:S:510:TYR:OH    | 2.15                     | 0.46              |
| 1:S:817:LEU:HD23  | 1:S:818:PHE:CD1   | 2.51                     | 0.46              |
| 7:M:234:VAL:HG11  | 7:M:259:VAL:CG1   | 2.46                     | 0.46              |
| 11:U:481:VAL:HG12 | 11:U:485:PHE:CZ   | 2.51                     | 0.46              |
| 14:Z:47:DT:H2"    | 14:Z:48:DG:C8     | 2.50                     | 0.46              |
| 1:A:134:PRO:HA    | 1:A:220:GLN:HE22  | 1.81                     | 0.46              |
| 1:A:1252:GLU:O    | 1:A:1298:ARG:NH1  | 2.47                     | 0.46              |
| 2:B:183:LEU:HD12  | 2:B:191:LEU:HD12  | 1.97                     | 0.46              |
| 4:E:355:LEU:HD23  | 4:E:360:ALA:HA    | 1.96                     | 0.46              |
| 6:H:513:ARG:O     | 6:H:517:LEU:HG    | 2.16                     | 0.46              |
| 2:O:66:THR:O      | 2:O:68:LYS:NZ     | 2.42                     | 0.46              |
| 8:P:531:ASN:HB2   | 8:P:572:LEU:HD21  | 1.98                     | 0.46              |
| 10:X:57:ILE:HG23  | 10:X:61:TYR:CD2   | 2.50                     | 0.46              |
| 11:U:537:VAL:HG12 | 11:U:541:LEU:HD12 | 1.97                     | 0.46              |
| 11:U:595:LEU:CD1  | 11:U:626:THR:HG22 | 2.46                     | 0.46              |
| 12:V:193:THR:CA   | 12:V:196:ILE:HG22 | 2.45                     | 0.46              |
| 1:A:1358:VAL:O    | 1:A:1362:LEU:HG   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:392:PRO:HB2   | 7:L:131:THR:HG22  | 1.98                     | 0.46              |
| 3:C:315:ILE:CG2   | 3:C:399:HIS:CD2   | 2.99                     | 0.46              |
| 6:G:473:ILE:HD11  | 6:G:523:GLU:HB3   | 1.97                     | 0.46              |
| 6:H:387:SER:OG    | 6:H:388:PRO:HD2   | 2.16                     | 0.46              |
| 2:O:47:ARG:HH21   | 2:O:112:LEU:HD21  | 1.79                     | 0.46              |
| 2:O:759:MET:HE3   | 2:O:763:LEU:CD1   | 2.46                     | 0.46              |
| 2:O:851:PHE:CZ    | 8:Q:550:SER:HB2   | 2.51                     | 0.46              |
| 8:P:366:LEU:HD23  | 8:P:366:LEU:C     | 2.41                     | 0.46              |
| 8:P:373:ARG:NH1   | 8:P:383:PRO:O     | 2.48                     | 0.46              |
| 1:S:163:ARG:CG    | 1:S:191:VAL:HG13  | 2.46                     | 0.46              |
| 7:M:267:LEU:HD13  | 7:M:288:LEU:HD21  | 1.98                     | 0.46              |
| 11:U:742:SER:O    | 11:U:746:VAL:HG23 | 2.16                     | 0.46              |
| 1:A:424:LEU:O     | 1:A:428:VAL:HG23  | 2.16                     | 0.46              |
| 2:B:507:SER:OG    | 2:B:600:GLN:NE2   | 2.49                     | 0.46              |
| 2:B:637:PRO:HB3   | 2:B:701:TYR:CZ    | 2.51                     | 0.46              |
| 6:H:538:LEU:O     | 6:H:542:GLN:NE2   | 2.49                     | 0.46              |
| 8:P:311:CYS:HA    | 8:P:324:ILE:O     | 2.16                     | 0.46              |
| 1:S:1220:PRO:O    | 1:S:1253:ARG:NH2  | 2.49                     | 0.46              |
| 2:B:295:GLY:O     | 2:B:297:LEU:HD12  | 2.16                     | 0.46              |
| 2:B:330:ILE:CG2   | 2:B:339:GLU:OE1   | 2.64                     | 0.46              |
| 2:B:609:CYS:SG    | 8:P:644:ARG:NH2   | 2.89                     | 0.46              |
| 5:F:289:LEU:HD12  | 6:G:539:LEU:HD23  | 1.94                     | 0.46              |
| 2:O:487:LEU:HB2   | 2:O:584:LEU:HD21  | 1.97                     | 0.46              |
| 2:O:759:MET:HE3   | 2:O:763:LEU:HD11  | 1.98                     | 0.46              |
| 2:O:770:LEU:O     | 2:O:773:LEU:HB3   | 2.16                     | 0.46              |
| 8:P:510:THR:HG22  | 8:P:527:CYS:HA    | 1.98                     | 0.46              |
| 8:Q:486:LEU:CD2   | 8:Q:490:MET:HE3   | 2.44                     | 0.46              |
| 7:M:253:PHE:CE2   | 7:M:263:LEU:HB3   | 2.51                     | 0.46              |
| 11:U:109:ALA:HB1  | 11:U:160:LEU:HD11 | 1.98                     | 0.46              |
| 1:A:818:PHE:CG    | 1:A:864:LEU:HD11  | 2.51                     | 0.46              |
| 1:A:1269:LEU:HD21 | 1:A:1330:LEU:HB2  | 1.97                     | 0.46              |
| 2:B:711:THR:O     | 2:B:714:GLU:N     | 2.49                     | 0.46              |
| 3:C:248:PRO:O     | 3:C:252:LYS:HB2   | 2.15                     | 0.46              |
| 4:E:339:LEU:HD13  | 12:V:309:HIS:ND1  | 2.30                     | 0.46              |
| 5:F:158:GLN:OE1   | 5:F:158:GLN:N     | 2.38                     | 0.46              |
| 6:H:186:PRO:HB3   | 6:H:200:ALA:HB3   | 1.98                     | 0.46              |
| 2:O:584:LEU:HB3   | 2:O:588:LEU:HD11  | 1.98                     | 0.46              |
| 2:O:602:MET:HE2   | 8:Q:548:LEU:CD1   | 2.43                     | 0.46              |
| 8:P:152:MET:O     | 8:P:172:GLU:HA    | 2.16                     | 0.46              |
| 8:Q:508:CYS:O     | 8:Q:643:SER:HB2   | 2.16                     | 0.46              |
| 8:Q:773:MET:HB3   | 8:Q:776:LEU:HG    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:S:988:LEU:CD2   | 1:S:1077:MET:HE2   | 2.44                     | 0.46              |
| 7:M:197:LEU:CD1   | 7:M:201:TRP:HZ2    | 2.22                     | 0.46              |
| 12:V:199:LEU:HD23 | 12:V:199:LEU:C     | 2.41                     | 0.46              |
| 12:V:382:LEU:HD11 | 12:V:416:LEU:HB3   | 1.98                     | 0.46              |
| 1:A:78:ILE:HG22   | 1:A:79:ASP:N       | 2.31                     | 0.45              |
| 1:A:174:GLN:HE21  | 1:A:209:TRP:CD1    | 2.33                     | 0.45              |
| 1:A:651:GLY:O     | 1:A:654:THR:OG1    | 2.34                     | 0.45              |
| 2:B:139:GLY:O     | 2:B:141:LEU:HB2    | 2.16                     | 0.45              |
| 2:B:330:ILE:HG22  | 2:B:339:GLU:OE1    | 2.16                     | 0.45              |
| 2:B:584:LEU:HD12  | 2:O:725:THR:HG21   | 1.97                     | 0.45              |
| 7:L:326:ASN:HD22  | 7:L:364:LYS:HG3    | 1.80                     | 0.45              |
| 8:P:143:LEU:C     | 8:P:143:LEU:HD23   | 2.41                     | 0.45              |
| 8:P:150:TRP:HZ3   | 8:P:195:PRO:HG3    | 1.82                     | 0.45              |
| 8:P:424:SER:OG    | 8:P:428:ARG:HB2    | 2.17                     | 0.45              |
| 8:P:679:PHE:CD2   | 8:P:679:PHE:O      | 2.69                     | 0.45              |
| 1:S:57:LEU:CD1    | 1:S:101:GLN:HE21   | 2.29                     | 0.45              |
| 10:X:44:THR:CG2   | 10:X:116:SER:HA    | 2.37                     | 0.45              |
| 11:U:646:LYS:HG3  | 11:U:649:ALA:HB3   | 1.98                     | 0.45              |
| 11:U:1146:HIS:CD2 | 11:U:1208:LEU:HD13 | 2.51                     | 0.45              |
| 12:V:1238:MET:HE2 | 12:V:1278:LEU:HD21 | 1.98                     | 0.45              |
| 1:A:286:GLN:HB3   | 1:A:292:HIS:HB2    | 1.98                     | 0.45              |
| 1:A:375:LEU:HD11  | 1:A:392:PHE:CE1    | 2.51                     | 0.45              |
| 1:A:661:ARG:NH2   | 1:A:728:GLN:HB3    | 2.30                     | 0.45              |
| 2:B:331:ASP:CB    | 2:B:333:PHE:CE1    | 2.99                     | 0.45              |
| 3:C:200:VAL:O     | 3:C:201:GLU:C      | 2.58                     | 0.45              |
| 3:C:280:SER:O     | 3:C:283:GLN:HB2    | 2.16                     | 0.45              |
| 4:E:429:LEU:HB3   | 4:E:460:ARG:HH12   | 1.80                     | 0.45              |
| 4:E:516:LEU:HD21  | 4:E:527:LEU:HD13   | 1.97                     | 0.45              |
| 6:G:372:ALA:O     | 6:G:373:LEU:C      | 2.58                     | 0.45              |
| 6:H:342:THR:CB    | 6:H:384:PRO:HG3    | 2.43                     | 0.45              |
| 7:L:66:TYR:HA     | 7:L:69:ILE:HG12    | 1.97                     | 0.45              |
| 2:O:94:ILE:HG22   | 2:O:96:ILE:HG12    | 1.99                     | 0.45              |
| 2:O:521:LEU:HD23  | 2:O:523:CYS:SG     | 2.55                     | 0.45              |
| 8:P:137:ASP:N     | 8:P:137:ASP:OD1    | 2.49                     | 0.45              |
| 8:P:540:GLY:HA2   | 8:P:608:GLU:CG     | 2.46                     | 0.45              |
| 1:S:239:VAL:HG11  | 1:S:301:VAL:HG22   | 1.98                     | 0.45              |
| 1:S:1266:MET:HE3  | 1:S:1323:ALA:HB1   | 1.97                     | 0.45              |
| 11:U:962:PHE:CD2  | 11:U:992:LEU:HD11  | 2.50                     | 0.45              |
| 12:V:1077:GLY:O   | 12:V:1083:ASN:ND2  | 2.47                     | 0.45              |
| 12:V:1136:ARG:HA  | 12:V:1139:MET:HE2  | 1.99                     | 0.45              |
| 2:B:836:ARG:CZ    | 8:P:822:ALA:HB2    | 2.47                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:C:169:PHE:CZ    | 4:E:17:ALA:HB2     | 2.51                     | 0.45              |
| 4:E:358:SER:O     | 4:E:362:VAL:HG23   | 2.17                     | 0.45              |
| 4:E:361:THR:HG23  | 4:E:401:ALA:CB     | 2.45                     | 0.45              |
| 4:E:387:LEU:O     | 4:E:391:CYS:SG     | 2.74                     | 0.45              |
| 5:F:156:ASN:C     | 5:F:158:GLN:OE1    | 2.59                     | 0.45              |
| 6:G:416:LEU:HD13  | 1:S:22:TRP:CH2     | 2.52                     | 0.45              |
| 6:G:518:ILE:HD11  | 6:G:550:THR:HA     | 1.98                     | 0.45              |
| 2:O:156:GLN:O     | 2:O:156:GLN:NE2    | 2.49                     | 0.45              |
| 2:O:592:LYS:HG2   | 2:O:593:PHE:N      | 2.31                     | 0.45              |
| 2:O:843:ALA:CB    | 8:Q:809:GLN:HE21   | 2.30                     | 0.45              |
| 8:P:27:ARG:N      | 8:P:38:SER:OG      | 2.45                     | 0.45              |
| 8:P:341:TYR:C     | 8:P:342:CYS:SG     | 2.98                     | 0.45              |
| 1:S:1033:ASP:CG   | 1:S:1093:SER:HB2   | 2.42                     | 0.45              |
| 11:U:1099:VAL:HA  | 11:U:1102:LEU:HD12 | 1.96                     | 0.45              |
| 12:V:1078:PHE:O   | 12:V:1084:GLN:NE2  | 2.40                     | 0.45              |
| 12:V:1092:HIS:O   | 12:V:1096:SER:OG   | 2.31                     | 0.45              |
| 1:A:392:PHE:CE1   | 1:A:396:LEU:HD13   | 2.51                     | 0.45              |
| 2:B:40:THR:HG23   | 2:B:70:GLU:CD      | 2.41                     | 0.45              |
| 2:B:228:ILE:HG22  | 2:B:229:ILE:H      | 1.81                     | 0.45              |
| 2:B:695:GLU:HA    | 2:B:701:TYR:CE1    | 2.50                     | 0.45              |
| 4:E:384:THR:OG1   | 4:E:385:THR:N      | 2.50                     | 0.45              |
| 6:G:393:MET:HE2   | 8:P:236:LEU:CD2    | 2.46                     | 0.45              |
| 6:G:458:LEU:CD2   | 6:G:596:TYR:CD2    | 2.99                     | 0.45              |
| 6:H:31:GLN:NE2    | 6:H:320:GLN:OE1    | 2.50                     | 0.45              |
| 7:L:208:ASP:O     | 7:L:295:ARG:NH2    | 2.49                     | 0.45              |
| 2:O:641:PRO:O     | 2:O:643:GLU:HG3    | 2.17                     | 0.45              |
| 2:O:704:LEU:HB2   | 2:O:720:TYR:HB2    | 1.99                     | 0.45              |
| 1:A:61:LEU:HD23   | 1:A:105:LEU:HD21   | 1.97                     | 0.45              |
| 1:A:163:ARG:N     | 8:P:849:ASP:OD2    | 2.49                     | 0.45              |
| 1:A:1122:HIS:N    | 1:A:1125:ALA:O     | 2.44                     | 0.45              |
| 1:A:1376:VAL:HG11 | 1:A:1392:PRO:HG3   | 1.98                     | 0.45              |
| 2:B:31:ASN:O      | 2:B:38:THR:N       | 2.50                     | 0.45              |
| 2:B:398:LEU:HA    | 8:P:462:ILE:HG12   | 1.98                     | 0.45              |
| 5:F:181:GLU:HA    | 5:F:184:ARG:HH12   | 1.81                     | 0.45              |
| 6:H:67:LEU:O      | 6:H:68:PRO:C       | 2.58                     | 0.45              |
| 6:H:590:PRO:HB2   | 6:H:592:TYR:CE2    | 2.51                     | 0.45              |
| 2:O:69:GLU:O      | 2:O:71:ASN:N       | 2.50                     | 0.45              |
| 1:S:316:LEU:HD11  | 1:S:320:PHE:CZ     | 2.52                     | 0.45              |
| 1:S:992:HIS:NE2   | 1:S:1077:MET:HE1   | 2.32                     | 0.45              |
| 1:S:1029:GLU:OE2  | 1:S:1089:VAL:N     | 2.49                     | 0.45              |
| 11:U:322:PHE:N    | 11:U:322:PHE:CD1   | 2.84                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:U:420:LYS:N    | 11:U:420:LYS:HD3  | 2.31                     | 0.45              |
| 12:V:215:LEU:O    | 12:V:219:LEU:HG   | 2.16                     | 0.45              |
| 12:V:243:VAL:CG2  | 12:V:244:PRO:HD3  | 2.47                     | 0.45              |
| 1:A:474:PHE:CD2   | 1:A:510:TYR:CE2   | 3.05                     | 0.45              |
| 1:A:733:ALA:HB1   | 1:A:742:GLN:CD    | 2.42                     | 0.45              |
| 2:B:91:LEU:HD13   | 2:B:111:ILE:HG21  | 1.97                     | 0.45              |
| 2:B:144:TRP:CH2   | 2:B:151:PHE:HB2   | 2.51                     | 0.45              |
| 3:C:171:THR:HG22  | 4:E:14:VAL:HB     | 1.99                     | 0.45              |
| 4:E:117:VAL:O     | 4:E:120:ILE:HB    | 2.17                     | 0.45              |
| 6:G:279:TRP:C     | 6:G:282:PRO:HD2   | 2.41                     | 0.45              |
| 6:G:296:THR:CG2   | 6:G:357:THR:HG21  | 2.47                     | 0.45              |
| 6:H:220:LEU:HD23  | 6:H:220:LEU:C     | 2.42                     | 0.45              |
| 7:L:51:ALA:HB3    | 7:L:74:MET:SD     | 2.57                     | 0.45              |
| 7:L:170:PRO:HD2   | 7:L:197:LEU:HD13  | 1.98                     | 0.45              |
| 2:O:522:LYS:CG    | 2:O:523:CYS:N     | 2.79                     | 0.45              |
| 8:P:429:LEU:HD23  | 8:P:429:LEU:C     | 2.42                     | 0.45              |
| 8:P:658:LEU:CD2   | 8:P:745:VAL:CG1   | 2.95                     | 0.45              |
| 1:S:291:THR:HA    | 1:S:294:ILE:HD12  | 1.99                     | 0.45              |
| 1:S:449:ALA:HB2   | 1:S:492:HIS:ND1   | 2.31                     | 0.45              |
| 1:S:1211:LEU:HD12 | 1:S:1233:ALA:HB1  | 1.99                     | 0.45              |
| 11:U:537:VAL:HG13 | 11:U:605:LEU:HD23 | 1.98                     | 0.45              |
| 12:V:532:LEU:HA   | 12:V:535:VAL:HG12 | 1.98                     | 0.45              |
| 1:A:32:ARG:CB     | 6:H:311:ASN:HD21  | 2.30                     | 0.45              |
| 1:A:415:MET:O     | 1:A:419:PHE:CD2   | 2.70                     | 0.45              |
| 1:A:1173:TRP:O    | 1:A:1177:LEU:HG   | 2.16                     | 0.45              |
| 2:B:500:SER:O     | 2:B:604:ARG:NH1   | 2.49                     | 0.45              |
| 2:B:713:PHE:CE2   | 6:H:242:ARG:NH2   | 2.85                     | 0.45              |
| 6:G:459:GLN:O     | 6:G:462:ALA:HB3   | 2.16                     | 0.45              |
| 6:H:164:GLU:HG2   | 6:H:171:SER:O     | 2.16                     | 0.45              |
| 8:P:471:PHE:C     | 8:P:471:PHE:HD1   | 2.24                     | 0.45              |
| 1:S:556:MET:HE3   | 1:S:1010:GLY:CA   | 2.47                     | 0.45              |
| 1:S:1302:TRP:CH2  | 1:S:1348:ILE:HG21 | 2.52                     | 0.45              |
| 12:V:110:PHE:CE2  | 12:V:114:LEU:HD11 | 2.51                     | 0.45              |
| 12:V:979:MET:O    | 12:V:979:MET:HE3  | 2.17                     | 0.45              |
| 1:A:286:GLN:O     | 1:A:288:GLU:N     | 2.46                     | 0.45              |
| 1:A:1305:LEU:HA   | 1:A:1308:LEU:HD21 | 1.98                     | 0.45              |
| 1:A:1361:TYR:CD1  | 1:A:1361:TYR:C    | 2.94                     | 0.45              |
| 3:C:165:HIS:HB2   | 3:C:206:CYS:HB3   | 1.99                     | 0.45              |
| 6:G:287:SER:OG    | 6:G:288:ARG:N     | 2.49                     | 0.45              |
| 7:L:9:LEU:HD11    | 8:P:491:ASN:ND2   | 2.32                     | 0.45              |
| 7:L:185:SER:O     | 7:L:188:SER:OG    | 2.30                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:O:17:CYS:O      | 2:O:81:CYS:SG     | 2.75                     | 0.45              |
| 8:P:524:MET:HA    | 8:P:582:LEU:O     | 2.17                     | 0.45              |
| 8:Q:726:VAL:HA    | 8:Q:727:PRO:HD2   | 1.67                     | 0.45              |
| 1:S:568:VAL:HG22  | 1:S:1069:LEU:HD11 | 1.99                     | 0.45              |
| 1:S:776:LEU:HD22  | 1:S:780:HIS:HB3   | 1.99                     | 0.45              |
| 1:S:1139:LEU:HD21 | 1:S:1181:LEU:HD22 | 1.99                     | 0.45              |
| 1:S:1246:LEU:HD22 | 1:S:1249:LEU:HD22 | 1.98                     | 0.45              |
| 1:S:1266:MET:HE2  | 1:S:1266:MET:HA   | 1.99                     | 0.45              |
| 10:X:62:PRO:HD2   | 10:X:63:PHE:CD2   | 2.52                     | 0.45              |
| 10:X:87:LEU:HD23  | 10:X:90:LEU:HG    | 1.99                     | 0.45              |
| 11:U:525:MET:HE1  | 11:U:590:SER:HB3  | 1.99                     | 0.45              |
| 11:U:748:GLY:O    | 11:U:752:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:1163:CYS:HB3  | 1:A:1166:ILE:HD12 | 1.99                     | 0.45              |
| 2:B:330:ILE:HG22  | 2:B:339:GLU:OE2   | 2.16                     | 0.45              |
| 2:B:630:GLY:O     | 2:B:631:LYS:HB3   | 2.17                     | 0.45              |
| 4:E:41:ARG:O      | 4:E:44:LEU:N      | 2.49                     | 0.45              |
| 6:H:178:LEU:O     | 6:H:182:LYS:HG3   | 2.16                     | 0.45              |
| 8:P:29:LEU:N      | 8:P:36:PHE:O      | 2.45                     | 0.45              |
| 8:P:243:CYS:SG    | 8:P:243:CYS:O     | 2.75                     | 0.45              |
| 8:P:260:THR:HB    | 8:P:264:ALA:O     | 2.16                     | 0.45              |
| 8:Q:229:PHE:HE1   | 8:Q:252:CYS:SG    | 2.40                     | 0.45              |
| 10:X:77:PRO:HD2   | 10:X:118:PRO:HB3  | 1.99                     | 0.45              |
| 11:U:115:ALA:HB1  | 11:U:121:LEU:HD21 | 1.99                     | 0.45              |
| 12:V:570:TYR:HA   | 12:V:573:ILE:HD12 | 1.99                     | 0.45              |
| 1:A:733:ALA:O     | 1:A:736:VAL:C     | 2.60                     | 0.45              |
| 1:A:835:LYS:HE2   | 1:A:903:TRP:CE2   | 2.51                     | 0.45              |
| 1:A:1220:PRO:HG2  | 1:A:1226:SER:CB   | 2.47                     | 0.45              |
| 2:B:172:TRP:HZ3   | 2:B:176:ILE:HD11  | 1.81                     | 0.45              |
| 2:B:292:SER:OG    | 2:B:292:SER:O     | 2.35                     | 0.45              |
| 2:B:342:LEU:HG    | 2:B:344:LEU:CD2   | 2.46                     | 0.45              |
| 2:B:667:TYR:CE2   | 6:H:239:LEU:HD11  | 2.51                     | 0.45              |
| 4:E:404:ASP:O     | 4:E:408:GLN:N     | 2.36                     | 0.45              |
| 6:G:354:CYS:O     | 6:G:357:THR:OG1   | 2.34                     | 0.45              |
| 6:H:388:PRO:HD2   | 6:H:389:PRO:HD3   | 1.98                     | 0.45              |
| 8:P:120:PRO:O     | 8:P:123:CYS:HB3   | 2.17                     | 0.45              |
| 8:P:228:LEU:HD11  | 8:P:312:LEU:HD22  | 1.98                     | 0.45              |
| 7:M:295:ARG:C     | 7:M:297:ILE:H     | 2.25                     | 0.45              |
| 10:X:57:ILE:CG2   | 10:X:61:TYR:CD2   | 2.99                     | 0.45              |
| 11:U:658:ILE:HD13 | 11:U:734:SER:HA   | 1.97                     | 0.45              |
| 14:Z:45:DT:H2"    | 14:Z:46:DC:C6     | 2.52                     | 0.45              |
| 2:B:294:GLY:C     | 2:B:409:ARG:HH22  | 2.24                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:850:ASP:OD2    | 8:P:801:HIS:ND1   | 2.49                     | 0.44              |
| 4:E:123:GLN:OE1    | 4:E:129:PRO:HA    | 2.17                     | 0.44              |
| 4:E:379:ALA:HB2    | 4:E:419:LEU:HD11  | 1.98                     | 0.44              |
| 7:L:315:LEU:HD23   | 7:L:336:ILE:HD13  | 1.97                     | 0.44              |
| 8:Q:563:ILE:HG21   | 8:Q:565:TYR:CZ    | 2.52                     | 0.44              |
| 1:S:476:PHE:CZ     | 1:S:480:LEU:HD13  | 2.52                     | 0.44              |
| 10:X:54:GLU:HB2    | 10:X:71:LEU:HD11  | 1.99                     | 0.44              |
| 11:U:491:LEU:HB2   | 11:U:496:VAL:CG2  | 2.48                     | 0.44              |
| 11:U:1019:ARG:O    | 11:U:1025:CYS:SG  | 2.75                     | 0.44              |
| 11:U:1248:LYS:N    | 11:U:1249:PRO:CD  | 2.80                     | 0.44              |
| 12:V:350:ILE:HG21  | 12:V:384:MET:HE1  | 1.99                     | 0.44              |
| 1:A:1063:TRP:NE1   | 1:A:1329:ARG:NH2  | 2.65                     | 0.44              |
| 1:A:1266:MET:HE1   | 1:A:1323:ALA:HB1  | 1.98                     | 0.44              |
| 1:A:1345:ASP:OD1   | 1:A:1345:ASP:N    | 2.50                     | 0.44              |
| 3:C:127:PHE:CZ     | 3:C:153:MET:HE1   | 2.51                     | 0.44              |
| 5:F:345:SER:O      | 5:F:346:ILE:C     | 2.61                     | 0.44              |
| 2:O:397:GLY:HA3    | 7:M:111:TYR:CE2   | 2.52                     | 0.44              |
| 8:P:327:SER:OG     | 8:P:335:VAL:O     | 2.23                     | 0.44              |
| 8:P:678:THR:O      | 8:P:679:PHE:C     | 2.60                     | 0.44              |
| 8:P:861:ALA:O      | 8:P:865:ARG:CB    | 2.64                     | 0.44              |
| 8:Q:141:VAL:HG11   | 8:Q:241:VAL:HG11  | 2.00                     | 0.44              |
| 1:S:773:GLY:N      | 1:S:774:PRO:HD2   | 2.32                     | 0.44              |
| 1:S:874:ARG:O      | 1:S:874:ARG:CG    | 2.64                     | 0.44              |
| 1:S:1033:ASP:OD2   | 1:S:1093:SER:CB   | 2.60                     | 0.44              |
| 7:M:361:TYR:HA     | 10:X:101:SER:CB   | 2.46                     | 0.44              |
| 11:U:230:LEU:HD11  | 11:U:285:LEU:HD11 | 1.98                     | 0.44              |
| 11:U:806:SER:HA    | 11:U:862:PRO:HD2  | 1.99                     | 0.44              |
| 11:U:1095:VAL:HG13 | 11:U:1137:GLN:NE2 | 2.32                     | 0.44              |
| 11:U:1151:THR:O    | 11:U:1212:PHE:HE2 | 2.01                     | 0.44              |
| 12:V:412:ILE:HA    | 12:V:416:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:230:VAL:HG12   | 1:A:234:MET:HE3   | 1.99                     | 0.44              |
| 2:B:96:ILE:O       | 2:B:107:TYR:HA    | 2.18                     | 0.44              |
| 4:E:106:ARG:O      | 4:E:107:PRO:C     | 2.60                     | 0.44              |
| 7:L:101:LEU:HB2    | 7:L:102:TYR:CD2   | 2.53                     | 0.44              |
| 2:O:486:SER:HA     | 2:O:582:THR:O     | 2.18                     | 0.44              |
| 8:P:251:CYS:SG     | 8:P:274:ILE:HB    | 2.57                     | 0.44              |
| 8:P:516:ARG:NH1    | 8:Q:579:GLU:O     | 2.49                     | 0.44              |
| 8:P:874:ARG:HA     | 8:P:874:ARG:HE    | 1.82                     | 0.44              |
| 1:S:240:GLN:HA     | 1:S:311:ILE:HD11  | 1.99                     | 0.44              |
| 1:S:1167:LEU:O     | 1:S:1171:LEU:HG   | 2.17                     | 0.44              |
| 7:M:39:ARG:NH1     | 7:M:55:CYS:O      | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:108:PRO:HG2   | 1:A:111:ILE:HD12  | 1.99                     | 0.44              |
| 1:A:900:SER:OG    | 1:A:903:TRP:NE1   | 2.51                     | 0.44              |
| 1:A:1101:ILE:HD13 | 1:A:1154:PHE:CE2  | 2.52                     | 0.44              |
| 2:B:307:ASN:C     | 2:B:325:LEU:HD12  | 2.42                     | 0.44              |
| 3:C:216:GLN:O     | 3:C:219:PHE:HB3   | 2.17                     | 0.44              |
| 5:F:203:LYS:O     | 5:F:207:VAL:HG23  | 2.18                     | 0.44              |
| 1:S:599:SER:CB    | 1:S:1009:GLY:HA3  | 2.47                     | 0.44              |
| 1:S:777:SER:C     | 1:S:779:PRO:HD2   | 2.42                     | 0.44              |
| 1:S:911:TRP:CE3   | 1:S:917:ARG:NH1   | 2.85                     | 0.44              |
| 1:S:1175:PRO:HD3  | 1:S:1204:ARG:NH1  | 2.32                     | 0.44              |
| 12:V:154:PHE:CD2  | 12:V:195:LYS:HB3  | 2.53                     | 0.44              |
| 12:V:463:LYS:HE2  | 12:V:502:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:403:ALA:O     | 1:A:407:LEU:HB2   | 2.18                     | 0.44              |
| 2:B:266:ILE:HG22  | 2:B:267:SER:O     | 2.18                     | 0.44              |
| 2:B:315:SER:O     | 2:B:315:SER:OG    | 2.33                     | 0.44              |
| 3:C:163:GLU:O     | 3:C:164:ASN:C     | 2.60                     | 0.44              |
| 4:E:106:ARG:N     | 4:E:107:PRO:CD    | 2.81                     | 0.44              |
| 4:E:282:LYS:CD    | 4:E:282:LYS:N     | 2.81                     | 0.44              |
| 6:H:99:SER:O      | 6:H:103:VAL:HG23  | 2.18                     | 0.44              |
| 6:H:146:GLN:NE2   | 6:H:150:TRP:CE2   | 2.86                     | 0.44              |
| 7:L:126:LEU:HD12  | 7:L:127:VAL:N     | 2.32                     | 0.44              |
| 2:O:265:LEU:HD22  | 2:O:311:VAL:HG21  | 1.98                     | 0.44              |
| 2:O:624:LEU:HD12  | 2:O:624:LEU:HA    | 1.78                     | 0.44              |
| 8:Q:466:SER:HB2   | 7:M:108:PRO:HD3   | 1.98                     | 0.44              |
| 1:S:992:HIS:CD2   | 1:S:1073:ARG:NH2  | 2.85                     | 0.44              |
| 11:U:867:PRO:O    | 11:U:923:TYR:OH   | 2.33                     | 0.44              |
| 12:V:383:VAL:CG2  | 12:V:420:THR:HG23 | 2.47                     | 0.44              |
| 12:V:686:LEU:HD12 | 12:V:757:ASP:HA   | 1.98                     | 0.44              |
| 1:A:1117:ARG:O    | 1:A:1324:PRO:HB3  | 2.17                     | 0.44              |
| 2:B:324:LYS:O     | 2:B:325:LEU:C     | 2.60                     | 0.44              |
| 2:B:651:LEU:HD23  | 2:B:655:PHE:CE1   | 2.52                     | 0.44              |
| 3:C:55:MET:CE     | 3:C:60:VAL:HG21   | 2.48                     | 0.44              |
| 3:C:490:LEU:O     | 3:C:493:ASN:HB2   | 2.17                     | 0.44              |
| 4:E:368:PHE:O     | 4:E:371:ARG:N     | 2.50                     | 0.44              |
| 4:E:501:GLN:CG    | 4:E:502:ALA:N     | 2.80                     | 0.44              |
| 5:F:292:GLY:HA3   | 6:G:485:ARG:HD2   | 2.00                     | 0.44              |
| 6:G:147:ALA:CA    | 6:G:159:LEU:HD11  | 2.47                     | 0.44              |
| 6:H:23:LEU:HD22   | 6:H:46:ALA:HA     | 1.99                     | 0.44              |
| 7:L:69:ILE:O      | 7:L:73:ARG:HG2    | 2.18                     | 0.44              |
| 8:P:604:TYR:HB3   | 8:P:638:VAL:HG23  | 1.99                     | 0.44              |
| 1:S:847:LYS:HG2   | 1:S:848:PHE:CD2   | 2.53                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 7:M:214:LEU:HD12  | 7:M:229:ALA:HB2    | 1.99                     | 0.44              |
| 10:X:9:ARG:O      | 10:X:13:MET:HB2    | 2.18                     | 0.44              |
| 11:U:439:GLU:HG2  | 11:U:440:ILE:N     | 2.32                     | 0.44              |
| 11:U:485:PHE:HA   | 11:U:488:LEU:HB2   | 1.99                     | 0.44              |
| 11:U:731:GLN:NE2  | 11:U:792:ALA:CB    | 2.81                     | 0.44              |
| 11:U:1033:PHE:CE2 | 11:U:1087:LEU:HD22 | 2.53                     | 0.44              |
| 12:V:208:GLN:O    | 12:V:212:ILE:HG12  | 2.17                     | 0.44              |
| 12:V:278:LEU:N    | 12:V:279:PRO:HD3   | 2.33                     | 0.44              |
| 12:V:1348:HIS:O   | 12:V:1350:ASP:N    | 2.49                     | 0.44              |
| 1:A:32:ARG:HB3    | 6:H:311:ASN:ND2    | 2.32                     | 0.44              |
| 3:C:12:TYR:CE2    | 3:C:63:ARG:HB3     | 2.53                     | 0.44              |
| 3:C:525:PHE:CD1   | 3:C:525:PHE:C      | 2.95                     | 0.44              |
| 4:E:108:SER:O     | 4:E:109:LEU:HD23   | 2.18                     | 0.44              |
| 4:E:467:GLU:O     | 4:E:471:VAL:HG23   | 2.18                     | 0.44              |
| 6:G:505:SER:HB3   | 6:G:508:ALA:H      | 1.83                     | 0.44              |
| 6:H:104:LEU:HD13  | 6:H:121:LEU:HD23   | 1.99                     | 0.44              |
| 7:L:4:THR:HB      | 7:L:81:MET:HB2     | 1.98                     | 0.44              |
| 7:L:338:LEU:HD11  | 7:L:342:LEU:CD1    | 2.46                     | 0.44              |
| 8:P:778:PRO:HD3   | 8:P:824:ASP:O      | 2.18                     | 0.44              |
| 1:S:430:ALA:O     | 1:S:434:VAL:HG23   | 2.16                     | 0.44              |
| 1:S:818:PHE:CD2   | 1:S:864:LEU:HD11   | 2.52                     | 0.44              |
| 10:X:49:GLY:HA3   | 10:X:147:THR:HG23  | 1.99                     | 0.44              |
| 11:U:506:LEU:HD13 | 11:U:513:MET:SD    | 2.58                     | 0.44              |
| 11:U:643:PRO:CB   | 11:U:721:PHE:CE1   | 3.01                     | 0.44              |
| 12:V:189:GLY:O    | 12:V:192:LEU:HB3   | 2.17                     | 0.44              |
| 12:V:452:SER:O    | 12:V:455:SER:OG    | 2.28                     | 0.44              |
| 2:B:146:HIS:O     | 2:B:148:LYS:N      | 2.51                     | 0.44              |
| 2:B:430:VAL:HG21  | 8:P:638:VAL:HG12   | 1.99                     | 0.44              |
| 2:B:480:TYR:CD1   | 2:B:480:TYR:N      | 2.86                     | 0.44              |
| 2:B:817:GLN:HE21  | 2:B:821:LYS:HE3    | 1.81                     | 0.44              |
| 5:F:313:SER:O     | 5:F:316:GLN:N      | 2.50                     | 0.44              |
| 6:G:267:LEU:HD21  | 1:S:60:LEU:HD11    | 1.99                     | 0.44              |
| 6:G:393:MET:CE    | 8:P:236:LEU:HD21   | 2.48                     | 0.44              |
| 6:H:368:LEU:HD11  | 6:H:404:LEU:HD11   | 2.00                     | 0.44              |
| 8:P:67:LEU:HD22   | 8:P:76:LEU:HD21    | 1.99                     | 0.44              |
| 1:S:342:MET:HB3   | 1:S:346:TRP:CZ2    | 2.52                     | 0.44              |
| 11:U:295:VAL:HA   | 11:U:301:SER:HB3   | 1.99                     | 0.44              |
| 12:V:368:ILE:HD13 | 12:V:381:ASP:HB3   | 2.00                     | 0.44              |
| 5:F:168:GLU:OE2   | 5:F:211:GLN:HG3    | 2.18                     | 0.44              |
| 7:L:354:ILE:HG23  | 7:L:367:THR:CG2    | 2.47                     | 0.44              |
| 2:O:17:CYS:SG     | 2:O:331:ASP:HB2    | 2.58                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:O:287:VAL:HB     | 2:O:301:VAL:HG22   | 1.99                     | 0.44              |
| 8:P:269:ASN:N      | 8:P:269:ASN:HD22   | 2.16                     | 0.44              |
| 1:S:566:VAL:CG1    | 1:S:1273:LEU:HD21  | 2.48                     | 0.44              |
| 7:M:69:ILE:O       | 7:M:73:ARG:HG2     | 2.18                     | 0.44              |
| 11:U:324:ASP:N     | 11:U:324:ASP:OD1   | 2.50                     | 0.44              |
| 11:U:1081:ALA:HB3  | 11:U:1082:PRO:HD3  | 2.00                     | 0.44              |
| 11:U:1146:HIS:ND1  | 11:U:1204:HIS:HB3  | 2.33                     | 0.44              |
| 12:V:298:ILE:O     | 12:V:302:ARG:HB2   | 2.17                     | 0.44              |
| 12:V:801:CYS:SG    | 12:V:802:GLN:N     | 2.91                     | 0.44              |
| 12:V:1306:LEU:HG   | 12:V:1367:LEU:HD13 | 1.99                     | 0.44              |
| 12:V:1355:GLN:HE22 | 14:Z:35:DG:H5"     | 1.82                     | 0.44              |
| 12:V:1357:VAL:HB   | 12:V:1358:PRO:HD3  | 2.00                     | 0.44              |
| 1:A:197:LEU:HD22   | 1:A:206:VAL:HG13   | 1.99                     | 0.43              |
| 2:B:665:PRO:HD2    | 2:B:741:ASN:HB2    | 1.99                     | 0.43              |
| 4:E:71:GLU:HB3     | 4:E:72:PRO:CD      | 2.48                     | 0.43              |
| 5:F:346:ILE:HG23   | 5:F:347:TRP:CD2    | 2.53                     | 0.43              |
| 6:G:447:TYR:CD1    | 6:G:488:PRO:O      | 2.71                     | 0.43              |
| 2:O:423:TYR:CD1    | 8:Q:606:LEU:HD12   | 2.51                     | 0.43              |
| 8:P:423:LEU:HA     | 8:P:428:ARG:O      | 2.17                     | 0.43              |
| 8:P:704:SER:N      | 8:P:791:SER:O      | 2.51                     | 0.43              |
| 1:S:218:CYS:HB3    | 1:S:294:ILE:HA     | 1.99                     | 0.43              |
| 1:S:731:MET:SD     | 1:S:779:PRO:HB3    | 2.58                     | 0.43              |
| 7:M:21:SER:O       | 7:M:23:THR:N       | 2.51                     | 0.43              |
| 7:M:165:TYR:CE1    | 7:M:175:ALA:HB3    | 2.53                     | 0.43              |
| 11:U:448:VAL:O     | 11:U:456:ILE:CD1   | 2.66                     | 0.43              |
| 11:U:473:VAL:HG13  | 11:U:474:LEU:N     | 2.33                     | 0.43              |
| 11:U:504:GLN:HE22  | 11:U:543:LEU:HA    | 1.83                     | 0.43              |
| 1:A:744:PRO:HB2    | 1:A:747:ALA:HB3    | 2.00                     | 0.43              |
| 2:B:534:PRO:HA     | 2:B:572:LYS:NZ     | 2.32                     | 0.43              |
| 4:E:381:ARG:N      | 12:V:272:SER:HA    | 2.32                     | 0.43              |
| 8:P:170:ILE:CG2    | 8:P:259:VAL:HG22   | 2.47                     | 0.43              |
| 8:Q:42:GLU:OE1     | 8:Q:62:ASP:N       | 2.50                     | 0.43              |
| 1:S:393:VAL:HA     | 1:S:396:LEU:HD12   | 2.00                     | 0.43              |
| 11:U:86:VAL:HA     | 11:U:89:ILE:HG22   | 2.00                     | 0.43              |
| 11:U:499:LEU:HG    | 11:U:500:LEU:HD23  | 2.00                     | 0.43              |
| 1:A:313:THR:HA     | 1:A:316:LEU:HB3    | 2.01                     | 0.43              |
| 1:A:1232:PHE:O     | 1:A:1236:GLN:OE1   | 2.36                     | 0.43              |
| 2:B:669:LEU:HB3    | 2:B:712:PRO:O      | 2.19                     | 0.43              |
| 3:C:492:LEU:HD13   | 3:C:522:ILE:HG23   | 1.99                     | 0.43              |
| 4:E:517:GLU:HB2    | 4:E:518:PRO:HD3    | 2.01                     | 0.43              |
| 7:L:109:GLN:NE2    | 7:L:113:SER:OG     | 2.51                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 8:P:276:HIS:ND1    | 8:P:277:HIS:N     | 2.66                     | 0.43              |
| 8:Q:284:PHE:HB3    | 8:Q:315:PHE:CD2   | 2.54                     | 0.43              |
| 7:M:343:ARG:NH1    | 12:V:472:GLU:OE1  | 2.51                     | 0.43              |
| 11:U:2:ASP:HB2     | 11:U:35:ASN:HD21  | 1.84                     | 0.43              |
| 11:U:422:GLY:HA2   | 11:U:425:ILE:HD12 | 1.99                     | 0.43              |
| 12:V:342:CYS:HA    | 12:V:345:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:1034:LEU:CD2   | 1:S:1188:HIS:CD2  | 3.02                     | 0.43              |
| 1:A:1331:LEU:HB3   | 1:A:1332:PRO:HD3  | 2.01                     | 0.43              |
| 1:A:1368:PHE:CZ    | 1:A:1393:VAL:HG22 | 2.54                     | 0.43              |
| 2:B:725:THR:CG2    | 2:O:485:ASP:HA    | 2.49                     | 0.43              |
| 3:C:315:ILE:CG2    | 3:C:399:HIS:HA    | 2.46                     | 0.43              |
| 3:C:365:LEU:CD1    | 3:C:422:LEU:HD11  | 2.48                     | 0.43              |
| 5:F:116:PHE:HD1    | 5:F:130:GLN:HG3   | 1.82                     | 0.43              |
| 6:G:367:TYR:HD1    | 6:G:370:LEU:HD23  | 1.83                     | 0.43              |
| 6:H:450:LEU:O      | 6:H:453:SER:OG    | 2.34                     | 0.43              |
| 2:O:519:ARG:HG3    | 2:O:520:LEU:N     | 2.33                     | 0.43              |
| 8:P:35:VAL:HG12    | 8:P:47:TYR:HB2    | 1.99                     | 0.43              |
| 8:P:74:ARG:C       | 8:P:90:LEU:HG     | 2.44                     | 0.43              |
| 8:P:253:VAL:HG23   | 8:P:272:VAL:CA    | 2.48                     | 0.43              |
| 8:P:321:MET:HG2    | 8:P:322:LEU:N     | 2.33                     | 0.43              |
| 11:U:1:MET:HE1     | 11:U:24:LEU:HD11  | 1.99                     | 0.43              |
| 11:U:717:GLU:C     | 11:U:719:GLU:H    | 2.26                     | 0.43              |
| 11:U:1254:ILE:O    | 11:U:1258:GLU:HG2 | 2.19                     | 0.43              |
| 12:V:752:ILE:O     | 12:V:755:LEU:N    | 2.45                     | 0.43              |
| 12:V:1013:VAL:HG21 | 12:V:1075:TRP:CE3 | 2.53                     | 0.43              |
| 3:C:207:HIS:CD2    | 4:E:93:ILE:HG13   | 2.53                     | 0.43              |
| 7:L:66:TYR:O       | 7:L:70:VAL:HG23   | 2.18                     | 0.43              |
| 8:P:474:LYS:O      | 8:P:477:ASP:HB2   | 2.18                     | 0.43              |
| 10:X:40:GLY:HA3    | 10:X:46:TYR:O     | 2.19                     | 0.43              |
| 12:V:686:LEU:HD13  | 12:V:811:LYS:HG2  | 2.01                     | 0.43              |
| 2:B:240:VAL:HG13   | 2:B:256:LEU:HD11  | 1.99                     | 0.43              |
| 2:B:742:CYS:O      | 8:P:684:ARG:HD2   | 2.18                     | 0.43              |
| 3:C:188:VAL:CG2    | 3:C:219:PHE:HA    | 2.48                     | 0.43              |
| 2:O:83:SER:HA      | 2:O:89:ILE:O      | 2.18                     | 0.43              |
| 8:P:143:LEU:HB2    | 8:P:197:LEU:HD11  | 2.01                     | 0.43              |
| 8:P:361:SER:CB     | 8:P:398:SER:O     | 2.66                     | 0.43              |
| 8:Q:348:LEU:HD11   | 8:Q:363:PRO:HD3   | 2.00                     | 0.43              |
| 1:S:328:LEU:HD22   | 1:S:389:VAL:CG2   | 2.48                     | 0.43              |
| 1:S:772:GLN:NE2    | 9:W:95:TRP:CZ2    | 2.87                     | 0.43              |
| 1:S:1262:PHE:CD2   | 1:S:1319:LEU:HD22 | 2.54                     | 0.43              |
| 7:M:121:LEU:HD11   | 7:M:183:LEU:HB3   | 2.01                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 11:U:537:VAL:CG1   | 11:U:541:LEU:HD12 | 2.49                     | 0.43              |
| 11:U:854:LYS:HD2   | 11:U:914:LYS:HB3  | 2.01                     | 0.43              |
| 12:V:1186:LEU:HD21 | 12:V:1234:PHE:CE2 | 2.54                     | 0.43              |
| 1:A:59:ALA:O       | 1:A:63:GLU:HG3    | 2.19                     | 0.43              |
| 1:A:327:ILE:HG23   | 1:A:388:ARG:HD3   | 2.01                     | 0.43              |
| 1:A:361:ARG:HB3    | 1:A:365:MET:HE1   | 2.00                     | 0.43              |
| 2:B:242:ILE:HG12   | 2:B:243:CYS:N     | 2.34                     | 0.43              |
| 2:B:480:TYR:HE2    | 2:B:622:LEU:HD11  | 1.82                     | 0.43              |
| 3:C:501:GLY:O      | 3:C:502:HIS:ND1   | 2.52                     | 0.43              |
| 6:G:458:LEU:HD22   | 6:G:596:TYR:CD2   | 2.53                     | 0.43              |
| 6:H:128:ALA:HA     | 6:H:131:LEU:HD12  | 2.00                     | 0.43              |
| 6:H:362:ASP:OD1    | 6:H:362:ASP:N     | 2.52                     | 0.43              |
| 8:Q:764:VAL:HG23   | 8:Q:791:SER:HB2   | 1.99                     | 0.43              |
| 1:S:598:ASP:O      | 1:S:601:VAL:HB    | 2.19                     | 0.43              |
| 1:S:661:ARG:HD2    | 9:W:78:PHE:CE1    | 2.53                     | 0.43              |
| 1:S:1266:MET:HE3   | 1:S:1323:ALA:CB   | 2.49                     | 0.43              |
| 11:U:283:TYR:CE1   | 12:V:483:SER:HB2  | 2.54                     | 0.43              |
| 11:U:1045:LEU:HG   | 11:U:1072:PHE:CZ  | 2.54                     | 0.43              |
| 11:U:1155:SER:HA   | 11:U:1159:VAL:CG1 | 2.48                     | 0.43              |
| 12:V:277:ASP:C     | 12:V:279:PRO:HD2  | 2.44                     | 0.43              |
| 12:V:463:LYS:CE    | 12:V:502:LEU:HD11 | 2.49                     | 0.43              |
| 1:A:82:SER:HB2     | 1:A:116:MET:HE1   | 2.01                     | 0.43              |
| 1:A:101:GLN:CG     | 1:A:112:LEU:HD13  | 2.49                     | 0.43              |
| 1:A:152:ALA:HA     | 1:A:155:LEU:HD12  | 2.00                     | 0.43              |
| 1:A:286:GLN:CB     | 1:A:288:GLU:HG3   | 2.48                     | 0.43              |
| 6:G:468:ALA:O      | 6:G:469:GLN:C     | 2.61                     | 0.43              |
| 6:H:122:TRP:HE1    | 6:H:146:GLN:CD    | 2.27                     | 0.43              |
| 6:H:300:LEU:HD13   | 6:H:359:ARG:HD2   | 2.00                     | 0.43              |
| 7:L:144:SER:OG     | 7:L:146:ARG:NH2   | 2.51                     | 0.43              |
| 2:O:13:GLU:CD      | 2:O:353:CYS:SG    | 3.02                     | 0.43              |
| 8:P:148:ALA:O      | 8:P:180:PRO:HD2   | 2.19                     | 0.43              |
| 8:Q:141:VAL:HG22   | 8:Q:154:LEU:CD1   | 2.48                     | 0.43              |
| 8:Q:339:ARG:HE     | 7:M:101:LEU:HD21  | 1.84                     | 0.43              |
| 1:S:113:SER:HB2    | 1:S:155:LEU:HD13  | 2.01                     | 0.43              |
| 7:M:215:GLU:CB     | 7:M:227:ARG:HB3   | 2.49                     | 0.43              |
| 11:U:466:ILE:HG22  | 11:U:467:VAL:HG23 | 2.01                     | 0.43              |
| 11:U:668:LEU:HD11  | 11:U:749:VAL:HG13 | 2.00                     | 0.43              |
| 11:U:1050:SER:HB3  | 11:U:1144:PHE:CD1 | 2.53                     | 0.43              |
| 12:V:94:GLU:OE1    | 12:V:94:GLU:N     | 2.49                     | 0.43              |
| 12:V:1128:PHE:CE2  | 12:V:1181:GLN:HB3 | 2.52                     | 0.43              |
| 1:A:262:MET:HB3    | 1:A:264:GLN:HE21  | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1079:LYS:HG3  | 1:A:1130:ILE:HD13 | 2.01                     | 0.43              |
| 2:B:13:GLU:HG2    | 2:B:26:GLN:HG3    | 2.01                     | 0.43              |
| 5:F:289:LEU:HD13  | 6:G:484:PHE:CE2   | 2.54                     | 0.43              |
| 6:H:54:LEU:O      | 6:H:58:GLN:HG2    | 2.19                     | 0.43              |
| 2:O:79:CYS:CB     | 2:O:94:ILE:HD13   | 2.49                     | 0.43              |
| 2:O:706:THR:O     | 2:O:717:LEU:HD12  | 2.19                     | 0.43              |
| 8:Q:325:LYS:HE2   | 8:Q:384:GLU:HB3   | 2.01                     | 0.43              |
| 1:S:935:LEU:O     | 1:S:938:GLU:HB2   | 2.19                     | 0.43              |
| 1:S:1056:LEU:O    | 1:S:1071:ARG:NH2  | 2.51                     | 0.43              |
| 7:M:311:TYR:HE2   | 10:X:6:ARG:HD3    | 1.65                     | 0.43              |
| 11:U:430:PHE:CE2  | 11:U:466:ILE:HG23 | 2.54                     | 0.43              |
| 12:V:611:THR:HG23 | 12:V:651:TRP:CZ2  | 2.54                     | 0.43              |
| 1:A:504:ARG:HE    | 1:A:504:ARG:N     | 2.16                     | 0.43              |
| 1:A:1075:LEU:HD12 | 1:A:1119:PHE:CD2  | 2.54                     | 0.43              |
| 2:B:298:PHE:CD2   | 2:B:362:LEU:HD12  | 2.54                     | 0.43              |
| 2:B:682:CYS:HA    | 2:B:693:PHE:O     | 2.19                     | 0.43              |
| 3:C:223:VAL:O     | 3:C:224:ASN:C     | 2.60                     | 0.43              |
| 3:C:283:GLN:O     | 3:C:284:ALA:C     | 2.62                     | 0.43              |
| 3:C:348:LEU:HD23  | 3:C:396:LEU:HD22  | 2.00                     | 0.43              |
| 4:E:19:TRP:CD1    | 4:E:19:TRP:C      | 2.96                     | 0.43              |
| 6:G:257:ARG:NE    | 6:G:285:GLU:OE2   | 2.44                     | 0.43              |
| 6:G:382:PHE:CE2   | 8:P:139:VAL:HG21  | 2.54                     | 0.43              |
| 2:O:218:GLU:HB2   | 2:O:220:GLN:HE21  | 1.83                     | 0.43              |
| 8:Q:563:ILE:CG2   | 8:Q:564:THR:N     | 2.82                     | 0.43              |
| 7:M:212:TRP:HA    | 7:M:295:ARG:HD3   | 2.01                     | 0.43              |
| 11:U:746:VAL:HG11 | 11:U:781:LEU:HD11 | 2.00                     | 0.43              |
| 11:U:962:PHE:CD1  | 11:U:988:VAL:HG11 | 2.54                     | 0.43              |
| 1:A:364:VAL:N     | 2:B:817:GLN:HE22  | 2.17                     | 0.42              |
| 1:A:1372:ASP:CG   | 1:A:1372:ASP:O    | 2.61                     | 0.42              |
| 3:C:64:PHE:N      | 3:C:65:PRO:HD2    | 2.34                     | 0.42              |
| 4:E:387:LEU:HD12  | 4:E:391:CYS:SG    | 2.59                     | 0.42              |
| 7:L:320:PRO:HA    | 7:L:333:PHE:O     | 2.19                     | 0.42              |
| 2:O:184:LEU:HD23  | 2:O:184:LEU:HA    | 1.85                     | 0.42              |
| 8:Q:488:GLU:HA    | 8:Q:491:ASN:HD22  | 1.83                     | 0.42              |
| 1:S:1368:PHE:CD2  | 1:S:1396:ILE:HD11 | 2.54                     | 0.42              |
| 11:U:134:LEU:HD21 | 11:U:160:LEU:HD23 | 2.01                     | 0.42              |
| 11:U:530:LEU:CD1  | 11:U:598:GLN:HE21 | 2.31                     | 0.42              |
| 11:U:758:PHE:N    | 11:U:771:ILE:HD11 | 2.34                     | 0.42              |
| 1:A:108:PRO:CG    | 1:A:111:ILE:HD12  | 2.49                     | 0.42              |
| 1:A:327:ILE:O     | 1:A:388:ARG:HD2   | 2.19                     | 0.42              |
| 1:A:818:PHE:HE2   | 1:A:861:SER:HG    | 1.60                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:669:LEU:C     | 2:B:669:LEU:HD12 | 2.44                     | 0.42              |
| 4:E:332:GLN:C     | 4:E:334:PRO:HD2  | 2.44                     | 0.42              |
| 4:E:457:LEU:O     | 4:E:462:VAL:HG13 | 2.19                     | 0.42              |
| 6:G:280:GLY:N     | 6:G:281:PRO:HD2  | 2.34                     | 0.42              |
| 7:L:55:CYS:HB3    | 7:L:59:LEU:HB3   | 1.99                     | 0.42              |
| 7:L:226:ARG:HA    | 7:L:226:ARG:HD3  | 1.90                     | 0.42              |
| 8:P:288:LEU:N     | 8:P:311:CYS:O    | 2.49                     | 0.42              |
| 8:P:341:TYR:C     | 8:P:342:CYS:HG   | 2.26                     | 0.42              |
| 8:P:470:SER:O     | 8:P:471:PHE:C    | 2.61                     | 0.42              |
| 8:Q:140:LEU:HD23  | 8:Q:155:PHE:HB2  | 2.01                     | 0.42              |
| 8:Q:312:LEU:HD23  | 8:Q:324:ILE:HD12 | 2.02                     | 0.42              |
| 8:Q:642:LEU:O     | 8:Q:643:SER:C    | 2.62                     | 0.42              |
| 1:S:485:SER:OG    | 1:S:521:LEU:HD13 | 2.20                     | 0.42              |
| 12:V:505:SER:O    | 12:V:508:MET:HB2 | 2.18                     | 0.42              |
| 1:A:476:PHE:CZ    | 1:A:480:LEU:HD11 | 2.54                     | 0.42              |
| 1:A:1407:ILE:N    | 1:A:1408:PRO:HD2 | 2.35                     | 0.42              |
| 2:B:592:LYS:HG2   | 2:B:593:PHE:N    | 2.34                     | 0.42              |
| 3:C:159:SER:O     | 3:C:162:ARG:HB2  | 2.19                     | 0.42              |
| 4:E:510:LEU:O     | 4:E:514:MET:HG2  | 2.19                     | 0.42              |
| 4:E:516:LEU:HD21  | 4:E:527:LEU:HD22 | 2.01                     | 0.42              |
| 6:G:384:PRO:HB2   | 6:G:385:PRO:HD2  | 2.01                     | 0.42              |
| 6:H:69:LEU:O      | 6:H:72:THR:HB    | 2.19                     | 0.42              |
| 2:O:422:SER:HA    | 7:M:18:GLN:NE2   | 2.35                     | 0.42              |
| 8:P:424:SER:HB3   | 8:P:428:ARG:HB2  | 2.02                     | 0.42              |
| 8:Q:227:LEU:HD11  | 8:Q:336:PRO:HD3  | 2.01                     | 0.42              |
| 1:S:589:THR:O     | 1:S:625:CYS:SG   | 2.76                     | 0.42              |
| 11:U:541:LEU:HD22 | 11:U:608:GLY:C   | 2.45                     | 0.42              |
| 11:U:665:ASP:OD1  | 11:U:665:ASP:N   | 2.52                     | 0.42              |
| 1:A:1063:TRP:CE2  | 1:A:1329:ARG:CZ  | 3.02                     | 0.42              |
| 1:A:1143:LEU:HD21 | 1:A:1185:TRP:CE3 | 2.53                     | 0.42              |
| 2:B:573:GLU:CD    | 2:B:573:GLU:N    | 2.77                     | 0.42              |
| 3:C:61:ILE:HA     | 3:C:64:PHE:HB2   | 2.01                     | 0.42              |
| 4:E:26:ALA:O      | 4:E:29:LEU:N     | 2.53                     | 0.42              |
| 6:G:416:LEU:HD22  | 1:S:22:TRP:CZ3   | 2.52                     | 0.42              |
| 7:L:307:CYS:CB    | 7:L:310:CYS:SG   | 3.06                     | 0.42              |
| 2:O:239:TYR:HD2   | 2:O:259:LEU:HD21 | 1.84                     | 0.42              |
| 2:O:627:LEU:O     | 2:O:630:GLY:N    | 2.53                     | 0.42              |
| 2:O:680:MET:SD    | 2:O:700:PHE:CD2  | 3.12                     | 0.42              |
| 2:O:777:ILE:HG21  | 8:Q:830:LEU:CD1  | 2.48                     | 0.42              |
| 8:P:451:ALA:O     | 8:P:454:LYS:HB3  | 2.19                     | 0.42              |
| 1:S:57:LEU:HD12   | 1:S:101:GLN:HE21 | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:S:1220:PRO:HG2   | 1:S:1226:SER:CB    | 2.50                     | 0.42              |
| 7:M:320:PRO:HA     | 7:M:333:PHE:O      | 2.19                     | 0.42              |
| 11:U:638:LYS:O     | 11:U:712:ARG:CZ    | 2.66                     | 0.42              |
| 11:U:1042:PRO:O    | 11:U:1046:LEU:HG   | 2.19                     | 0.42              |
| 11:U:1060:ILE:HG23 | 11:U:1215:TYR:CD1  | 2.54                     | 0.42              |
| 11:U:1213:ILE:HG21 | 11:U:1285:ARG:HH22 | 1.84                     | 0.42              |
| 12:V:1035:GLN:HB2  | 12:V:1124:SER:HB2  | 2.00                     | 0.42              |
| 1:A:832:PHE:O      | 1:A:835:LYS:HB3    | 2.20                     | 0.42              |
| 1:A:1034:LEU:HD22  | 1:S:1188:HIS:CG    | 2.55                     | 0.42              |
| 1:A:1118:ASN:HA    | 1:A:1324:PRO:HB3   | 2.00                     | 0.42              |
| 1:A:1331:LEU:N     | 1:A:1332:PRO:HD2   | 2.34                     | 0.42              |
| 4:E:429:LEU:HD21   | 4:E:437:MET:HG3    | 2.01                     | 0.42              |
| 4:E:516:LEU:HD12   | 4:E:531:LEU:HD22   | 2.01                     | 0.42              |
| 6:G:521:GLY:HA3    | 6:G:537:PHE:CZ     | 2.54                     | 0.42              |
| 6:H:72:THR:C       | 6:H:76:ASN:ND2     | 2.78                     | 0.42              |
| 6:H:134:GLU:OE1    | 6:H:134:GLU:HA     | 2.20                     | 0.42              |
| 6:H:537:PHE:O      | 6:H:540:SER:OG     | 2.30                     | 0.42              |
| 7:L:81:MET:O       | 7:L:81:MET:HE3     | 2.19                     | 0.42              |
| 2:O:308:ALA:N      | 2:O:325:LEU:HD12   | 2.34                     | 0.42              |
| 8:P:317:HIS:O      | 8:P:346:PRO:HA     | 2.18                     | 0.42              |
| 8:P:402:CYS:O      | 8:P:420:LEU:HB2    | 2.19                     | 0.42              |
| 8:Q:317:HIS:C      | 8:Q:319:GLY:H      | 2.27                     | 0.42              |
| 1:S:276:PHE:HE2    | 1:S:294:ILE:HG21   | 1.84                     | 0.42              |
| 1:S:346:TRP:CD2    | 1:S:387:GLN:HA     | 2.53                     | 0.42              |
| 7:M:8:LEU:CD2      | 7:M:25:TYR:HE2     | 2.30                     | 0.42              |
| 7:M:159:PRO:O      | 7:M:179:PRO:HA     | 2.18                     | 0.42              |
| 11:U:959:ILE:HG13  | 11:U:992:LEU:HD22  | 2.01                     | 0.42              |
| 11:U:1014:CYS:HA   | 11:U:1074:ILE:HD12 | 2.02                     | 0.42              |
| 12:V:657:CYS:SG    | 12:V:658:ASN:N     | 2.91                     | 0.42              |
| 1:A:823:THR:HG21   | 1:A:829:SER:HB2    | 2.02                     | 0.42              |
| 1:A:1142:CYS:SG    | 1:A:1152:VAL:HG22  | 2.60                     | 0.42              |
| 1:A:1200:LEU:O     | 1:A:1204:ARG:HG2   | 2.19                     | 0.42              |
| 2:B:18:TYR:HB3     | 2:B:23:LEU:HD11    | 2.02                     | 0.42              |
| 3:C:49:TYR:CE1     | 3:C:92:TRP:HB3     | 2.54                     | 0.42              |
| 3:C:367:THR:HG21   | 3:C:403:TRP:CH2    | 2.54                     | 0.42              |
| 4:E:121:ALA:C      | 4:E:123:GLN:N      | 2.77                     | 0.42              |
| 6:H:296:THR:HG21   | 6:H:357:THR:HG23   | 2.01                     | 0.42              |
| 2:O:423:TYR:CD1    | 8:Q:606:LEU:CD1    | 3.02                     | 0.42              |
| 2:O:483:ILE:O      | 2:O:484:ASP:C      | 2.63                     | 0.42              |
| 8:P:571:GLN:O      | 8:P:572:LEU:C      | 2.61                     | 0.42              |
| 8:Q:135:LEU:HD12   | 8:Q:140:LEU:HD12   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:S:767:GLN:HA    | 1:S:767:GLN:NE2   | 2.34                     | 0.42              |
| 1:S:1305:LEU:O    | 1:S:1308:LEU:HG   | 2.19                     | 0.42              |
| 11:U:169:TRP:HH2  | 11:U:194:VAL:HG23 | 1.84                     | 0.42              |
| 12:V:942:THR:HG21 | 12:V:1058:MET:HE1 | 2.01                     | 0.42              |
| 1:A:776:LEU:HD13  | 1:A:784:LEU:CD1   | 2.49                     | 0.42              |
| 3:C:145:TYR:O     | 3:C:146:TYR:C     | 2.62                     | 0.42              |
| 3:C:462:LEU:O     | 3:C:504:ILE:HD13  | 2.19                     | 0.42              |
| 7:L:126:LEU:HD12  | 7:L:127:VAL:H     | 1.85                     | 0.42              |
| 7:L:187:TYR:CE2   | 7:L:191:LEU:HD21  | 2.55                     | 0.42              |
| 2:O:592:LYS:HG3   | 2:O:622:LEU:O     | 2.19                     | 0.42              |
| 8:P:37:LEU:HD12   | 8:P:429:LEU:HD12  | 2.01                     | 0.42              |
| 8:Q:479:ARG:HA    | 8:Q:479:ARG:HD3   | 1.73                     | 0.42              |
| 7:M:361:TYR:CE1   | 10:X:101:SER:N    | 2.87                     | 0.42              |
| 11:U:660:LEU:HD13 | 11:U:745:LEU:HD11 | 2.02                     | 0.42              |
| 12:V:420:THR:HG22 | 12:V:428:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:1112:VAL:HG12 | 1:A:1165:LEU:HD12 | 2.02                     | 0.42              |
| 2:B:187:LYS:HG2   | 2:B:229:ILE:CG1   | 2.49                     | 0.42              |
| 2:B:281:PHE:CD2   | 2:B:307:ASN:CG    | 2.98                     | 0.42              |
| 6:G:81:ARG:CG     | 6:G:92:GLN:HE21   | 2.32                     | 0.42              |
| 6:G:160:ALA:O     | 6:G:164:GLU:HB2   | 2.20                     | 0.42              |
| 6:G:389:PRO:C     | 6:G:501:GLN:HE22  | 2.27                     | 0.42              |
| 6:G:588:SER:O     | 6:G:588:SER:OG    | 2.34                     | 0.42              |
| 1:S:61:LEU:HD11   | 1:S:116:MET:HE3   | 2.02                     | 0.42              |
| 1:S:1404:LEU:HD21 | 1:S:1432:VAL:HG22 | 2.02                     | 0.42              |
| 7:M:309:ILE:HG12  | 7:M:333:PHE:CD1   | 2.49                     | 0.42              |
| 11:U:653:THR:HG23 | 11:U:658:ILE:HG13 | 2.01                     | 0.42              |
| 12:V:1316:SER:HB2 | 12:V:1320:HIS:ND1 | 2.34                     | 0.42              |
| 1:A:156:LEU:HD22  | 1:A:163:ARG:HH22  | 1.85                     | 0.42              |
| 1:A:1363:LYS:HA   | 1:A:1366:GLN:OE1  | 2.20                     | 0.42              |
| 2:B:534:PRO:HA    | 2:B:572:LYS:CE    | 2.50                     | 0.42              |
| 2:B:580:ALA:C     | 2:B:581:VAL:CG2   | 2.92                     | 0.42              |
| 2:B:774:SER:HB2   | 8:P:834:HIS:ND1   | 2.35                     | 0.42              |
| 5:F:289:LEU:HD13  | 6:G:484:PHE:HE2   | 1.85                     | 0.42              |
| 7:L:313:TYR:CD1   | 7:L:320:PRO:HD2   | 2.55                     | 0.42              |
| 8:Q:746:VAL:HG13  | 8:Q:751:LEU:HB3   | 2.02                     | 0.42              |
| 1:S:145:LEU:HG    | 1:S:149:LEU:CD1   | 2.50                     | 0.42              |
| 11:U:430:PHE:CZ   | 11:U:466:ILE:HG23 | 2.55                     | 0.42              |
| 11:U:836:ASN:O    | 11:U:839:MET:HB2  | 2.19                     | 0.42              |
| 12:V:149:ILE:O    | 12:V:152:THR:HG22 | 2.19                     | 0.42              |
| 12:V:468:TYR:CD2  | 12:V:469:CYS:SG   | 3.02                     | 0.42              |
| 14:Z:36:DA:C2     | 14:Z:37:DA:C5     | 3.08                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:B:89:ILE:O     | 2:B:90:ASN:C      | 2.63                     | 0.42              |
| 2:B:667:TYR:HE2  | 6:H:239:LEU:HD11  | 1.85                     | 0.42              |
| 5:F:2:GLU:O      | 5:F:6:GLN:OE1     | 2.38                     | 0.42              |
| 5:F:341:VAL:HG13 | 5:F:344:LEU:HD12  | 2.01                     | 0.42              |
| 6:H:240:CYS:O    | 6:H:242:ARG:N     | 2.53                     | 0.42              |
| 7:L:42:LEU:HD12  | 7:L:46:LEU:HD23   | 2.02                     | 0.42              |
| 7:L:228:ILE:HD12 | 7:L:238:ILE:HD12  | 2.02                     | 0.42              |
| 2:O:478:ILE:O    | 2:O:478:ILE:HG23  | 2.20                     | 0.42              |
| 8:P:74:ARG:HA    | 8:P:74:ARG:HD3    | 1.80                     | 0.42              |
| 8:P:601:THR:HG22 | 8:P:641:PRO:HA    | 2.01                     | 0.42              |
| 1:S:346:TRP:CZ3  | 1:S:390:LEU:HD22  | 2.55                     | 0.42              |
| 1:S:998:TYR:HB3  | 1:S:1007:VAL:HG22 | 2.00                     | 0.42              |
| 1:S:1210:PHE:HE1 | 1:S:1246:LEU:HD23 | 1.85                     | 0.42              |
| 1:S:1261:PHE:HB2 | 1:S:1291:ILE:HG21 | 2.01                     | 0.42              |
| 7:M:12:CYS:O     | 7:M:13:PRO:C      | 2.62                     | 0.42              |
| 11:U:324:ASP:CG  | 11:U:325:GLN:N    | 2.78                     | 0.42              |
| 11:U:507:LEU:CD1 | 11:U:517:LEU:HD22 | 2.50                     | 0.42              |
| 12:V:1332:GLN:O  | 12:V:1335:THR:HB  | 2.20                     | 0.42              |
| 2:B:52:ARG:O     | 2:B:55:LYS:NZ     | 2.32                     | 0.41              |
| 2:B:365:ILE:HG23 | 2:B:367:TYR:CD2   | 2.54                     | 0.41              |
| 2:B:423:TYR:CE2  | 8:P:606:LEU:HB3   | 2.55                     | 0.41              |
| 4:E:501:GLN:HG3  | 4:E:502:ALA:N     | 2.35                     | 0.41              |
| 5:F:90:ASP:O     | 5:F:93:LEU:HB3    | 2.20                     | 0.41              |
| 6:G:296:THR:HG21 | 6:G:357:THR:HG21  | 2.01                     | 0.41              |
| 7:L:170:PRO:HD2  | 7:L:197:LEU:CD1   | 2.50                     | 0.41              |
| 8:P:37:LEU:CD1   | 8:P:429:LEU:HD12  | 2.50                     | 0.41              |
| 1:S:44:LYS:O     | 1:S:48:VAL:HG23   | 2.20                     | 0.41              |
| 1:S:1266:MET:CE  | 1:S:1323:ALA:HB1  | 2.50                     | 0.41              |
| 7:M:15:LEU:HD23  | 7:M:15:LEU:HA     | 1.89                     | 0.41              |
| 7:M:342:LEU:O    | 7:M:348:SER:CB    | 2.68                     | 0.41              |
| 11:U:113:ILE:O   | 11:U:117:ARG:HG2  | 2.20                     | 0.41              |
| 12:V:355:ARG:HA  | 12:V:391:THR:HG21 | 2.02                     | 0.41              |
| 1:A:814:VAL:HB   | 1:A:815:PRO:HD3   | 2.01                     | 0.41              |
| 2:B:525:ASN:HD22 | 2:B:525:ASN:N     | 2.17                     | 0.41              |
| 2:B:614:TYR:O    | 2:B:615:VAL:HG23  | 2.20                     | 0.41              |
| 4:E:380:SER:C    | 4:E:382:LEU:N     | 2.77                     | 0.41              |
| 6:G:306:LEU:CD2  | 6:G:346:THR:HG21  | 2.51                     | 0.41              |
| 6:H:69:LEU:O     | 6:H:73:VAL:HG23   | 2.20                     | 0.41              |
| 6:H:250:THR:HG22 | 6:H:282:PRO:CA    | 2.49                     | 0.41              |
| 6:H:388:PRO:N    | 6:H:389:PRO:CD    | 2.84                     | 0.41              |
| 2:O:306:ASN:O    | 2:O:324:LYS:N     | 2.52                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 8:P:311:CYS:SG    | 8:P:324:ILE:O      | 2.77                     | 0.41              |
| 8:Q:580:VAL:HG12  | 8:Q:582:LEU:HD23   | 2.01                     | 0.41              |
| 1:S:573:ILE:HG22  | 1:S:574:PHE:CE1    | 2.56                     | 0.41              |
| 1:S:1014:ASN:ND2  | 1:S:1016:ASP:OD2   | 2.53                     | 0.41              |
| 7:M:356:PHE:CE2   | 11:U:376:ASP:OD2   | 2.73                     | 0.41              |
| 11:U:676:ALA:O    | 11:U:680:ASN:ND2   | 2.53                     | 0.41              |
| 12:V:98:SER:HA    | 12:V:101:GLU:CD    | 2.44                     | 0.41              |
| 12:V:157:LEU:N    | 12:V:158:PRO:CD    | 2.83                     | 0.41              |
| 12:V:684:TYR:O    | 12:V:815:ARG:NH1   | 2.53                     | 0.41              |
| 1:A:818:PHE:CZ    | 1:A:861:SER:HB2    | 2.50                     | 0.41              |
| 2:B:134:LEU:CD1   | 2:B:142:ILE:HG23   | 2.51                     | 0.41              |
| 2:B:339:GLU:C     | 2:B:340:GLN:NE2    | 2.78                     | 0.41              |
| 2:B:494:THR:OG1   | 2:B:496:SER:OG     | 2.34                     | 0.41              |
| 6:G:97:GLN:HB2    | 6:G:118:LEU:HD21   | 2.03                     | 0.41              |
| 6:H:60:LEU:HD21   | 2:O:232:ALA:HB1    | 2.01                     | 0.41              |
| 2:O:426:LEU:HG    | 8:Q:490:MET:CE     | 2.50                     | 0.41              |
| 8:P:133:PHE:HE1   | 8:P:135:LEU:HD12   | 1.85                     | 0.41              |
| 8:P:472:LEU:O     | 8:P:476:VAL:HG23   | 2.19                     | 0.41              |
| 8:Q:288:LEU:HD11  | 8:Q:358:VAL:HG23   | 2.03                     | 0.41              |
| 1:S:1295:LEU:HD23 | 1:S:1300:ILE:HD12  | 2.02                     | 0.41              |
| 11:U:391:ASP:HB3  | 12:V:394:GLN:HE22  | 1.86                     | 0.41              |
| 11:U:757:ASN:ND2  | 11:U:770:ASP:OD2   | 2.53                     | 0.41              |
| 12:V:1137:LEU:O   | 12:V:1140:VAL:HG12 | 2.20                     | 0.41              |
| 2:B:83:SER:HB2    | 8:P:15:CYS:CB      | 2.50                     | 0.41              |
| 3:C:361:ARG:HD2   | 3:C:538:ILE:HD12   | 2.02                     | 0.41              |
| 4:E:109:LEU:HD12  | 4:E:114:LEU:HD21   | 2.02                     | 0.41              |
| 4:E:319:CYS:SG    | 4:E:327:LEU:HD22   | 2.60                     | 0.41              |
| 6:G:340:CYS:O     | 8:P:263:SER:OG     | 2.33                     | 0.41              |
| 6:G:447:TYR:CE1   | 6:G:488:PRO:O      | 2.72                     | 0.41              |
| 8:P:13:GLY:HA2    | 8:P:427:GLY:O      | 2.20                     | 0.41              |
| 8:P:249:GLN:HG2   | 8:P:277:HIS:NE2    | 2.35                     | 0.41              |
| 8:P:678:THR:OG1   | 8:P:679:PHE:N      | 2.54                     | 0.41              |
| 11:U:986:VAL:O    | 11:U:990:THR:OG1   | 2.31                     | 0.41              |
| 12:V:523:ASN:C    | 12:V:524:ILE:HG13  | 2.44                     | 0.41              |
| 1:A:652:GLN:O     | 1:A:683:ARG:NH1    | 2.53                     | 0.41              |
| 1:A:728:GLN:O     | 1:A:731:MET:HB2    | 2.20                     | 0.41              |
| 2:B:418:ILE:HA    | 2:B:421:LYS:HB3    | 2.03                     | 0.41              |
| 2:B:680:MET:HE1   | 2:B:700:PHE:CE2    | 2.56                     | 0.41              |
| 4:E:135:ALA:O     | 4:E:138:GLU:HB2    | 2.21                     | 0.41              |
| 4:E:464:MET:HE3   | 4:E:500:TYR:CE2    | 2.55                     | 0.41              |
| 5:F:301:ASP:O     | 5:F:302:VAL:C      | 2.64                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:H:55:HIS:O      | 2:O:264:GLN:NE2   | 2.54                     | 0.41              |
| 2:O:176:ILE:HD12  | 2:O:182:VAL:HG21  | 2.01                     | 0.41              |
| 2:O:655:PHE:CD2   | 2:O:721:SER:C     | 2.98                     | 0.41              |
| 8:Q:177:SER:HB2   | 8:Q:274:ILE:HD13  | 2.02                     | 0.41              |
| 8:Q:517:LEU:O     | 8:Q:518:GLN:C     | 2.63                     | 0.41              |
| 1:S:955:HIS:HB3   | 1:S:1020:ARG:HE   | 1.86                     | 0.41              |
| 1:A:1174:TRP:HB3  | 1:A:1204:ARG:NH1  | 2.36                     | 0.41              |
| 4:E:130:ASP:OD1   | 4:E:130:ASP:C     | 2.64                     | 0.41              |
| 4:E:418:GLU:O     | 4:E:421:CYS:HB2   | 2.20                     | 0.41              |
| 5:F:323:ASP:OD1   | 5:F:324:LYS:N     | 2.54                     | 0.41              |
| 8:P:284:PHE:CD1   | 8:P:350:ALA:HB3   | 2.56                     | 0.41              |
| 1:S:568:VAL:CG2   | 1:S:1069:LEU:HD11 | 2.50                     | 0.41              |
| 1:S:570:GLU:OE1   | 1:S:574:PHE:CD2   | 2.74                     | 0.41              |
| 1:S:772:GLN:HE22  | 9:W:95:TRP:HH2    | 1.65                     | 0.41              |
| 1:S:989:MET:HG3   | 1:S:1055:ARG:HD3  | 2.02                     | 0.41              |
| 1:S:1139:LEU:CD2  | 1:S:1181:LEU:HD22 | 2.50                     | 0.41              |
| 12:V:139:LEU:HA   | 12:V:142:ILE:HD12 | 2.02                     | 0.41              |
| 1:A:60:LEU:HG     | 6:H:263:GLN:HB3   | 2.03                     | 0.41              |
| 1:A:1109:PHE:HA   | 1:A:1163:CYS:SG   | 2.60                     | 0.41              |
| 1:A:1336:TYR:HB3  | 1:A:1395:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:583:SER:OG    | 2:B:584:LEU:N     | 2.54                     | 0.41              |
| 2:B:723:ASN:ND2   | 2:B:725:THR:HG23  | 2.36                     | 0.41              |
| 3:C:145:TYR:C     | 3:C:147:PRO:CD    | 2.93                     | 0.41              |
| 3:C:150:LEU:O     | 3:C:151:LYS:C     | 2.63                     | 0.41              |
| 3:C:188:VAL:HB    | 3:C:189:PRO:HD3   | 2.03                     | 0.41              |
| 3:C:200:VAL:HA    | 3:C:203:LEU:HD12  | 2.03                     | 0.41              |
| 3:C:370:HIS:NE2   | 3:C:374:LEU:HD11  | 2.35                     | 0.41              |
| 6:G:64:VAL:N      | 6:G:65:PRO:HD2    | 2.36                     | 0.41              |
| 6:G:415:THR:HG21  | 1:S:21:ALA:HB1    | 2.03                     | 0.41              |
| 6:G:479:CYS:O     | 6:G:482:LEU:N     | 2.53                     | 0.41              |
| 7:L:307:CYS:HB3   | 7:L:310:CYS:SG    | 2.59                     | 0.41              |
| 2:O:777:ILE:HD13  | 8:Q:830:LEU:HD13  | 2.03                     | 0.41              |
| 8:P:131:CYS:SG    | 8:P:145:GLN:HB2   | 2.61                     | 0.41              |
| 8:P:284:PHE:CD2   | 8:P:284:PHE:C     | 2.98                     | 0.41              |
| 7:M:155:LYS:NZ    | 7:M:162:SER:O     | 2.48                     | 0.41              |
| 7:M:297:ILE:HG22  | 7:M:298:LEU:HD22  | 2.02                     | 0.41              |
| 7:M:352:PHE:CD1   | 11:U:439:GLU:OE1  | 2.73                     | 0.41              |
| 11:U:137:LEU:HD11 | 11:U:156:CYS:HB3  | 2.03                     | 0.41              |
| 11:U:865:GLN:O    | 11:U:867:PRO:HD3  | 2.21                     | 0.41              |
| 12:V:51:LEU:HA    | 12:V:54:ILE:HD12  | 2.02                     | 0.41              |
| 12:V:408:ARG:C    | 12:V:410:GLY:H    | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:240:GLN:HA    | 1:A:311:ILE:HD11  | 2.01                     | 0.41              |
| 1:A:275:ILE:HG12  | 1:A:330:HIS:CE1   | 2.56                     | 0.41              |
| 1:A:1075:LEU:CD1  | 1:A:1119:PHE:HD2  | 2.33                     | 0.41              |
| 2:B:170:ILE:HG23  | 2:B:170:ILE:O     | 2.21                     | 0.41              |
| 2:B:357:PHE:CD2   | 2:B:357:PHE:C     | 2.98                     | 0.41              |
| 2:B:745:LYS:HG2   | 2:B:746:ASN:N     | 2.32                     | 0.41              |
| 3:C:509:ILE:HD13  | 3:C:509:ILE:N     | 2.36                     | 0.41              |
| 4:E:31:GLN:HB3    | 7:L:341:TRP:CH2   | 2.56                     | 0.41              |
| 8:P:465:ILE:CG2   | 8:P:466:SER:N     | 2.82                     | 0.41              |
| 8:P:801:HIS:O     | 8:P:805:VAL:HG23  | 2.21                     | 0.41              |
| 1:S:419:PHE:CE2   | 1:S:463:HIS:ND1   | 2.89                     | 0.41              |
| 1:S:1056:LEU:HD13 | 1:S:1115:GLU:HG3  | 2.02                     | 0.41              |
| 1:S:1326:GLN:HA   | 1:S:1329:ARG:HH21 | 1.86                     | 0.41              |
| 11:U:670:CYS:O    | 11:U:674:CYS:SG   | 2.76                     | 0.41              |
| 11:U:1052:ASP:OD1 | 11:U:1071:HIS:HB2 | 2.21                     | 0.41              |
| 1:A:517:ARG:O     | 1:A:521:LEU:HG    | 2.21                     | 0.41              |
| 1:A:713:PRO:O     | 1:A:717:MET:HG2   | 2.21                     | 0.41              |
| 1:A:1103:ALA:O    | 1:A:1104:ARG:HB2  | 2.20                     | 0.41              |
| 2:B:74:LEU:CD2    | 2:B:98:LYS:HD3    | 2.51                     | 0.41              |
| 2:B:82:VAL:O      | 2:B:83:SER:OG     | 2.36                     | 0.41              |
| 2:B:124:PHE:O     | 2:B:124:PHE:CD1   | 2.74                     | 0.41              |
| 2:B:487:LEU:HB2   | 2:B:584:LEU:HD23  | 2.02                     | 0.41              |
| 2:B:522:LYS:O     | 2:B:582:THR:OG1   | 2.28                     | 0.41              |
| 2:B:530:LEU:HD12  | 2:B:649:PHE:CE1   | 2.56                     | 0.41              |
| 2:B:725:THR:O     | 2:B:728:PHE:N     | 2.54                     | 0.41              |
| 4:E:396:TYR:HB3   | 4:E:397:PRO:HD3   | 2.03                     | 0.41              |
| 4:E:485:THR:OG1   | 4:E:520:THR:HG21  | 2.21                     | 0.41              |
| 6:G:448:CYS:O     | 6:G:448:CYS:SG    | 2.79                     | 0.41              |
| 6:G:483:LEU:HD21  | 6:G:512:LEU:HD23  | 2.03                     | 0.41              |
| 6:G:484:PHE:HZ    | 6:G:543:MET:HE1   | 1.86                     | 0.41              |
| 6:H:266:LEU:O     | 6:H:270:VAL:HG23  | 2.20                     | 0.41              |
| 7:L:107:PRO:N     | 7:L:108:PRO:CD    | 2.84                     | 0.41              |
| 7:L:113:SER:O     | 7:L:116:GLU:HB3   | 2.20                     | 0.41              |
| 7:L:169:PHE:CZ    | 7:L:193:ALA:CB    | 3.04                     | 0.41              |
| 7:L:256:ALA:HB1   | 7:L:258:HIS:CE1   | 2.56                     | 0.41              |
| 7:L:313:TYR:CZ    | 7:L:319:ILE:HG23  | 2.52                     | 0.41              |
| 2:O:170:ILE:O     | 2:O:170:ILE:CG2   | 2.69                     | 0.41              |
| 2:O:524:GLN:HE21  | 2:O:524:GLN:HB3   | 1.48                     | 0.41              |
| 8:P:51:GLY:O      | 8:P:53:LEU:N      | 2.54                     | 0.41              |
| 8:P:236:LEU:O     | 8:P:237:GLN:C     | 2.63                     | 0.41              |
| 8:P:486:LEU:O     | 8:P:489:ALA:HB3   | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:P:593:ASP:O     | 8:P:594:LEU:HD23  | 2.20                     | 0.41              |
| 8:P:709:LYS:HB2   | 8:P:879:ILE:HG22  | 2.03                     | 0.41              |
| 8:P:717:ALA:HB3   | 8:P:815:GLN:NE2   | 2.36                     | 0.41              |
| 8:Q:337:GLU:OE2   | 8:Q:339:ARG:NH1   | 2.54                     | 0.41              |
| 1:S:346:TRP:CZ2   | 1:S:387:GLN:HG2   | 2.55                     | 0.41              |
| 1:S:874:ARG:O     | 1:S:875:LEU:HD23  | 2.21                     | 0.41              |
| 7:M:55:CYS:HB3    | 7:M:59:LEU:HB3    | 2.02                     | 0.41              |
| 11:U:286:GLY:O    | 11:U:290:VAL:HG23 | 2.21                     | 0.41              |
| 12:V:305:LEU:HD22 | 12:V:307:LEU:HD21 | 2.03                     | 0.41              |
| 12:V:571:LYS:NZ   | 12:V:620:CYS:O    | 2.43                     | 0.41              |
| 12:V:611:THR:HG23 | 12:V:651:TRP:CH2  | 2.56                     | 0.41              |
| 12:V:1276:SER:O   | 12:V:1280:ASN:ND2 | 2.53                     | 0.41              |
| 1:A:281:LEU:HA    | 1:A:286:GLN:HE21  | 1.86                     | 0.41              |
| 2:B:279:LEU:HA    | 2:B:280:PRO:HD3   | 1.87                     | 0.41              |
| 2:B:338:THR:O     | 2:B:340:GLN:NE2   | 2.53                     | 0.41              |
| 2:B:773:LEU:CA    | 2:B:838:ILE:HG21  | 2.50                     | 0.41              |
| 2:B:818:ARG:NH1   | 2:B:821:LYS:HD3   | 2.36                     | 0.41              |
| 4:E:374:SER:O     | 4:E:376:THR:HG23  | 2.21                     | 0.41              |
| 6:G:360:ALA:HB1   | 6:G:406:GLN:HB2   | 2.02                     | 0.41              |
| 6:G:458:LEU:O     | 6:G:459:GLN:C     | 2.64                     | 0.41              |
| 6:H:191:LEU:HD12  | 6:H:192:ASP:N     | 2.36                     | 0.41              |
| 2:O:61:SER:OG     | 2:O:62:THR:N      | 2.53                     | 0.41              |
| 2:O:391:VAL:HB    | 2:O:392:PRO:HD3   | 2.03                     | 0.41              |
| 2:O:478:ILE:HD11  | 2:O:620:VAL:HG13  | 2.02                     | 0.41              |
| 2:O:533:ASN:O     | 2:O:572:LYS:NZ    | 2.41                     | 0.41              |
| 8:P:504:ARG:O     | 8:P:532:SER:OG    | 2.32                     | 0.41              |
| 8:P:679:PHE:O     | 8:P:682:THR:OG1   | 2.38                     | 0.41              |
| 8:Q:510:THR:HG21  | 8:Q:598:VAL:CG2   | 2.50                     | 0.41              |
| 8:Q:733:LEU:HD13  | 8:Q:751:LEU:O     | 2.21                     | 0.41              |
| 7:M:32:GLN:O      | 7:M:34:ARG:HG3    | 2.21                     | 0.41              |
| 11:U:281:LEU:O    | 12:V:523:ASN:ND2  | 2.54                     | 0.41              |
| 11:U:924:GLN:N    | 11:U:925:PRO:CD   | 2.84                     | 0.41              |
| 1:A:486:PRO:HG2   | 1:A:489:LEU:HD12  | 2.03                     | 0.40              |
| 1:A:770:ARG:HD3   | 1:A:821:LEU:HA    | 2.03                     | 0.40              |
| 2:B:332:ASP:OD1   | 2:B:335:GLY:N     | 2.53                     | 0.40              |
| 6:H:37:LEU:O      | 6:H:41:GLN:HG3    | 2.21                     | 0.40              |
| 6:H:310:LEU:HD11  | 6:H:340:CYS:SG    | 2.60                     | 0.40              |
| 7:L:313:TYR:CE1   | 7:L:319:ILE:CG2   | 2.92                     | 0.40              |
| 2:O:130:MET:CE    | 2:O:134:LEU:HD22  | 2.51                     | 0.40              |
| 8:P:43:LEU:HB3    | 8:P:45:TYR:CE1    | 2.56                     | 0.40              |
| 8:P:124:ILE:O     | 8:P:125:LEU:C     | 2.63                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:Q:366:LEU:HD23  | 8:Q:366:LEU:C     | 2.46                     | 0.40              |
| 8:Q:451:ALA:O     | 8:Q:455:ILE:HG12  | 2.21                     | 0.40              |
| 1:S:349:ALA:HB2   | 1:S:682:GLU:HG3   | 2.03                     | 0.40              |
| 10:X:58:PRO:HD3   | 10:X:67:GLN:NE2   | 2.36                     | 0.40              |
| 11:U:651:ILE:HD13 | 11:U:738:LYS:CG   | 2.51                     | 0.40              |
| 11:U:668:LEU:HB3  | 11:U:752:VAL:HG11 | 2.02                     | 0.40              |
| 11:U:843:VAL:O    | 11:U:846:ALA:N    | 2.54                     | 0.40              |
| 12:V:72:GLN:NE2   | 12:V:132:SER:OG   | 2.55                     | 0.40              |
| 12:V:816:LEU:HD11 | 12:V:935:ILE:HD13 | 2.02                     | 0.40              |
| 1:A:1224:TRP:CH2  | 1:A:1225:LEU:HD13 | 2.56                     | 0.40              |
| 3:C:125:LEU:C     | 3:C:127:PHE:H     | 2.28                     | 0.40              |
| 4:E:408:GLN:HE21  | 4:E:444:LEU:HD13  | 1.86                     | 0.40              |
| 7:L:303:PHE:O     | 7:L:305:MET:N     | 2.54                     | 0.40              |
| 2:O:592:LYS:CG    | 2:O:593:PHE:N     | 2.84                     | 0.40              |
| 2:O:843:ALA:HB3   | 8:Q:809:GLN:HE21  | 1.86                     | 0.40              |
| 1:S:933:LEU:HD21  | 1:S:984:LEU:HD12  | 2.03                     | 0.40              |
| 1:S:1092:GLY:HA2  | 1:S:1104:ARG:HH21 | 1.86                     | 0.40              |
| 7:M:56:SER:HG     | 7:M:59:LEU:H      | 1.70                     | 0.40              |
| 11:U:94:MET:HE1   | 11:U:128:GLU:O    | 2.21                     | 0.40              |
| 11:U:308:PHE:O    | 11:U:311:ALA:HB3  | 2.21                     | 0.40              |
| 11:U:970:LEU:O    | 11:U:1019:ARG:NH2 | 2.54                     | 0.40              |
| 12:V:252:LEU:HD23 | 12:V:252:LEU:HA   | 1.99                     | 0.40              |
| 2:B:362:LEU:O     | 8:P:468:ARG:NH2   | 2.54                     | 0.40              |
| 4:E:280:LEU:O     | 4:E:285:GLN:NE2   | 2.54                     | 0.40              |
| 6:G:39:ARG:NH2    | 6:G:319:PRO:O     | 2.54                     | 0.40              |
| 6:G:414:LEU:HD21  | 6:G:459:GLN:O     | 2.21                     | 0.40              |
| 8:P:505:PRO:HA    | 8:P:533:SER:HB3   | 2.03                     | 0.40              |
| 8:P:640:LEU:HA    | 8:P:641:PRO:HD3   | 1.81                     | 0.40              |
| 1:S:910:LEU:C     | 1:S:910:LEU:HD23  | 2.46                     | 0.40              |
| 10:X:24:CYS:SG    | 10:X:34:LEU:HB3   | 2.62                     | 0.40              |
| 11:U:504:GLN:HE22 | 11:U:543:LEU:HD23 | 1.86                     | 0.40              |
| 11:U:1206:THR:O   | 11:U:1209:CYS:HB2 | 2.21                     | 0.40              |
| 1:A:822:LEU:HD12  | 1:A:867:LYS:CE    | 2.52                     | 0.40              |
| 5:F:116:PHE:CD1   | 5:F:130:GLN:HG3   | 2.57                     | 0.40              |
| 7:L:98:ARG:HD2    | 7:L:101:LEU:HD11  | 2.03                     | 0.40              |
| 2:O:426:LEU:CD1   | 8:Q:490:MET:HE1   | 2.48                     | 0.40              |
| 8:P:48:ASP:HB3    | 8:P:53:LEU:HD23   | 2.03                     | 0.40              |
| 8:P:86:TYR:CD1    | 8:P:86:TYR:N      | 2.89                     | 0.40              |
| 8:P:353:GLY:O     | 8:P:354:GLY:C     | 2.64                     | 0.40              |
| 8:P:423:LEU:HD12  | 8:P:423:LEU:C     | 2.47                     | 0.40              |
| 8:Q:508:CYS:SG    | 8:Q:600:CYS:SG    | 3.17                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:S:765:LEU:HD21   | 1:S:787:LEU:CD2   | 2.51                     | 0.40              |
| 1:S:974:ASP:O      | 1:S:975:GLY:C     | 2.65                     | 0.40              |
| 7:M:90:LEU:C       | 7:M:90:LEU:HD23   | 2.47                     | 0.40              |
| 10:X:57:ILE:HG23   | 10:X:61:TYR:CG    | 2.57                     | 0.40              |
| 11:U:385:LEU:HA    | 11:U:388:ILE:HD12 | 2.03                     | 0.40              |
| 11:U:434:GLU:HG3   | 11:U:437:ARG:NH2  | 2.37                     | 0.40              |
| 11:U:1259:GLN:HE21 | 12:V:1358:PRO:HG2 | 1.86                     | 0.40              |
| 12:V:347:PHE:HA    | 12:V:350:ILE:HD12 | 2.03                     | 0.40              |
| 12:V:479:THR:O     | 12:V:483:SER:CB   | 2.68                     | 0.40              |
| 1:A:1027:ASP:OD2   | 1:S:1184:ARG:NH2  | 2.43                     | 0.40              |
| 1:A:1174:TRP:N     | 1:A:1175:PRO:CD   | 2.85                     | 0.40              |
| 1:A:1213:PRO:O     | 1:A:1215:ALA:N    | 2.54                     | 0.40              |
| 1:A:1315:LEU:O     | 1:A:1319:LEU:HD12 | 2.22                     | 0.40              |
| 4:E:332:GLN:HA     | 4:E:334:PRO:HD2   | 2.03                     | 0.40              |
| 6:G:84:LEU:O       | 6:G:86:GLN:HG2    | 2.22                     | 0.40              |
| 2:O:520:LEU:HD22   | 8:P:518:GLN:O     | 2.22                     | 0.40              |
| 8:P:11:LEU:HD13    | 8:P:429:LEU:HD22  | 2.02                     | 0.40              |
| 8:P:193:PHE:HD1    | 8:P:193:PHE:HA    | 1.76                     | 0.40              |
| 8:P:424:SER:CB     | 8:P:428:ARG:HB2   | 2.51                     | 0.40              |
| 8:P:528:VAL:HA     | 8:P:579:GLU:HA    | 2.03                     | 0.40              |
| 1:S:975:GLY:O      | 1:S:976:ASP:C     | 2.64                     | 0.40              |
| 7:M:8:LEU:HD21     | 7:M:25:TYR:CE2    | 2.48                     | 0.40              |
| 11:U:90:ILE:HD13   | 11:U:93:LEU:HD12  | 2.02                     | 0.40              |
| 12:V:261:LYS:O     | 12:V:265:LEU:HG   | 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%) | 1060 (91%) | 92 (8%) | 8 (1%)   | 18 54       |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 1   | S     | 1224/1477 (83%)   | 1101 (90%) | 110 (9%)   | 13 (1%)  | 11          | 45  |
| 2   | B     | 685/884 (78%)     | 572 (84%)  | 100 (15%)  | 13 (2%)  | 6           | 32  |
| 2   | O     | 685/884 (78%)     | 587 (86%)  | 81 (12%)   | 17 (2%)  | 4           | 27  |
| 3   | C     | 546/583 (94%)     | 472 (86%)  | 66 (12%)   | 8 (2%)   | 8           | 38  |
| 4   | E     | 411/555 (74%)     | 366 (89%)  | 45 (11%)   | 0        | 100         | 100 |
| 5   | F     | 336/399 (84%)     | 295 (88%)  | 40 (12%)   | 1 (0%)   | 36          | 71  |
| 6   | G     | 567/641 (88%)     | 497 (88%)  | 65 (12%)   | 5 (1%)   | 14          | 49  |
| 6   | H     | 532/641 (83%)     | 473 (89%)  | 55 (10%)   | 4 (1%)   | 16          | 52  |
| 7   | L     | 368/394 (93%)     | 328 (89%)  | 37 (10%)   | 3 (1%)   | 16          | 52  |
| 7   | M     | 368/394 (93%)     | 328 (89%)  | 33 (9%)    | 7 (2%)   | 6           | 32  |
| 8   | P     | 726/906 (80%)     | 608 (84%)  | 90 (12%)   | 28 (4%)  | 2           | 19  |
| 8   | Q     | 732/906 (81%)     | 624 (85%)  | 94 (13%)   | 14 (2%)  | 6           | 32  |
| 9   | W     | 21/39 (54%)       | 12 (57%)   | 3 (14%)    | 6 (29%)  | 0           | 0   |
| 10  | X     | 151/197 (77%)     | 140 (93%)  | 10 (7%)    | 1 (1%)   | 18          | 54  |
| 11  | U     | 1180/1328 (89%)   | 1051 (89%) | 116 (10%)  | 13 (1%)  | 11          | 45  |
| 12  | V     | 1131/1451 (78%)   | 1042 (92%) | 80 (7%)    | 9 (1%)   | 16          | 52  |
| All | All   | 10823/13156 (82%) | 9556 (88%) | 1117 (10%) | 150 (1%) | 11          | 39  |

All (150) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 287 | GLU  |
| 1   | A     | 737 | ALA  |
| 2   | B     | 132 | ASP  |
| 2   | B     | 133 | GLY  |
| 2   | B     | 138 | ASN  |
| 2   | B     | 147 | VAL  |
| 3   | C     | 4   | ASP  |
| 3   | C     | 84  | ASP  |
| 6   | H     | 192 | ASP  |
| 6   | H     | 241 | PRO  |
| 6   | H     | 242 | ARG  |
| 2   | O     | 70  | GLU  |
| 2   | O     | 83  | SER  |
| 2   | O     | 147 | VAL  |
| 2   | O     | 249 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | O     | 354  | LEU  |
| 8   | P     | 857  | ALA  |
| 8   | Q     | 50   | GLU  |
| 8   | Q     | 539  | GLN  |
| 8   | Q     | 557  | ASP  |
| 8   | Q     | 649  | MET  |
| 1   | S     | 288  | GLU  |
| 1   | S     | 972  | GLY  |
| 1   | S     | 975  | GLY  |
| 9   | W     | 80   | VAL  |
| 11  | U     | 451  | ARG  |
| 11  | U     | 548  | LYS  |
| 11  | U     | 598  | GLN  |
| 1   | A     | 972  | GLY  |
| 1   | A     | 1214 | GLU  |
| 2   | B     | 196  | CYS  |
| 6   | G     | 192  | ASP  |
| 2   | O     | 251  | GLN  |
| 2   | O     | 314  | GLU  |
| 2   | O     | 324  | LYS  |
| 2   | O     | 631  | LYS  |
| 2   | O     | 636  | PHE  |
| 2   | O     | 637  | PRO  |
| 8   | P     | 137  | ASP  |
| 8   | P     | 383  | PRO  |
| 8   | P     | 518  | GLN  |
| 8   | P     | 595  | PRO  |
| 8   | P     | 781  | PRO  |
| 8   | Q     | 63   | GLN  |
| 8   | Q     | 397  | ALA  |
| 8   | Q     | 643  | SER  |
| 1   | S     | 592  | VAL  |
| 1   | S     | 689  | GLY  |
| 1   | S     | 947  | SER  |
| 1   | S     | 1003 | ASN  |
| 9   | W     | 86   | SER  |
| 7   | M     | 176  | SER  |
| 7   | M     | 296  | ALA  |
| 11  | U     | 374  | SER  |
| 11  | U     | 456  | ILE  |
| 11  | U     | 724  | ASP  |
| 1   | A     | 26   | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 670  | ARG  |
| 2   | B     | 140  | PRO  |
| 2   | B     | 314  | GLU  |
| 2   | B     | 316  | PHE  |
| 2   | B     | 325  | LEU  |
| 2   | B     | 637  | PRO  |
| 3   | C     | 2    | ALA  |
| 3   | C     | 128  | ASP  |
| 3   | C     | 173  | ARG  |
| 7   | L     | 304  | THR  |
| 2   | O     | 138  | ASN  |
| 8   | P     | 62   | ASP  |
| 8   | P     | 63   | GLN  |
| 8   | P     | 148  | ALA  |
| 8   | P     | 426  | LYS  |
| 8   | P     | 550  | SER  |
| 8   | P     | 557  | ASP  |
| 8   | P     | 642  | LEU  |
| 8   | P     | 782  | ILE  |
| 8   | Q     | 518  | GLN  |
| 9   | W     | 85   | PHE  |
| 7   | M     | 103  | ALA  |
| 7   | M     | 351  | SER  |
| 11  | U     | 1042 | PRO  |
| 12  | V     | 412  | ILE  |
| 12  | V     | 1348 | HIS  |
| 1   | A     | 484  | GLU  |
| 6   | G     | 445  | LEU  |
| 7   | L     | 227  | ARG  |
| 2   | O     | 223  | LEU  |
| 2   | O     | 325  | LEU  |
| 2   | O     | 495  | SER  |
| 8   | P     | 15   | CYS  |
| 8   | P     | 161  | GLY  |
| 8   | P     | 332  | GLY  |
| 8   | P     | 354  | GLY  |
| 8   | P     | 385  | GLU  |
| 8   | P     | 387  | PRO  |
| 8   | P     | 549  | THR  |
| 8   | P     | 875  | HIS  |
| 8   | Q     | 607  | ARG  |
| 8   | Q     | 757  | VAL  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S     | 1104 | ARG  |
| 7   | M     | 22   | LYS  |
| 11  | U     | 361  | SER  |
| 11  | U     | 975  | GLU  |
| 12  | V     | 166  | ASN  |
| 2   | B     | 82   | VAL  |
| 2   | B     | 273  | PRO  |
| 6   | G     | 343  | GLN  |
| 6   | H     | 61   | PRO  |
| 2   | O     | 140  | PRO  |
| 2   | O     | 711  | THR  |
| 8   | P     | 66   | HIS  |
| 8   | P     | 166  | PRO  |
| 8   | P     | 372  | SER  |
| 8   | P     | 822  | ALA  |
| 1   | S     | 338  | ASP  |
| 1   | S     | 1023 | GLU  |
| 10  | X     | 62   | PRO  |
| 11  | U     | 449  | VAL  |
| 11  | U     | 1019 | ARG  |
| 12  | V     | 296  | GLU  |
| 12  | V     | 411  | CYS  |
| 12  | V     | 466  | ASP  |
| 12  | V     | 753  | ASP  |
| 12  | V     | 1167 | TRP  |
| 12  | V     | 1349 | GLN  |
| 1   | A     | 314  | ASP  |
| 2   | B     | 711  | THR  |
| 3   | C     | 23   | ASP  |
| 3   | C     | 169  | PHE  |
| 3   | C     | 382  | GLN  |
| 6   | G     | 261  | ASN  |
| 8   | P     | 641  | PRO  |
| 8   | Q     | 92   | HIS  |
| 8   | Q     | 148  | ALA  |
| 8   | Q     | 758  | ALA  |
| 1   | S     | 564  | ILE  |
| 1   | S     | 1002 | GLU  |
| 9   | W     | 82   | PRO  |
| 7   | M     | 215  | GLU  |
| 11  | U     | 341  | LEU  |
| 11  | U     | 729  | PHE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 5   | F     | 23   | VAL  |
| 8   | Q     | 727  | PRO  |
| 1   | S     | 1331 | LEU  |
| 8   | P     | 6    | PRO  |
| 7   | M     | 216  | PRO  |
| 9   | W     | 74   | PRO  |
| 9   | W     | 92   | PRO  |
| 6   | G     | 242  | ARG  |
| 7   | L     | 106  | 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%) | 916 (89%)  | 118 (11%) | 5           | 21 |
| 1   | S     | 1092/1282 (85%) | 1007 (92%) | 85 (8%)   | 11          | 33 |
| 2   | B     | 644/810 (80%)   | 557 (86%)  | 87 (14%)  | 4           | 17 |
| 2   | O     | 641/810 (79%)   | 576 (90%)  | 65 (10%)  | 7           | 24 |
| 3   | C     | 480/507 (95%)   | 452 (94%)  | 28 (6%)   | 18          | 41 |
| 4   | E     | 358/467 (77%)   | 298 (83%)  | 60 (17%)  | 2           | 12 |
| 5   | F     | 288/336 (86%)   | 268 (93%)  | 20 (7%)   | 14          | 37 |
| 6   | G     | 483/538 (90%)   | 425 (88%)  | 58 (12%)  | 5           | 19 |
| 6   | H     | 454/538 (84%)   | 396 (87%)  | 58 (13%)  | 4           | 18 |
| 7   | L     | 334/354 (94%)   | 313 (94%)  | 21 (6%)   | 16          | 39 |
| 7   | M     | 334/354 (94%)   | 310 (93%)  | 24 (7%)   | 13          | 35 |
| 8   | P     | 627/749 (84%)   | 543 (87%)  | 84 (13%)  | 4           | 17 |
| 8   | Q     | 630/749 (84%)   | 567 (90%)  | 63 (10%)  | 7           | 24 |
| 9   | W     | 22/22 (100%)    | 20 (91%)   | 2 (9%)    | 9           | 29 |
| 10  | X     | 136/175 (78%)   | 130 (96%)  | 6 (4%)    | 25          | 48 |
| 11  | U     | 1092/1204 (91%) | 1041 (95%) | 51 (5%)   | 23          | 46 |
| 12  | V     | 1067/1324 (81%) | 1038 (97%) | 29 (3%)   | 39          | 60 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| All | All   | 9716/11501 (84%) | 8857 (91%) | 859 (9%) | 11          | 30 |

All (859) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 55  | GLN  |
| 1   | A     | 56  | ASP  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 105 | LEU  |
| 1   | A     | 109 | VAL  |
| 1   | A     | 137 | LEU  |
| 1   | A     | 139 | VAL  |
| 1   | A     | 147 | SER  |
| 1   | A     | 148 | LEU  |
| 1   | A     | 149 | LEU  |
| 1   | A     | 150 | GLU  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 176 | SER  |
| 1   | A     | 178 | LEU  |
| 1   | A     | 182 | VAL  |
| 1   | A     | 191 | VAL  |
| 1   | A     | 193 | LEU  |
| 1   | A     | 217 | LEU  |
| 1   | A     | 236 | SER  |
| 1   | A     | 239 | VAL  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 267 | VAL  |
| 1   | A     | 268 | ASP  |
| 1   | A     | 273 | MET  |
| 1   | A     | 274 | LEU  |
| 1   | A     | 289 | SER  |
| 1   | A     | 313 | THR  |
| 1   | A     | 318 | ARG  |
| 1   | A     | 333 | VAL  |
| 1   | A     | 342 | MET  |
| 1   | A     | 354 | LEU  |
| 1   | A     | 369 | GLU  |
| 1   | A     | 371 | LEU  |
| 1   | A     | 383 | GLU  |
| 1   | A     | 390 | LEU  |
| 1   | A     | 396 | LEU  |
| 1   | A     | 402 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 405 | GLN  |
| 1   | A     | 434 | VAL  |
| 1   | A     | 446 | LEU  |
| 1   | A     | 456 | PHE  |
| 1   | A     | 462 | TYR  |
| 1   | A     | 465 | CYS  |
| 1   | A     | 468 | LYS  |
| 1   | A     | 479 | GLU  |
| 1   | A     | 491 | VAL  |
| 1   | A     | 494 | LEU  |
| 1   | A     | 507 | LEU  |
| 1   | A     | 653 | LEU  |
| 1   | A     | 665 | THR  |
| 1   | A     | 671 | ASP  |
| 1   | A     | 723 | LEU  |
| 1   | A     | 741 | ARG  |
| 1   | A     | 762 | LEU  |
| 1   | A     | 767 | GLN  |
| 1   | A     | 775 | SER  |
| 1   | A     | 782 | LEU  |
| 1   | A     | 787 | LEU  |
| 1   | A     | 817 | LEU  |
| 1   | A     | 821 | LEU  |
| 1   | A     | 822 | LEU  |
| 1   | A     | 826 | THR  |
| 1   | A     | 852 | SER  |
| 1   | A     | 860 | LEU  |
| 1   | A     | 861 | SER  |
| 1   | A     | 877 | SER  |
| 1   | A     | 881 | GLN  |
| 1   | A     | 900 | SER  |
| 1   | A     | 904 | GLN  |
| 1   | A     | 923 | GLU  |
| 1   | A     | 928 | THR  |
| 1   | A     | 930 | GLN  |
| 1   | A     | 948 | ASP  |
| 1   | A     | 949 | THR  |
| 1   | A     | 953 | ASP  |
| 1   | A     | 961 | GLU  |
| 1   | A     | 964 | LEU  |
| 1   | A     | 968 | SER  |
| 1   | A     | 984 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 992  | HIS  |
| 1   | A     | 1012 | THR  |
| 1   | A     | 1014 | ASN  |
| 1   | A     | 1024 | MET  |
| 1   | A     | 1030 | LEU  |
| 1   | A     | 1031 | GLN  |
| 1   | A     | 1032 | GLN  |
| 1   | A     | 1060 | THR  |
| 1   | A     | 1069 | LEU  |
| 1   | A     | 1073 | ARG  |
| 1   | A     | 1076 | LEU  |
| 1   | A     | 1077 | MET  |
| 1   | A     | 1080 | ARG  |
| 1   | A     | 1098 | GLU  |
| 1   | A     | 1101 | ILE  |
| 1   | A     | 1126 | LEU  |
| 1   | A     | 1130 | ILE  |
| 1   | A     | 1139 | LEU  |
| 1   | A     | 1155 | ILE  |
| 1   | A     | 1163 | CYS  |
| 1   | A     | 1188 | HIS  |
| 1   | A     | 1190 | GLN  |
| 1   | A     | 1191 | SER  |
| 1   | A     | 1208 | SER  |
| 1   | A     | 1231 | HIS  |
| 1   | A     | 1241 | ASN  |
| 1   | A     | 1253 | ARG  |
| 1   | A     | 1269 | LEU  |
| 1   | A     | 1301 | SER  |
| 1   | A     | 1305 | LEU  |
| 1   | A     | 1310 | GLU  |
| 1   | A     | 1320 | LEU  |
| 1   | A     | 1345 | ASP  |
| 1   | A     | 1367 | LEU  |
| 1   | A     | 1391 | ASN  |
| 1   | A     | 1395 | LEU  |
| 1   | A     | 1413 | LYS  |
| 1   | A     | 1425 | ARG  |
| 1   | A     | 1427 | ASP  |
| 2   | B     | 9    | SER  |
| 2   | B     | 13   | GLU  |
| 2   | B     | 17   | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 28  | SER  |
| 2   | B     | 40  | THR  |
| 2   | B     | 47  | ARG  |
| 2   | B     | 66  | THR  |
| 2   | B     | 68  | LYS  |
| 2   | B     | 70  | GLU  |
| 2   | B     | 90  | ASN  |
| 2   | B     | 94  | ILE  |
| 2   | B     | 98  | LYS  |
| 2   | B     | 112 | LEU  |
| 2   | B     | 143 | LEU  |
| 2   | B     | 155 | SER  |
| 2   | B     | 187 | LYS  |
| 2   | B     | 197 | THR  |
| 2   | B     | 225 | ASP  |
| 2   | B     | 226 | ILE  |
| 2   | B     | 237 | VAL  |
| 2   | B     | 246 | GLU  |
| 2   | B     | 252 | LEU  |
| 2   | B     | 254 | ILE  |
| 2   | B     | 256 | LEU  |
| 2   | B     | 281 | PHE  |
| 2   | B     | 285 | CYS  |
| 2   | B     | 287 | VAL  |
| 2   | B     | 311 | VAL  |
| 2   | B     | 323 | GLU  |
| 2   | B     | 326 | SER  |
| 2   | B     | 329 | LEU  |
| 2   | B     | 331 | ASP  |
| 2   | B     | 341 | VAL  |
| 2   | B     | 349 | LEU  |
| 2   | B     | 353 | CYS  |
| 2   | B     | 354 | LEU  |
| 2   | B     | 364 | LYS  |
| 2   | B     | 396 | THR  |
| 2   | B     | 398 | LEU  |
| 2   | B     | 401 | CYS  |
| 2   | B     | 410 | GLN  |
| 2   | B     | 412 | LEU  |
| 2   | B     | 417 | LYS  |
| 2   | B     | 420 | SER  |
| 2   | B     | 422 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 428 | ASN  |
| 2   | B     | 471 | SER  |
| 2   | B     | 483 | ILE  |
| 2   | B     | 492 | LYS  |
| 2   | B     | 494 | THR  |
| 2   | B     | 498 | LYS  |
| 2   | B     | 504 | VAL  |
| 2   | B     | 505 | THR  |
| 2   | B     | 506 | LEU  |
| 2   | B     | 507 | SER  |
| 2   | B     | 510 | MET  |
| 2   | B     | 517 | ARG  |
| 2   | B     | 523 | CYS  |
| 2   | B     | 535 | PHE  |
| 2   | B     | 572 | LYS  |
| 2   | B     | 573 | GLU  |
| 2   | B     | 577 | ILE  |
| 2   | B     | 602 | MET  |
| 2   | B     | 604 | ARG  |
| 2   | B     | 605 | GLU  |
| 2   | B     | 609 | CYS  |
| 2   | B     | 619 | ARG  |
| 2   | B     | 622 | LEU  |
| 2   | B     | 631 | LYS  |
| 2   | B     | 638 | LYS  |
| 2   | B     | 663 | THR  |
| 2   | B     | 671 | SER  |
| 2   | B     | 677 | LEU  |
| 2   | B     | 678 | GLU  |
| 2   | B     | 706 | THR  |
| 2   | B     | 716 | ILE  |
| 2   | B     | 726 | VAL  |
| 2   | B     | 734 | LEU  |
| 2   | B     | 742 | CYS  |
| 2   | B     | 748 | LYS  |
| 2   | B     | 752 | GLU  |
| 2   | B     | 763 | LEU  |
| 2   | B     | 780 | HIS  |
| 2   | B     | 836 | ARG  |
| 2   | B     | 838 | ILE  |
| 2   | B     | 847 | LEU  |
| 2   | B     | 857 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 10  | CYS  |
| 3   | C     | 17  | GLN  |
| 3   | C     | 115 | GLN  |
| 3   | C     | 123 | SER  |
| 3   | C     | 126 | ARG  |
| 3   | C     | 150 | LEU  |
| 3   | C     | 153 | MET  |
| 3   | C     | 155 | LEU  |
| 3   | C     | 156 | SER  |
| 3   | C     | 162 | ARG  |
| 3   | C     | 182 | SER  |
| 3   | C     | 190 | LEU  |
| 3   | C     | 193 | LEU  |
| 3   | C     | 194 | THR  |
| 3   | C     | 195 | ASP  |
| 3   | C     | 205 | ILE  |
| 3   | C     | 224 | ASN  |
| 3   | C     | 241 | CYS  |
| 3   | C     | 245 | ARG  |
| 3   | C     | 266 | ARG  |
| 3   | C     | 306 | ASP  |
| 3   | C     | 319 | THR  |
| 3   | C     | 338 | LYS  |
| 3   | C     | 350 | MET  |
| 3   | C     | 396 | LEU  |
| 3   | C     | 398 | ILE  |
| 3   | C     | 488 | ARG  |
| 3   | C     | 509 | ILE  |
| 4   | E     | 12  | GLU  |
| 4   | E     | 21  | GLN  |
| 4   | E     | 23  | GLU  |
| 4   | E     | 30  | LEU  |
| 4   | E     | 41  | ARG  |
| 4   | E     | 44  | LEU  |
| 4   | E     | 68  | CYS  |
| 4   | E     | 83  | LEU  |
| 4   | E     | 86  | LEU  |
| 4   | E     | 87  | LEU  |
| 4   | E     | 88  | LEU  |
| 4   | E     | 91  | PRO  |
| 4   | E     | 94  | CYS  |
| 4   | E     | 98  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 100 | SER  |
| 4   | E     | 112 | SER  |
| 4   | E     | 123 | GLN  |
| 4   | E     | 125 | LEU  |
| 4   | E     | 141 | ARG  |
| 4   | E     | 142 | ARG  |
| 4   | E     | 148 | THR  |
| 4   | E     | 155 | PRO  |
| 4   | E     | 157 | SER  |
| 4   | E     | 160 | CYS  |
| 4   | E     | 161 | GLN  |
| 4   | E     | 276 | GLU  |
| 4   | E     | 287 | GLN  |
| 4   | E     | 293 | GLN  |
| 4   | E     | 313 | LEU  |
| 4   | E     | 318 | GLU  |
| 4   | E     | 319 | CYS  |
| 4   | E     | 330 | GLN  |
| 4   | E     | 332 | GLN  |
| 4   | E     | 344 | LEU  |
| 4   | E     | 346 | THR  |
| 4   | E     | 356 | SER  |
| 4   | E     | 357 | LEU  |
| 4   | E     | 363 | LEU  |
| 4   | E     | 378 | SER  |
| 4   | E     | 395 | THR  |
| 4   | E     | 404 | ASP  |
| 4   | E     | 429 | LEU  |
| 4   | E     | 432 | ASP  |
| 4   | E     | 438 | LEU  |
| 4   | E     | 443 | GLU  |
| 4   | E     | 447 | LYS  |
| 4   | E     | 453 | VAL  |
| 4   | E     | 463 | GLU  |
| 4   | E     | 474 | GLU  |
| 4   | E     | 484 | THR  |
| 4   | E     | 486 | SER  |
| 4   | E     | 487 | MET  |
| 4   | E     | 492 | LEU  |
| 4   | E     | 494 | LEU  |
| 4   | E     | 499 | LYS  |
| 4   | E     | 503 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 505 | THR  |
| 4   | E     | 519 | ASN  |
| 4   | E     | 523 | LEU  |
| 4   | E     | 527 | LEU  |
| 5   | F     | 12  | SER  |
| 5   | F     | 15  | LEU  |
| 5   | F     | 56  | THR  |
| 5   | F     | 60  | ARG  |
| 5   | F     | 68  | GLN  |
| 5   | F     | 90  | ASP  |
| 5   | F     | 121 | VAL  |
| 5   | F     | 125 | ASP  |
| 5   | F     | 129 | LEU  |
| 5   | F     | 140 | ARG  |
| 5   | F     | 173 | ARG  |
| 5   | F     | 191 | SER  |
| 5   | F     | 196 | LEU  |
| 5   | F     | 214 | LEU  |
| 5   | F     | 270 | LEU  |
| 5   | F     | 288 | ASP  |
| 5   | F     | 293 | ILE  |
| 5   | F     | 315 | CYS  |
| 5   | F     | 345 | SER  |
| 5   | F     | 355 | ARG  |
| 6   | G     | 13  | LEU  |
| 6   | G     | 48  | GLU  |
| 6   | G     | 57  | LEU  |
| 6   | G     | 80  | LEU  |
| 6   | G     | 104 | LEU  |
| 6   | G     | 118 | LEU  |
| 6   | G     | 120 | GLU  |
| 6   | G     | 136 | LEU  |
| 6   | G     | 149 | LEU  |
| 6   | G     | 156 | LEU  |
| 6   | G     | 161 | LEU  |
| 6   | G     | 166 | LEU  |
| 6   | G     | 169 | SER  |
| 6   | G     | 170 | GLN  |
| 6   | G     | 179 | LEU  |
| 6   | G     | 207 | LEU  |
| 6   | G     | 226 | ASP  |
| 6   | G     | 231 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | G     | 234 | GLU  |
| 6   | G     | 250 | THR  |
| 6   | G     | 259 | MET  |
| 6   | G     | 277 | SER  |
| 6   | G     | 301 | GLU  |
| 6   | G     | 326 | GLU  |
| 6   | G     | 327 | LEU  |
| 6   | G     | 343 | GLN  |
| 6   | G     | 352 | SER  |
| 6   | G     | 357 | THR  |
| 6   | G     | 359 | ARG  |
| 6   | G     | 362 | ASP  |
| 6   | G     | 371 | LEU  |
| 6   | G     | 376 | ASP  |
| 6   | G     | 378 | SER  |
| 6   | G     | 381 | ARG  |
| 6   | G     | 388 | PRO  |
| 6   | G     | 395 | GLU  |
| 6   | G     | 396 | VAL  |
| 6   | G     | 405 | ILE  |
| 6   | G     | 412 | ASP  |
| 6   | G     | 416 | LEU  |
| 6   | G     | 444 | GLU  |
| 6   | G     | 448 | CYS  |
| 6   | G     | 450 | LEU  |
| 6   | G     | 482 | LEU  |
| 6   | G     | 497 | PHE  |
| 6   | G     | 498 | ASN  |
| 6   | G     | 501 | GLN  |
| 6   | G     | 505 | SER  |
| 6   | G     | 524 | TRP  |
| 6   | G     | 531 | THR  |
| 6   | G     | 540 | SER  |
| 6   | G     | 565 | ASP  |
| 6   | G     | 573 | ARG  |
| 6   | G     | 586 | LEU  |
| 6   | G     | 588 | SER  |
| 6   | G     | 596 | TYR  |
| 6   | G     | 598 | SER  |
| 6   | G     | 603 | SER  |
| 6   | H     | 12  | CYS  |
| 6   | H     | 13  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 15  | LEU  |
| 6   | H     | 35  | LEU  |
| 6   | H     | 37  | LEU  |
| 6   | H     | 42  | LEU  |
| 6   | H     | 48  | GLU  |
| 6   | H     | 54  | LEU  |
| 6   | H     | 56  | SER  |
| 6   | H     | 89  | THR  |
| 6   | H     | 91  | ASP  |
| 6   | H     | 98  | ARG  |
| 6   | H     | 104 | LEU  |
| 6   | H     | 118 | LEU  |
| 6   | H     | 131 | LEU  |
| 6   | H     | 132 | LEU  |
| 6   | H     | 134 | GLU  |
| 6   | H     | 135 | LEU  |
| 6   | H     | 136 | LEU  |
| 6   | H     | 145 | LEU  |
| 6   | H     | 155 | ARG  |
| 6   | H     | 156 | LEU  |
| 6   | H     | 158 | ASP  |
| 6   | H     | 179 | LEU  |
| 6   | H     | 183 | THR  |
| 6   | H     | 191 | LEU  |
| 6   | H     | 230 | SER  |
| 6   | H     | 241 | PRO  |
| 6   | H     | 250 | THR  |
| 6   | H     | 258 | LYS  |
| 6   | H     | 277 | SER  |
| 6   | H     | 284 | LEU  |
| 6   | H     | 327 | LEU  |
| 6   | H     | 333 | ASP  |
| 6   | H     | 346 | THR  |
| 6   | H     | 350 | LEU  |
| 6   | H     | 359 | ARG  |
| 6   | H     | 362 | ASP  |
| 6   | H     | 365 | GLU  |
| 6   | H     | 378 | SER  |
| 6   | H     | 393 | MET  |
| 6   | H     | 395 | GLU  |
| 6   | H     | 404 | LEU  |
| 6   | H     | 405 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | H     | 416 | LEU  |
| 6   | H     | 469 | GLN  |
| 6   | H     | 470 | LYS  |
| 6   | H     | 478 | ARG  |
| 6   | H     | 483 | LEU  |
| 6   | H     | 505 | SER  |
| 6   | H     | 530 | ASP  |
| 6   | H     | 531 | THR  |
| 6   | H     | 550 | THR  |
| 6   | H     | 564 | ARG  |
| 6   | H     | 568 | THR  |
| 6   | H     | 586 | LEU  |
| 6   | H     | 605 | ARG  |
| 6   | H     | 606 | ASP  |
| 7   | L     | 10  | ARG  |
| 7   | L     | 25  | TYR  |
| 7   | L     | 35  | ASP  |
| 7   | L     | 39  | ARG  |
| 7   | L     | 56  | SER  |
| 7   | L     | 60  | ARG  |
| 7   | L     | 64  | SER  |
| 7   | L     | 74  | MET  |
| 7   | L     | 90  | LEU  |
| 7   | L     | 153 | LYS  |
| 7   | L     | 155 | LYS  |
| 7   | L     | 167 | VAL  |
| 7   | L     | 213 | VAL  |
| 7   | L     | 250 | GLU  |
| 7   | L     | 251 | CYS  |
| 7   | L     | 257 | ASP  |
| 7   | L     | 267 | LEU  |
| 7   | L     | 268 | SER  |
| 7   | L     | 291 | ASP  |
| 7   | L     | 345 | LEU  |
| 7   | L     | 350 | GLN  |
| 2   | O     | 29  | LYS  |
| 2   | O     | 39  | LYS  |
| 2   | O     | 40  | THR  |
| 2   | O     | 46  | ARG  |
| 2   | O     | 47  | ARG  |
| 2   | O     | 90  | ASN  |
| 2   | O     | 104 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 141 | LEU  |
| 2   | O     | 143 | LEU  |
| 2   | O     | 175 | GLU  |
| 2   | O     | 181 | MET  |
| 2   | O     | 213 | CYS  |
| 2   | O     | 237 | VAL  |
| 2   | O     | 246 | GLU  |
| 2   | O     | 252 | LEU  |
| 2   | O     | 253 | ARG  |
| 2   | O     | 256 | LEU  |
| 2   | O     | 257 | ILE  |
| 2   | O     | 267 | SER  |
| 2   | O     | 279 | LEU  |
| 2   | O     | 283 | ASP  |
| 2   | O     | 287 | VAL  |
| 2   | O     | 305 | SER  |
| 2   | O     | 323 | GLU  |
| 2   | O     | 326 | SER  |
| 2   | O     | 336 | SER  |
| 2   | O     | 354 | LEU  |
| 2   | O     | 390 | VAL  |
| 2   | O     | 424 | LYS  |
| 2   | O     | 475 | VAL  |
| 2   | O     | 478 | ILE  |
| 2   | O     | 486 | SER  |
| 2   | O     | 498 | LYS  |
| 2   | O     | 504 | VAL  |
| 2   | O     | 505 | THR  |
| 2   | O     | 507 | SER  |
| 2   | O     | 512 | GLN  |
| 2   | O     | 515 | ASP  |
| 2   | O     | 518 | PHE  |
| 2   | O     | 522 | LYS  |
| 2   | O     | 523 | CYS  |
| 2   | O     | 524 | GLN  |
| 2   | O     | 573 | GLU  |
| 2   | O     | 574 | CYS  |
| 2   | O     | 588 | LEU  |
| 2   | O     | 595 | CYS  |
| 2   | O     | 601 | ILE  |
| 2   | O     | 602 | MET  |
| 2   | O     | 622 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | O     | 624 | LEU  |
| 2   | O     | 626 | ASP  |
| 2   | O     | 628 | SER  |
| 2   | O     | 642 | ILE  |
| 2   | O     | 659 | CYS  |
| 2   | O     | 677 | LEU  |
| 2   | O     | 708 | LYS  |
| 2   | O     | 716 | ILE  |
| 2   | O     | 724 | GLN  |
| 2   | O     | 735 | ILE  |
| 2   | O     | 742 | CYS  |
| 2   | O     | 744 | LEU  |
| 2   | O     | 775 | SER  |
| 2   | O     | 780 | HIS  |
| 2   | O     | 782 | SER  |
| 2   | O     | 847 | LEU  |
| 8   | P     | 9   | ARG  |
| 8   | P     | 18  | LEU  |
| 8   | P     | 29  | LEU  |
| 8   | P     | 35  | VAL  |
| 8   | P     | 42  | GLU  |
| 8   | P     | 45  | TYR  |
| 8   | P     | 63  | GLN  |
| 8   | P     | 69  | LEU  |
| 8   | P     | 70  | LEU  |
| 8   | P     | 74  | ARG  |
| 8   | P     | 124 | ILE  |
| 8   | P     | 125 | LEU  |
| 8   | P     | 130 | LEU  |
| 8   | P     | 131 | CYS  |
| 8   | P     | 135 | LEU  |
| 8   | P     | 137 | ASP  |
| 8   | P     | 142 | THR  |
| 8   | P     | 144 | VAL  |
| 8   | P     | 162 | GLU  |
| 8   | P     | 173 | VAL  |
| 8   | P     | 177 | SER  |
| 8   | P     | 198 | CYS  |
| 8   | P     | 201 | SER  |
| 8   | P     | 215 | SER  |
| 8   | P     | 228 | LEU  |
| 8   | P     | 232 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | P     | 235 | LEU  |
| 8   | P     | 237 | GLN  |
| 8   | P     | 238 | SER  |
| 8   | P     | 246 | PRO  |
| 8   | P     | 247 | ASP  |
| 8   | P     | 251 | CYS  |
| 8   | P     | 253 | VAL  |
| 8   | P     | 254 | ILE  |
| 8   | P     | 261 | SER  |
| 8   | P     | 274 | ILE  |
| 8   | P     | 279 | GLU  |
| 8   | P     | 311 | CYS  |
| 8   | P     | 321 | MET  |
| 8   | P     | 347 | VAL  |
| 8   | P     | 360 | HIS  |
| 8   | P     | 364 | SER  |
| 8   | P     | 385 | GLU  |
| 8   | P     | 387 | PRO  |
| 8   | P     | 424 | SER  |
| 8   | P     | 465 | ILE  |
| 8   | P     | 468 | ARG  |
| 8   | P     | 481 | LYS  |
| 8   | P     | 494 | CYS  |
| 8   | P     | 522 | VAL  |
| 8   | P     | 527 | CYS  |
| 8   | P     | 543 | LEU  |
| 8   | P     | 560 | CYS  |
| 8   | P     | 564 | THR  |
| 8   | P     | 578 | ARG  |
| 8   | P     | 580 | VAL  |
| 8   | P     | 599 | SER  |
| 8   | P     | 600 | CYS  |
| 8   | P     | 638 | VAL  |
| 8   | P     | 644 | ARG  |
| 8   | P     | 646 | THR  |
| 8   | P     | 683 | CYS  |
| 8   | P     | 685 | GLU  |
| 8   | P     | 707 | SER  |
| 8   | P     | 710 | VAL  |
| 8   | P     | 744 | ASP  |
| 8   | P     | 745 | VAL  |
| 8   | P     | 749 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | P     | 754 | ILE  |
| 8   | P     | 766 | LEU  |
| 8   | P     | 768 | VAL  |
| 8   | P     | 769 | ARG  |
| 8   | P     | 777 | CYS  |
| 8   | P     | 789 | VAL  |
| 8   | P     | 797 | ILE  |
| 8   | P     | 804 | VAL  |
| 8   | P     | 809 | GLN  |
| 8   | P     | 812 | VAL  |
| 8   | P     | 836 | ASN  |
| 8   | P     | 842 | ARG  |
| 8   | P     | 854 | GLU  |
| 8   | P     | 856 | GLU  |
| 8   | P     | 864 | GLN  |
| 8   | P     | 879 | ILE  |
| 8   | Q     | 9   | ARG  |
| 8   | Q     | 50  | GLU  |
| 8   | Q     | 69  | LEU  |
| 8   | Q     | 125 | LEU  |
| 8   | Q     | 135 | LEU  |
| 8   | Q     | 142 | THR  |
| 8   | Q     | 144 | VAL  |
| 8   | Q     | 172 | GLU  |
| 8   | Q     | 219 | THR  |
| 8   | Q     | 250 | LEU  |
| 8   | Q     | 253 | VAL  |
| 8   | Q     | 274 | ILE  |
| 8   | Q     | 307 | VAL  |
| 8   | Q     | 329 | ASP  |
| 8   | Q     | 333 | LYS  |
| 8   | Q     | 334 | LEU  |
| 8   | Q     | 342 | CYS  |
| 8   | Q     | 352 | CYS  |
| 8   | Q     | 361 | SER  |
| 8   | Q     | 362 | THR  |
| 8   | Q     | 370 | ASP  |
| 8   | Q     | 372 | SER  |
| 8   | Q     | 403 | SER  |
| 8   | Q     | 406 | SER  |
| 8   | Q     | 462 | ILE  |
| 8   | Q     | 465 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | Q     | 483 | LEU  |
| 8   | Q     | 490 | MET  |
| 8   | Q     | 510 | THR  |
| 8   | Q     | 522 | VAL  |
| 8   | Q     | 529 | LEU  |
| 8   | Q     | 539 | GLN  |
| 8   | Q     | 543 | LEU  |
| 8   | Q     | 561 | SER  |
| 8   | Q     | 566 | THR  |
| 8   | Q     | 567 | ILE  |
| 8   | Q     | 570 | ASP  |
| 8   | Q     | 578 | ARG  |
| 8   | Q     | 582 | LEU  |
| 8   | Q     | 584 | LEU  |
| 8   | Q     | 598 | VAL  |
| 8   | Q     | 638 | VAL  |
| 8   | Q     | 642 | LEU  |
| 8   | Q     | 646 | THR  |
| 8   | Q     | 652 | CYS  |
| 8   | Q     | 683 | CYS  |
| 8   | Q     | 685 | GLU  |
| 8   | Q     | 701 | LEU  |
| 8   | Q     | 745 | VAL  |
| 8   | Q     | 751 | LEU  |
| 8   | Q     | 752 | SER  |
| 8   | Q     | 768 | VAL  |
| 8   | Q     | 769 | ARG  |
| 8   | Q     | 775 | ASP  |
| 8   | Q     | 782 | ILE  |
| 8   | Q     | 789 | VAL  |
| 8   | Q     | 797 | ILE  |
| 8   | Q     | 804 | VAL  |
| 8   | Q     | 810 | THR  |
| 8   | Q     | 812 | VAL  |
| 8   | Q     | 842 | ARG  |
| 8   | Q     | 852 | CYS  |
| 8   | Q     | 872 | GLN  |
| 1   | S     | 56  | ASP  |
| 1   | S     | 60  | LEU  |
| 1   | S     | 98  | LEU  |
| 1   | S     | 109 | VAL  |
| 1   | S     | 139 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | S     | 174 | GLN  |
| 1   | S     | 175 | SER  |
| 1   | S     | 179 | LEU  |
| 1   | S     | 182 | VAL  |
| 1   | S     | 191 | VAL  |
| 1   | S     | 239 | VAL  |
| 1   | S     | 267 | VAL  |
| 1   | S     | 274 | LEU  |
| 1   | S     | 312 | SER  |
| 1   | S     | 313 | THR  |
| 1   | S     | 333 | VAL  |
| 1   | S     | 334 | LEU  |
| 1   | S     | 337 | SER  |
| 1   | S     | 354 | LEU  |
| 1   | S     | 402 | GLU  |
| 1   | S     | 405 | GLN  |
| 1   | S     | 407 | LEU  |
| 1   | S     | 473 | LEU  |
| 1   | S     | 491 | VAL  |
| 1   | S     | 508 | THR  |
| 1   | S     | 648 | GLU  |
| 1   | S     | 653 | LEU  |
| 1   | S     | 665 | THR  |
| 1   | S     | 671 | ASP  |
| 1   | S     | 685 | ARG  |
| 1   | S     | 714 | ARG  |
| 1   | S     | 723 | LEU  |
| 1   | S     | 725 | SER  |
| 1   | S     | 766 | CYS  |
| 1   | S     | 775 | SER  |
| 1   | S     | 777 | SER  |
| 1   | S     | 795 | ARG  |
| 1   | S     | 800 | GLU  |
| 1   | S     | 818 | PHE  |
| 1   | S     | 821 | LEU  |
| 1   | S     | 847 | LYS  |
| 1   | S     | 850 | SER  |
| 1   | S     | 853 | ARG  |
| 1   | S     | 855 | THR  |
| 1   | S     | 856 | LEU  |
| 1   | S     | 859 | CYS  |
| 1   | S     | 911 | TRP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S     | 912  | THR  |
| 1   | S     | 924  | ASP  |
| 1   | S     | 930  | GLN  |
| 1   | S     | 948  | ASP  |
| 1   | S     | 949  | THR  |
| 1   | S     | 964  | LEU  |
| 1   | S     | 966  | GLU  |
| 1   | S     | 973  | CYS  |
| 1   | S     | 1007 | VAL  |
| 1   | S     | 1012 | THR  |
| 1   | S     | 1015 | GLU  |
| 1   | S     | 1016 | ASP  |
| 1   | S     | 1030 | LEU  |
| 1   | S     | 1031 | GLN  |
| 1   | S     | 1060 | THR  |
| 1   | S     | 1070 | GLN  |
| 1   | S     | 1076 | LEU  |
| 1   | S     | 1098 | GLU  |
| 1   | S     | 1126 | LEU  |
| 1   | S     | 1130 | ILE  |
| 1   | S     | 1139 | LEU  |
| 1   | S     | 1155 | ILE  |
| 1   | S     | 1183 | CYS  |
| 1   | S     | 1190 | GLN  |
| 1   | S     | 1202 | GLU  |
| 1   | S     | 1223 | ASP  |
| 1   | S     | 1241 | ASN  |
| 1   | S     | 1251 | CYS  |
| 1   | S     | 1253 | ARG  |
| 1   | S     | 1280 | ASP  |
| 1   | S     | 1308 | LEU  |
| 1   | S     | 1310 | GLU  |
| 1   | S     | 1339 | LEU  |
| 1   | S     | 1345 | ASP  |
| 1   | S     | 1367 | LEU  |
| 1   | S     | 1393 | VAL  |
| 1   | S     | 1395 | LEU  |
| 1   | S     | 1428 | CYS  |
| 9   | W     | 75   | THR  |
| 9   | W     | 90   | PHE  |
| 7   | M     | 10   | ARG  |
| 7   | M     | 25   | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | M     | 26  | GLU  |
| 7   | M     | 40  | ILE  |
| 7   | M     | 55  | CYS  |
| 7   | M     | 56  | SER  |
| 7   | M     | 60  | ARG  |
| 7   | M     | 72  | GLN  |
| 7   | M     | 82  | SER  |
| 7   | M     | 85  | MET  |
| 7   | M     | 131 | THR  |
| 7   | M     | 167 | VAL  |
| 7   | M     | 182 | SER  |
| 7   | M     | 213 | VAL  |
| 7   | M     | 217 | GLU  |
| 7   | M     | 232 | ASN  |
| 7   | M     | 277 | GLU  |
| 7   | M     | 286 | ASP  |
| 7   | M     | 291 | ASP  |
| 7   | M     | 303 | PHE  |
| 7   | M     | 343 | ARG  |
| 7   | M     | 345 | LEU  |
| 7   | M     | 347 | THR  |
| 7   | M     | 351 | SER  |
| 10  | X     | 9   | ARG  |
| 10  | X     | 32  | ASP  |
| 10  | X     | 64  | GLU  |
| 10  | X     | 86  | CYS  |
| 10  | X     | 122 | ASP  |
| 10  | X     | 153 | GLN  |
| 11  | U     | 56  | CYS  |
| 11  | U     | 265 | ARG  |
| 11  | U     | 275 | ILE  |
| 11  | U     | 284 | GLU  |
| 11  | U     | 312 | LEU  |
| 11  | U     | 317 | THR  |
| 11  | U     | 322 | PHE  |
| 11  | U     | 333 | SER  |
| 11  | U     | 337 | SER  |
| 11  | U     | 384 | GLU  |
| 11  | U     | 385 | LEU  |
| 11  | U     | 413 | MET  |
| 11  | U     | 419 | CYS  |
| 11  | U     | 420 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | U     | 437  | ARG  |
| 11  | U     | 440  | ILE  |
| 11  | U     | 453  | SER  |
| 11  | U     | 466  | ILE  |
| 11  | U     | 468  | MET  |
| 11  | U     | 481  | VAL  |
| 11  | U     | 490  | PHE  |
| 11  | U     | 505  | PRO  |
| 11  | U     | 528  | ASN  |
| 11  | U     | 531  | ASP  |
| 11  | U     | 603  | LEU  |
| 11  | U     | 607  | GLU  |
| 11  | U     | 627  | LEU  |
| 11  | U     | 628  | LEU  |
| 11  | U     | 632  | LYS  |
| 11  | U     | 741  | ILE  |
| 11  | U     | 760  | ILE  |
| 11  | U     | 777  | CYS  |
| 11  | U     | 783  | ASP  |
| 11  | U     | 812  | SER  |
| 11  | U     | 835  | SER  |
| 11  | U     | 836  | ASN  |
| 11  | U     | 837  | GLU  |
| 11  | U     | 872  | GLN  |
| 11  | U     | 996  | LEU  |
| 11  | U     | 1020 | GLU  |
| 11  | U     | 1034 | SER  |
| 11  | U     | 1064 | VAL  |
| 11  | U     | 1082 | PRO  |
| 11  | U     | 1141 | LEU  |
| 11  | U     | 1171 | THR  |
| 11  | U     | 1214 | SER  |
| 11  | U     | 1259 | GLN  |
| 11  | U     | 1261 | GLU  |
| 11  | U     | 1276 | MET  |
| 11  | U     | 1284 | SER  |
| 11  | U     | 1285 | ARG  |
| 12  | V     | 45   | ASP  |
| 12  | V     | 104  | ILE  |
| 12  | V     | 153  | LEU  |
| 12  | V     | 155  | GLU  |
| 12  | V     | 191  | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 12  | V     | 223  | GLN  |
| 12  | V     | 226  | ASP  |
| 12  | V     | 233  | ASP  |
| 12  | V     | 248  | VAL  |
| 12  | V     | 257  | ASN  |
| 12  | V     | 306  | ASP  |
| 12  | V     | 310  | CYS  |
| 12  | V     | 311  | VAL  |
| 12  | V     | 354  | ILE  |
| 12  | V     | 369  | GLU  |
| 12  | V     | 376  | GLU  |
| 12  | V     | 431  | MET  |
| 12  | V     | 432  | CYS  |
| 12  | V     | 472  | GLU  |
| 12  | V     | 493  | LEU  |
| 12  | V     | 496  | LEU  |
| 12  | V     | 559  | ILE  |
| 12  | V     | 657  | CYS  |
| 12  | V     | 781  | PHE  |
| 12  | V     | 1023 | MET  |
| 12  | V     | 1070 | HIS  |
| 12  | V     | 1079 | SER  |
| 12  | V     | 1346 | LYS  |
| 12  | V     | 1393 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (236) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 41  | GLN  |
| 1   | A     | 123 | GLN  |
| 1   | A     | 188 | GLN  |
| 1   | A     | 220 | GLN  |
| 1   | A     | 264 | GLN  |
| 1   | A     | 286 | GLN  |
| 1   | A     | 330 | HIS  |
| 1   | A     | 376 | GLN  |
| 1   | A     | 436 | GLN  |
| 1   | A     | 492 | HIS  |
| 1   | A     | 676 | GLN  |
| 1   | A     | 851 | GLN  |
| 1   | A     | 881 | GLN  |
| 1   | A     | 993 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1113 | ASN  |
| 1   | A     | 1128 | GLN  |
| 1   | A     | 1188 | HIS  |
| 1   | A     | 1327 | HIS  |
| 1   | A     | 1405 | GLN  |
| 2   | B     | 12   | GLN  |
| 2   | B     | 59   | GLN  |
| 2   | B     | 116  | ASN  |
| 2   | B     | 171  | GLN  |
| 2   | B     | 178  | ASN  |
| 2   | B     | 241  | HIS  |
| 2   | B     | 270  | ASN  |
| 2   | B     | 296  | ASN  |
| 2   | B     | 306  | ASN  |
| 2   | B     | 340  | GLN  |
| 2   | B     | 366  | ASN  |
| 2   | B     | 473  | GLN  |
| 2   | B     | 502  | ASN  |
| 2   | B     | 600  | GLN  |
| 2   | B     | 670  | ASN  |
| 2   | B     | 724  | GLN  |
| 2   | B     | 746  | ASN  |
| 2   | B     | 817  | GLN  |
| 2   | B     | 825  | GLN  |
| 2   | B     | 854  | GLN  |
| 3   | C     | 3    | GLN  |
| 3   | C     | 37   | HIS  |
| 3   | C     | 42   | GLN  |
| 3   | C     | 58   | ASN  |
| 3   | C     | 152  | ASN  |
| 3   | C     | 207  | HIS  |
| 3   | C     | 216  | GLN  |
| 3   | C     | 224  | ASN  |
| 3   | C     | 316  | GLN  |
| 3   | C     | 399  | HIS  |
| 3   | C     | 410  | GLN  |
| 3   | C     | 465  | GLN  |
| 3   | C     | 493  | ASN  |
| 4   | E     | 161  | GLN  |
| 4   | E     | 287  | GLN  |
| 4   | E     | 314  | GLN  |
| 4   | E     | 359  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | E     | 408 | GLN  |
| 4   | E     | 508 | GLN  |
| 5   | F     | 36  | GLN  |
| 5   | F     | 100 | ASN  |
| 5   | F     | 110 | HIS  |
| 5   | F     | 113 | GLN  |
| 5   | F     | 114 | GLN  |
| 5   | F     | 130 | GLN  |
| 5   | F     | 144 | HIS  |
| 5   | F     | 283 | GLN  |
| 5   | F     | 286 | HIS  |
| 5   | F     | 316 | GLN  |
| 6   | G     | 41  | GLN  |
| 6   | G     | 58  | GLN  |
| 6   | G     | 86  | GLN  |
| 6   | G     | 215 | GLN  |
| 6   | G     | 311 | ASN  |
| 6   | G     | 356 | GLN  |
| 6   | G     | 406 | GLN  |
| 6   | G     | 469 | GLN  |
| 6   | G     | 498 | ASN  |
| 6   | G     | 501 | GLN  |
| 6   | G     | 511 | GLN  |
| 6   | G     | 547 | ASN  |
| 6   | H     | 31  | GLN  |
| 6   | H     | 44  | GLN  |
| 6   | H     | 58  | GLN  |
| 6   | H     | 76  | ASN  |
| 6   | H     | 167 | ASN  |
| 6   | H     | 224 | ASN  |
| 6   | H     | 311 | ASN  |
| 6   | H     | 343 | GLN  |
| 6   | H     | 461 | GLN  |
| 6   | H     | 465 | GLN  |
| 6   | H     | 511 | GLN  |
| 6   | H     | 535 | GLN  |
| 6   | H     | 547 | ASN  |
| 7   | L     | 109 | GLN  |
| 7   | L     | 180 | GLN  |
| 7   | L     | 189 | GLN  |
| 7   | L     | 237 | ASN  |
| 7   | L     | 258 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | L     | 328 | GLN  |
| 7   | L     | 335 | GLN  |
| 2   | O     | 44  | HIS  |
| 2   | O     | 71  | ASN  |
| 2   | O     | 102 | ASN  |
| 2   | O     | 138 | ASN  |
| 2   | O     | 156 | GLN  |
| 2   | O     | 178 | ASN  |
| 2   | O     | 220 | GLN  |
| 2   | O     | 241 | HIS  |
| 2   | O     | 296 | ASN  |
| 2   | O     | 410 | GLN  |
| 2   | O     | 428 | ASN  |
| 2   | O     | 512 | GLN  |
| 2   | O     | 533 | ASN  |
| 2   | O     | 670 | ASN  |
| 2   | O     | 780 | HIS  |
| 8   | P     | 66  | HIS  |
| 8   | P     | 157 | GLN  |
| 8   | P     | 308 | HIS  |
| 8   | P     | 491 | ASN  |
| 8   | P     | 645 | HIS  |
| 8   | P     | 734 | GLN  |
| 8   | P     | 788 | GLN  |
| 8   | P     | 815 | GLN  |
| 8   | Q     | 66  | HIS  |
| 8   | Q     | 360 | HIS  |
| 8   | Q     | 400 | ASN  |
| 8   | Q     | 453 | GLN  |
| 8   | Q     | 478 | GLN  |
| 8   | Q     | 531 | ASN  |
| 8   | Q     | 539 | GLN  |
| 8   | Q     | 635 | GLN  |
| 8   | Q     | 651 | GLN  |
| 8   | Q     | 809 | GLN  |
| 1   | S     | 101 | GLN  |
| 1   | S     | 240 | GLN  |
| 1   | S     | 341 | GLN  |
| 1   | S     | 376 | GLN  |
| 1   | S     | 387 | GLN  |
| 1   | S     | 490 | GLN  |
| 1   | S     | 549 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S     | 771  | HIS  |
| 1   | S     | 772  | GLN  |
| 1   | S     | 851  | GLN  |
| 1   | S     | 940  | GLN  |
| 1   | S     | 962  | HIS  |
| 1   | S     | 992  | HIS  |
| 1   | S     | 993  | GLN  |
| 1   | S     | 1014 | ASN  |
| 1   | S     | 1113 | ASN  |
| 1   | S     | 1128 | GLN  |
| 1   | S     | 1140 | ASN  |
| 1   | S     | 1231 | HIS  |
| 1   | S     | 1327 | HIS  |
| 1   | S     | 1437 | GLN  |
| 1   | S     | 1440 | GLN  |
| 7   | M     | 32   | GLN  |
| 7   | M     | 109  | GLN  |
| 7   | M     | 232  | ASN  |
| 7   | M     | 328  | GLN  |
| 7   | M     | 331  | GLN  |
| 7   | M     | 335  | GLN  |
| 7   | M     | 350  | GLN  |
| 10  | X     | 67   | GLN  |
| 10  | X     | 103  | ASN  |
| 10  | X     | 150  | HIS  |
| 10  | X     | 153  | GLN  |
| 11  | U     | 22   | GLN  |
| 11  | U     | 31   | ASN  |
| 11  | U     | 36   | GLN  |
| 11  | U     | 82   | GLN  |
| 11  | U     | 98   | HIS  |
| 11  | U     | 143  | ASN  |
| 11  | U     | 171  | GLN  |
| 11  | U     | 172  | GLN  |
| 11  | U     | 208  | GLN  |
| 11  | U     | 244  | HIS  |
| 11  | U     | 266  | HIS  |
| 11  | U     | 302  | ASN  |
| 11  | U     | 320  | GLN  |
| 11  | U     | 323  | GLN  |
| 11  | U     | 345  | GLN  |
| 11  | U     | 380  | GLN  |

*Continued on next page...*

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | U     | 415  | ASN  |
| 11  | U     | 416  | GLN  |
| 11  | U     | 504  | GLN  |
| 11  | U     | 528  | ASN  |
| 11  | U     | 546  | ASN  |
| 11  | U     | 580  | ASN  |
| 11  | U     | 621  | ASN  |
| 11  | U     | 654  | GLN  |
| 11  | U     | 680  | ASN  |
| 11  | U     | 731  | GLN  |
| 11  | U     | 757  | ASN  |
| 11  | U     | 786  | ASN  |
| 11  | U     | 826  | GLN  |
| 11  | U     | 848  | GLN  |
| 11  | U     | 858  | HIS  |
| 11  | U     | 865  | GLN  |
| 11  | U     | 963  | GLN  |
| 11  | U     | 1017 | ASN  |
| 11  | U     | 1071 | HIS  |
| 11  | U     | 1137 | GLN  |
| 11  | U     | 1182 | GLN  |
| 11  | U     | 1185 | GLN  |
| 11  | U     | 1193 | ASN  |
| 11  | U     | 1217 | GLN  |
| 11  | U     | 1252 | ASN  |
| 11  | U     | 1259 | GLN  |
| 11  | U     | 1278 | HIS  |
| 12  | V     | 76   | GLN  |
| 12  | V     | 86   | HIS  |
| 12  | V     | 171  | ASN  |
| 12  | V     | 208  | GLN  |
| 12  | V     | 308  | GLN  |
| 12  | V     | 370  | ASN  |
| 12  | V     | 394  | GLN  |
| 12  | V     | 405  | ASN  |
| 12  | V     | 424  | HIS  |
| 12  | V     | 448  | GLN  |
| 12  | V     | 480  | HIS  |
| 12  | V     | 523  | ASN  |
| 12  | V     | 609  | GLN  |
| 12  | V     | 706  | GLN  |
| 12  | V     | 802  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 12  | V     | 922  | HIS  |
| 12  | V     | 1005 | GLN  |
| 12  | V     | 1056 | HIS  |
| 12  | V     | 1063 | GLN  |
| 12  | V     | 1105 | GLN  |
| 12  | V     | 1119 | GLN  |
| 12  | V     | 1129 | GLN  |
| 12  | V     | 1150 | GLN  |
| 12  | V     | 1151 | ASN  |
| 12  | V     | 1183 | HIS  |
| 12  | V     | 1280 | ASN  |
| 12  | V     | 1378 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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                |
| 7   | L     | 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      | 36.41        |
| 1     | W     | 95:TRP    | C      | 101:UNK   | N      | 6.57         |
| 1     | L     | 339:TYR   | C      | 340:GLU   | N      | 1.17         |
| 1     | L     | 332:PRO   | C      | 333:PHE   | N      | 1.15         |

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23090. These allow visual inspection of the internal detail of the map and identification of artifacts.

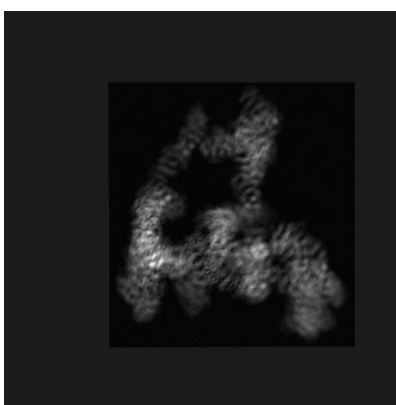
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

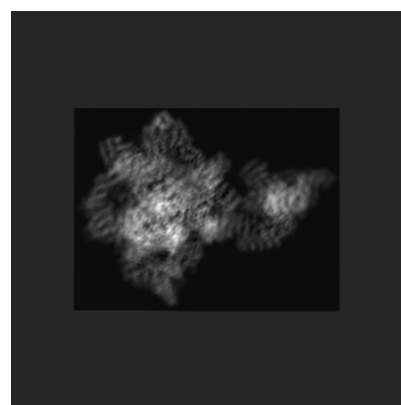
#### 6.1.1 Primary map



X



Y

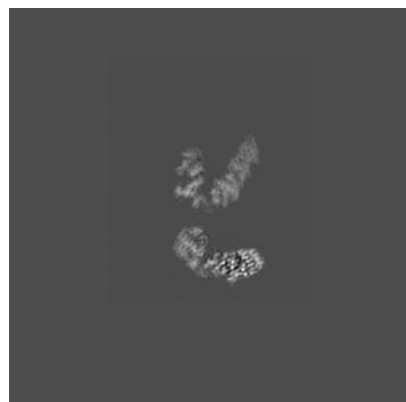


Z

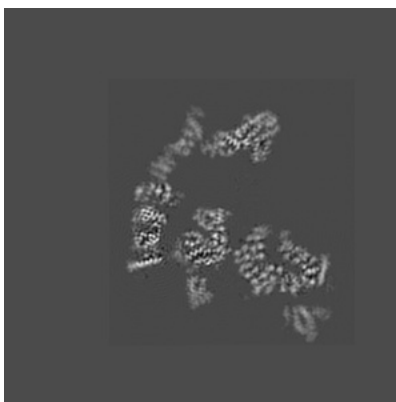
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

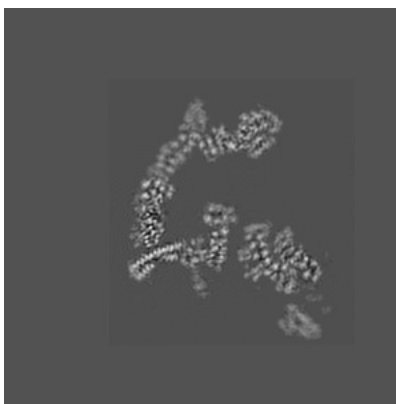
The images above show central slices of the map in three orthogonal directions.

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

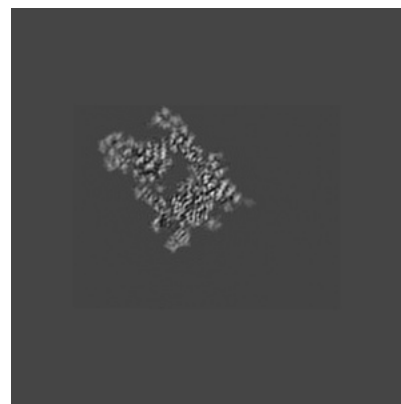
### 6.3.1 Primary map



X Index: 166



Y Index: 232

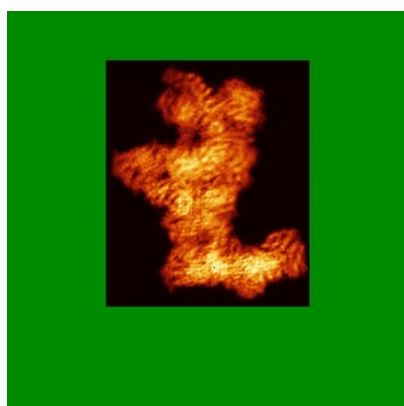


Z Index: 162

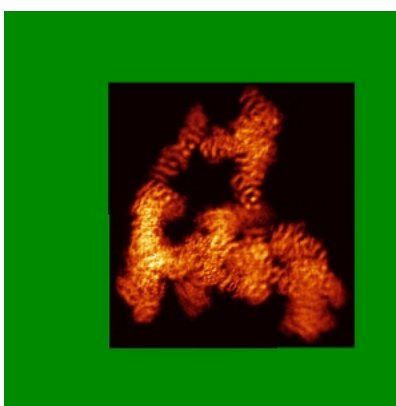
The images above show the largest variance slices of the map in three orthogonal directions.

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

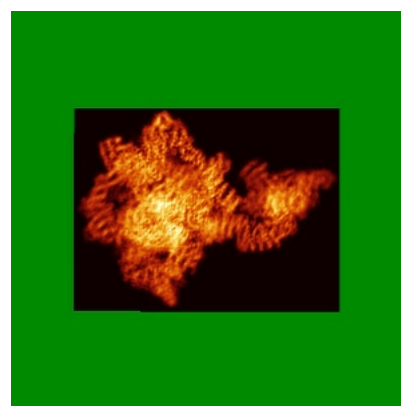
### 6.4.1 Primary map



X



Y

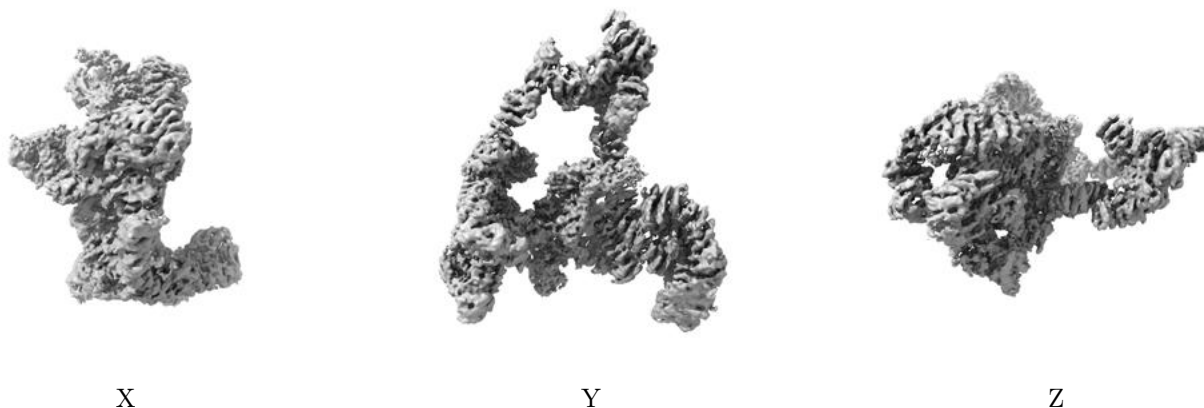


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

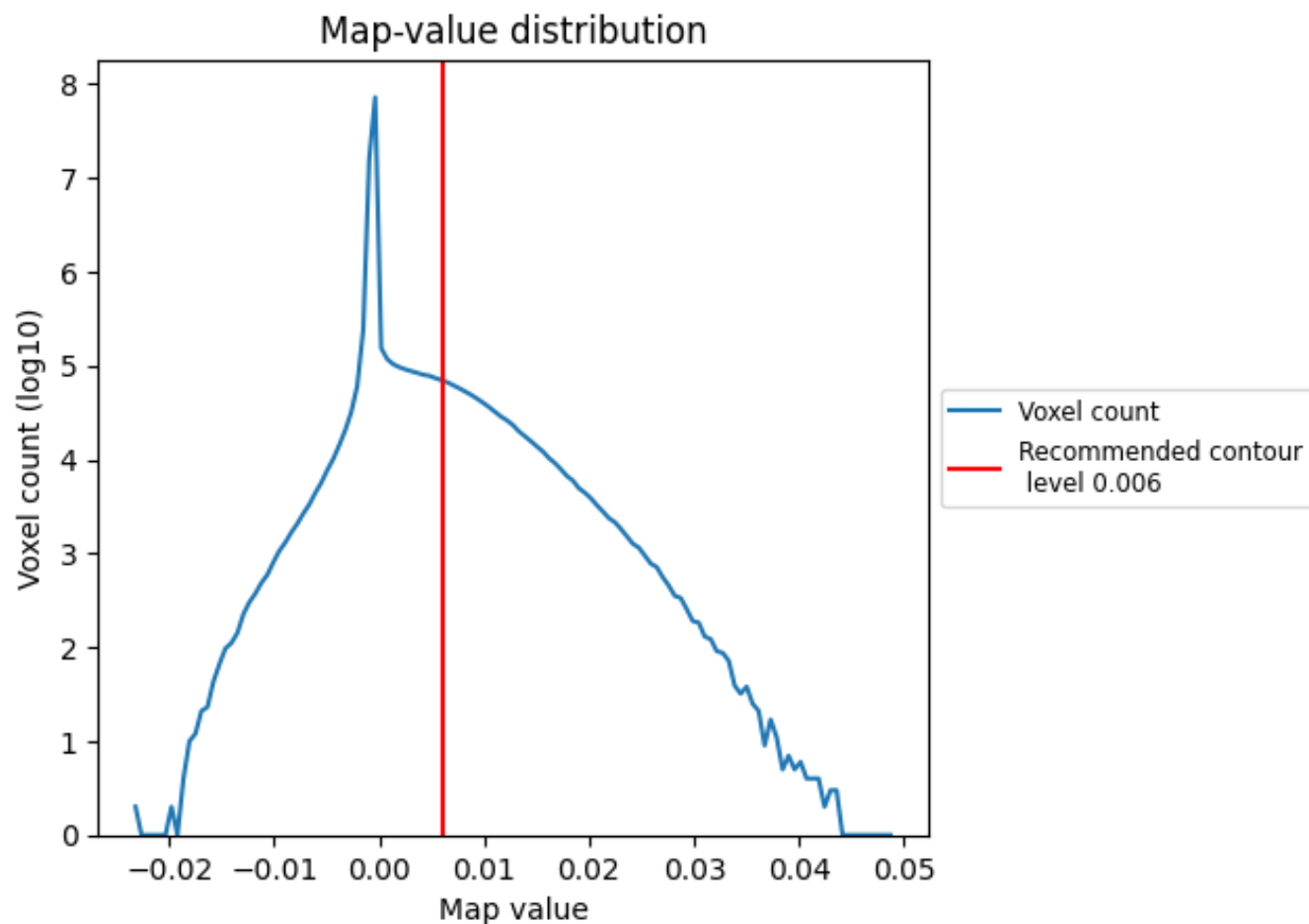
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

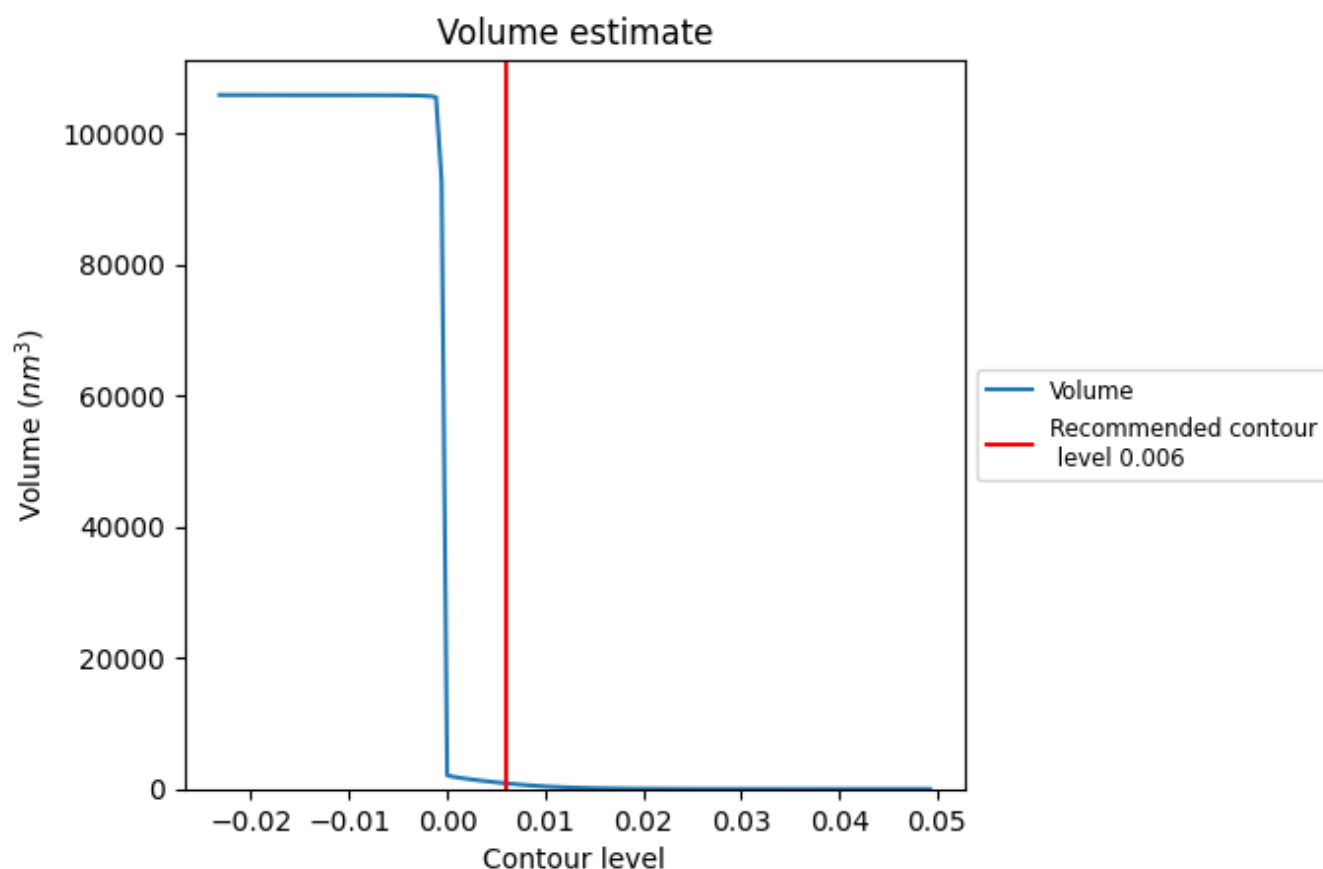
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

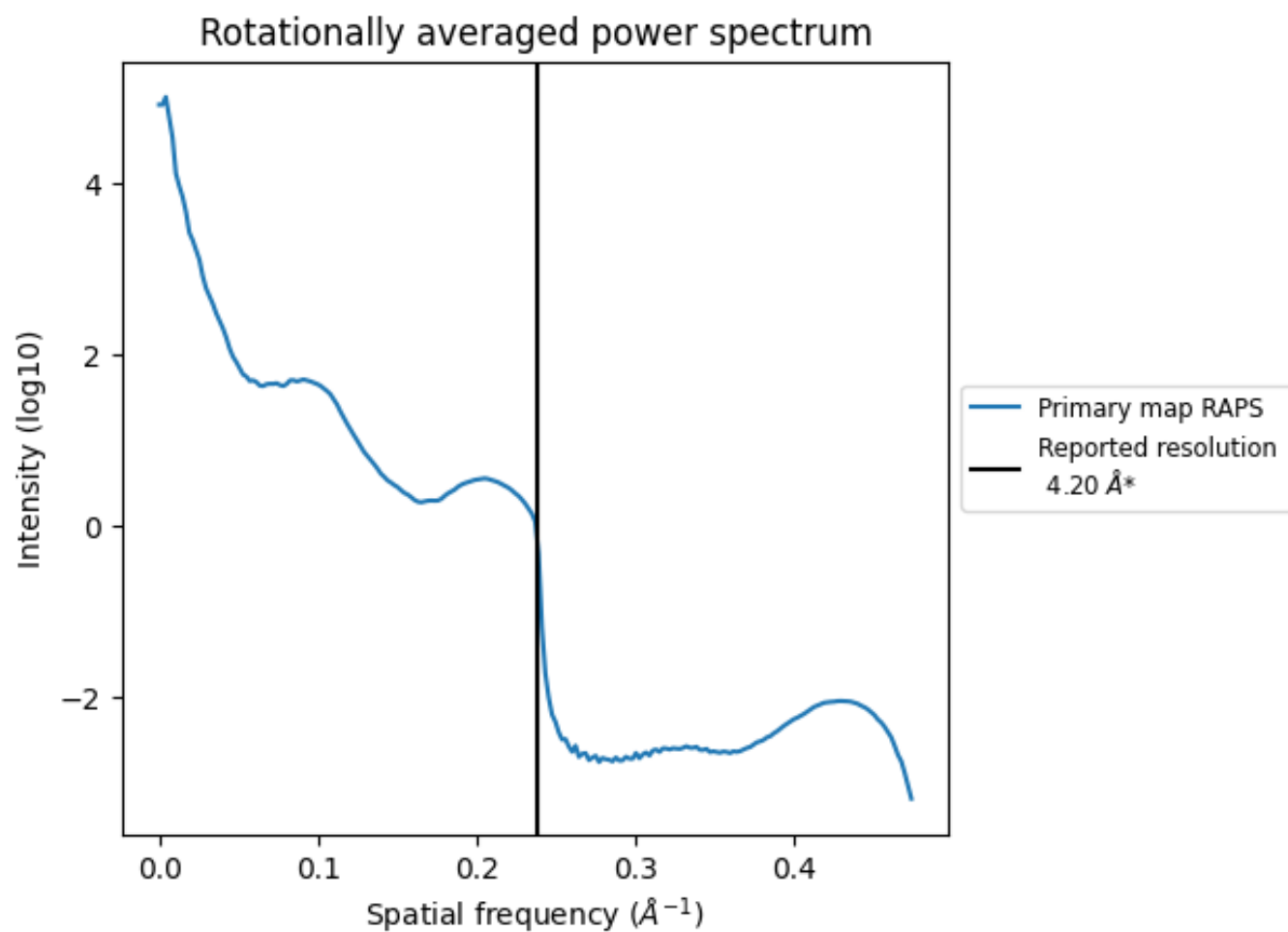
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 860  $\text{nm}^3$ ; this corresponds to an approximate mass of 777 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 0.238 Å<sup>-1</sup>

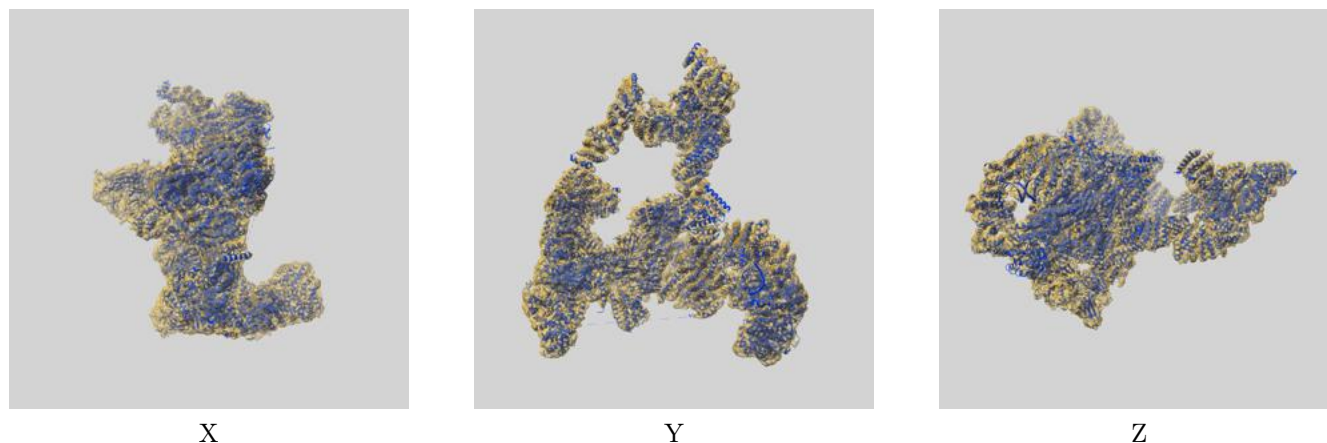
## 8 Fourier-Shell correlation

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

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

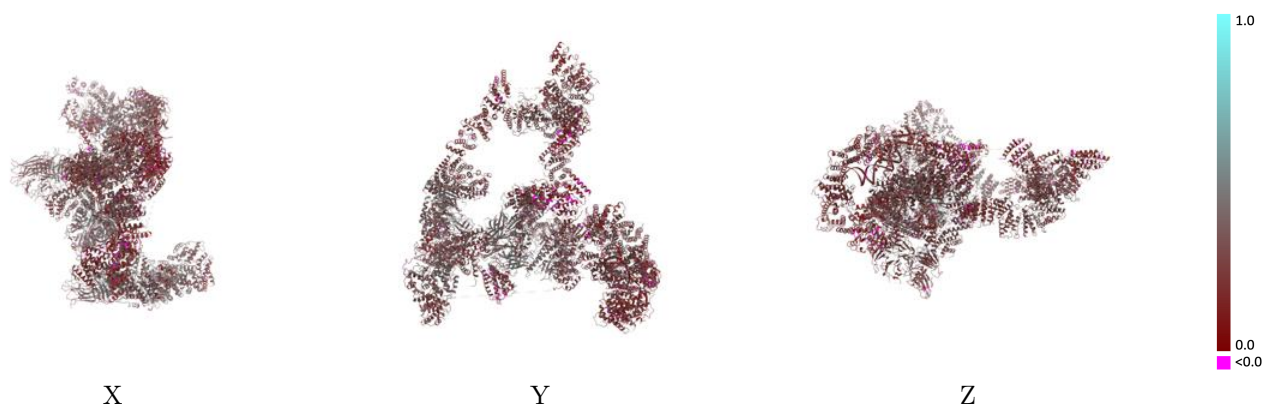
This section contains information regarding the fit between EMDB map EMD-23090 and PDB model 7KZV. Per-residue inclusion information can be found in section 3 on page 15.

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



The images above show the 3D surface view of the map at the recommended contour level 0.006 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](#)

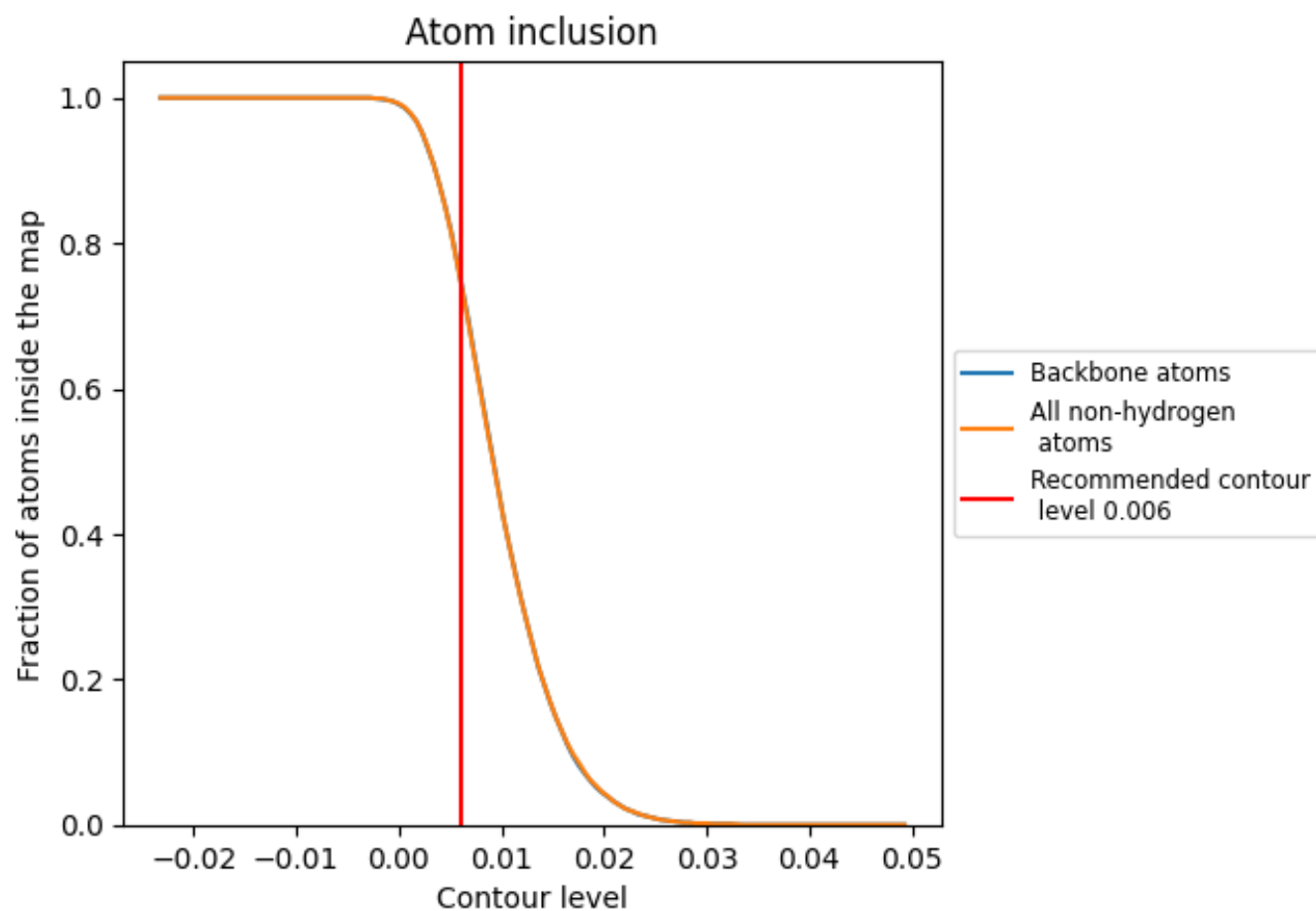


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 75% 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 (0.006) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7500   |  0.2930   |
| A     |  0.7080   |  0.2510   |
| B     |  0.8310   |  0.3630   |
| C     |  0.8750   |  0.3400   |
| E     |  0.7600   |  0.3100   |
| F     |  0.8750   |  0.3400   |
| G     |  0.8330   |  0.3180   |
| H     |  0.7810   |  0.2750   |
| L     |  0.8170   |  0.3350   |
| M     |  0.7330   |  0.2580   |
| O     |  0.8070   |  0.3070   |
| P     |  0.8500   |  0.3840   |
| Q     |  0.7640   |  0.3010   |
| S     |  0.7550   |  0.2700   |
| U     |  0.6530  |  0.2630  |
| V     |  0.7070 |  0.2530 |
| W     |  0.7290 |  0.3270 |
| X     |  0.6710 |  0.2410 |
| Y     |  0.3890 |  0.1710 |
| Z     |  0.4290 |  0.1980 |

