



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:16 PM UTC

PDB ID : 5CYL / pdb\_00005cyl  
Title : Crystal structure of the CupB6 tip adhesin from *Pseudomonas aeruginosa*  
Authors : Rasheed, M.; Garnett, J.A.; Perez-Dorado, I.; Matthews, S.J.  
Deposited on : 2015-07-30  
Resolution : 2.77 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

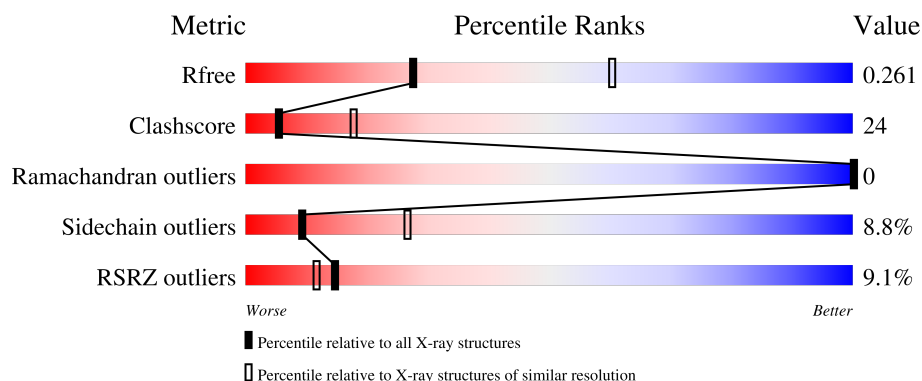
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 5248 (2.80-2.76)                                      |
| Clashscore            | 190562                      | 5693 (2.80-2.76)                                      |
| Ramachandran outliers | 187476                      | 5590 (2.80-2.76)                                      |
| Sidechain outliers    | 187428                      | 5592 (2.80-2.76)                                      |
| RSRZ outliers         | 180081                      | 5251 (2.80-2.76)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 370    |                  |
| 1   | B     | 370    |                  |
| 1   | C     | 370    |                  |
| 1   | D     | 370    |                  |
| 1   | E     | 370    |                  |

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| Mol | Chain | Length | Quality of chain                                                                           |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 1   | F     | 370    | <div><div></div><div>15%</div><div>52%</div><div>34%</div><div>6%</div><div>8%</div></div> |
| 1   | G     | 370    | <div><div></div><div>12%</div><div>57%</div><div>33%</div><div>5%</div><div>5%</div></div> |
| 1   | H     | 370    | <div><div></div><div>3%</div><div>73%</div><div>21%</div><div></div><div></div></div>      |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Fimbrial subunit CupB6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 361      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2637  | 1664 | 455 | 513 | 5 |         |         |       |
| 1   | B     | 355      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2608  | 1650 | 444 | 509 | 5 |         |         |       |
| 1   | C     | 353      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2574  | 1630 | 439 | 500 | 5 |         |         |       |
| 1   | D     | 359      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2616  | 1654 | 446 | 511 | 5 |         |         |       |
| 1   | E     | 355      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2602  | 1643 | 448 | 506 | 5 |         |         |       |
| 1   | F     | 342      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2452  | 1549 | 419 | 479 | 5 |         |         |       |
| 1   | G     | 353      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2550  | 1617 | 434 | 494 | 5 |         |         |       |
| 1   | H     | 359      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2644  | 1673 | 455 | 511 | 5 |         |         |       |

There are 208 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| A     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| A     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| A     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| A     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| A     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| A     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| A     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| A     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| A     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| A     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| A     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| A     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| A     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| A     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| A     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| A     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| A     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| A     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| A     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| A     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| B     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| B     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| B     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| B     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| B     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| B     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| B     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| B     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| B     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| B     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| B     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| B     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| B     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| B     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| B     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| B     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| B     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| B     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| B     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| B     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| C     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| C     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| C     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| C     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| C     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| C     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| C     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| C     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| C     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| C     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| C     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| C     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| C     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| C     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| C     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| C     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| C     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| C     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| C     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| C     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| D     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| D     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| D     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| D     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| D     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| D     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| D     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| D     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| D     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| D     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| D     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| D     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| D     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| D     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| D     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| D     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| D     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| D     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| D     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| D     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| E     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| E     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| E     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| E     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| E     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| E     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| E     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| E     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| E     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| E     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| E     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| E     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| E     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| E     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| E     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| E     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| E     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| E     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| E     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| E     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| F     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| F     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| F     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| F     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| F     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| F     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| F     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| F     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| F     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| F     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| F     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| F     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| F     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| F     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| F     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| F     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| F     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| F     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| F     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| F     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| G     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| G     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| G     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| G     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| G     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| G     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| G     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| G     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| G     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| G     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| G     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| G     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| G     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| G     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| G     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| G     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| G     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| G     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| G     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| G     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |

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| Chain | Residue | Modelled | Actual | Comment               | Reference  |
|-------|---------|----------|--------|-----------------------|------------|
| G     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 0       | MET      | -      | initiating methionine | UNP Q9HWU7 |
| H     | 345     | SER      | -      | expression tag        | UNP Q9HWU7 |
| H     | 346     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| H     | 347     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| H     | 348     | LYS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 349     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| H     | 350     | ASP      | -      | expression tag        | UNP Q9HWU7 |
| H     | 351     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| H     | 352     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| H     | 353     | VAL      | -      | expression tag        | UNP Q9HWU7 |
| H     | 354     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| H     | 355     | PHE      | -      | expression tag        | UNP Q9HWU7 |
| H     | 356     | SER      | -      | expression tag        | UNP Q9HWU7 |
| H     | 357     | GLY      | -      | expression tag        | UNP Q9HWU7 |
| H     | 358     | ASN      | -      | expression tag        | UNP Q9HWU7 |
| H     | 359     | ILE      | -      | expression tag        | UNP Q9HWU7 |
| H     | 360     | THR      | -      | expression tag        | UNP Q9HWU7 |
| H     | 361     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| H     | 362     | LEU      | -      | expression tag        | UNP Q9HWU7 |
| H     | 363     | GLU      | -      | expression tag        | UNP Q9HWU7 |
| H     | 364     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 365     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 366     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 367     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 368     | HIS      | -      | expression tag        | UNP Q9HWU7 |
| H     | 369     | HIS      | -      | expression tag        | UNP Q9HWU7 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2   | A     | 39       | Total O<br>39 39 | 0       | 0       |
| 2   | B     | 62       | Total O<br>62 62 | 0       | 0       |
| 2   | C     | 40       | Total O<br>40 40 | 0       | 0       |
| 2   | D     | 68       | Total O<br>68 68 | 0       | 0       |
| 2   | E     | 26       | Total O<br>26 26 | 0       | 0       |
| 2   | F     | 13       | Total O<br>13 13 | 0       | 0       |

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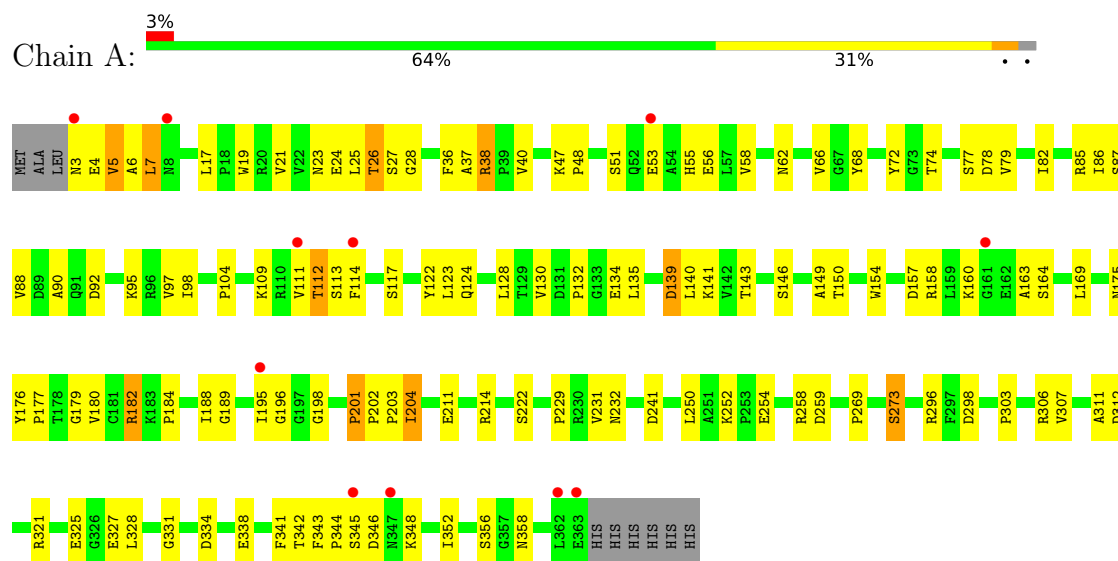
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | G     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 2   | H     | 41       | Total | O  | 0       | 0       |
|     |       |          | 41    | 41 |         |         |

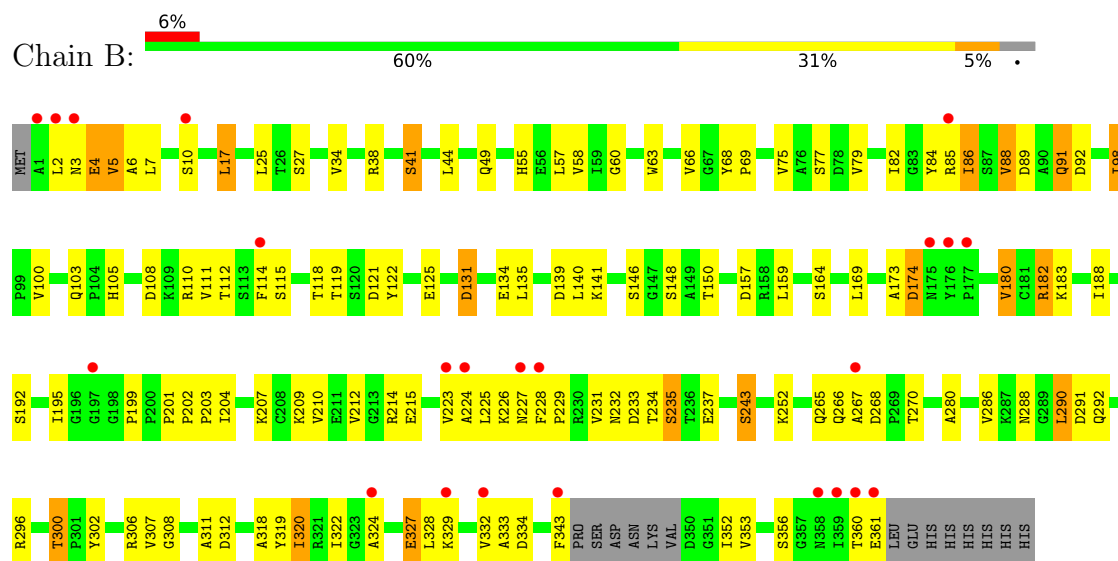
### 3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

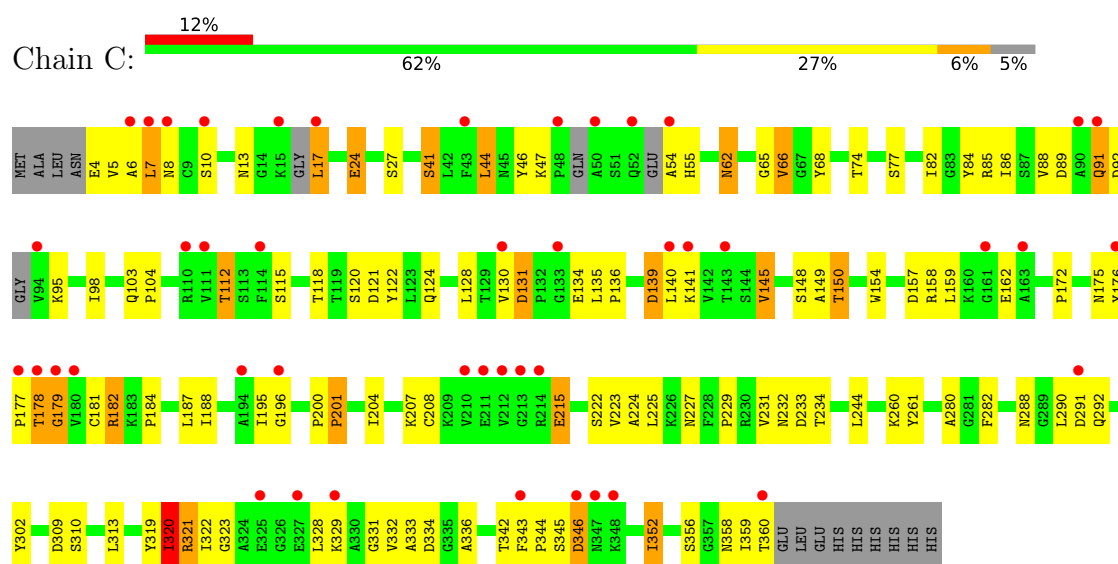
#### • Molecule 1: Fimbrial subunit CupB6



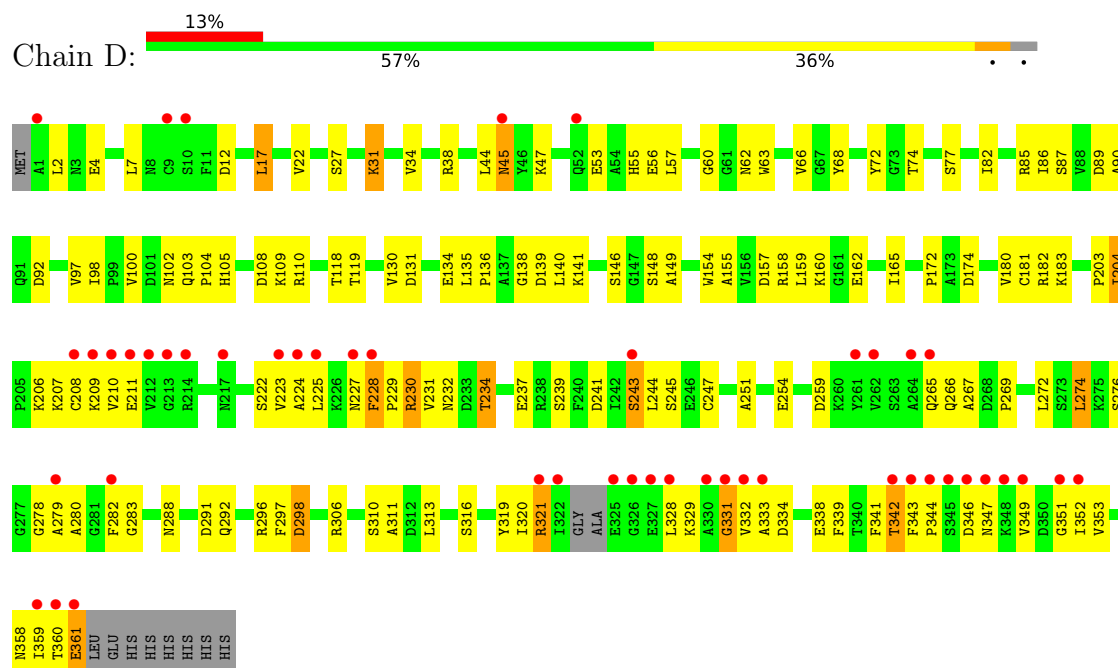
#### • Molecule 1: Fimbrial subunit CupB6



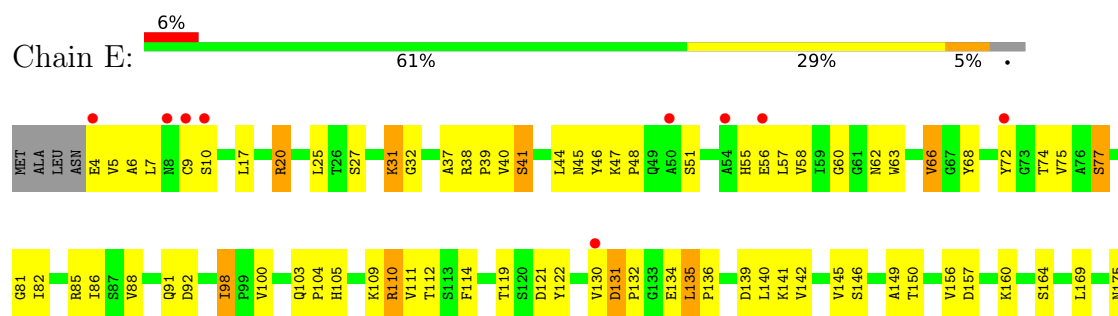
#### • Molecule 1: Fimbrial subunit CupB6

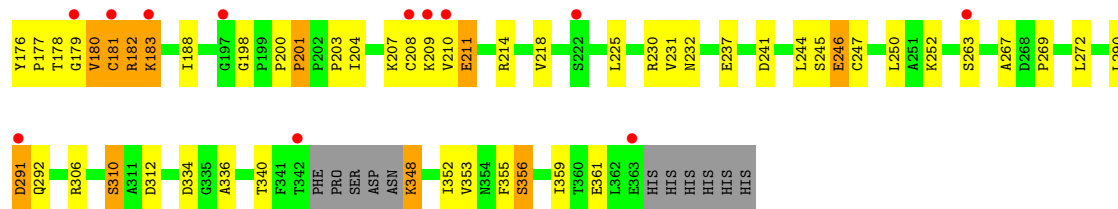


• Molecule 1: Fimbrial subunit CupB6

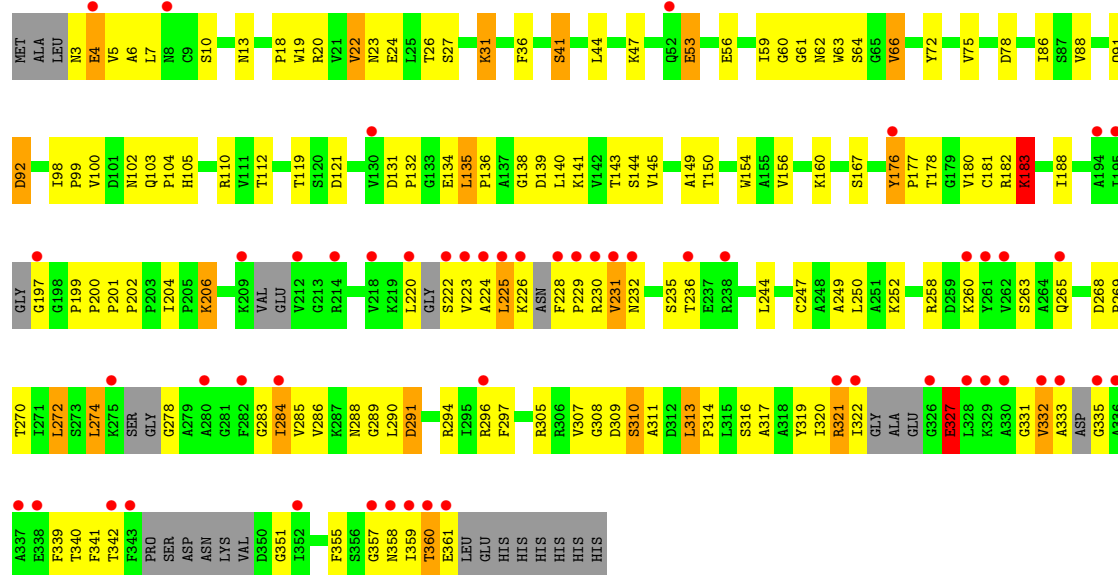


• Molecule 1: Fimbrial subunit CupB6

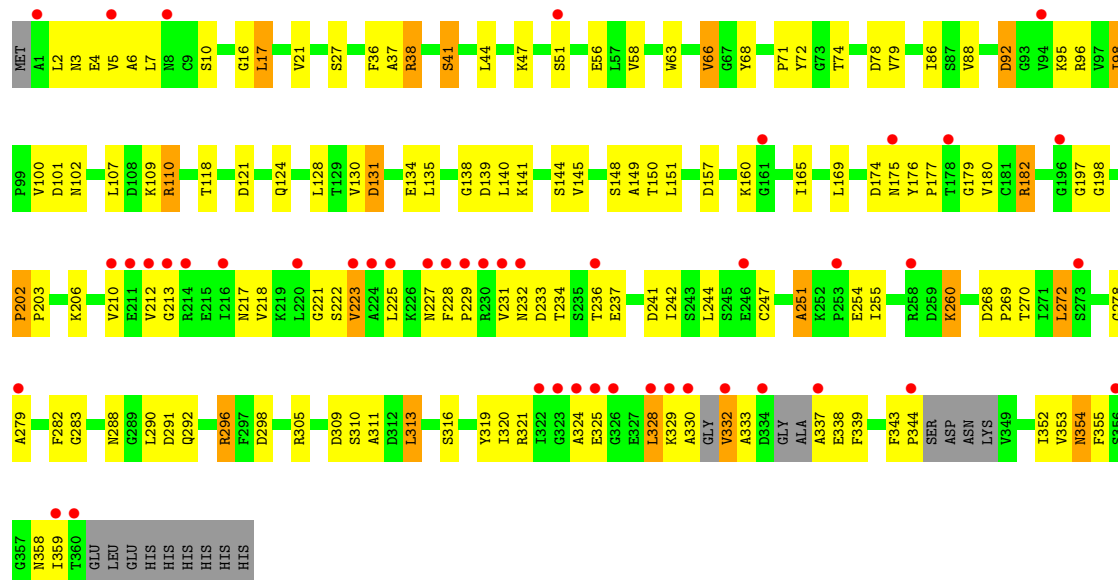




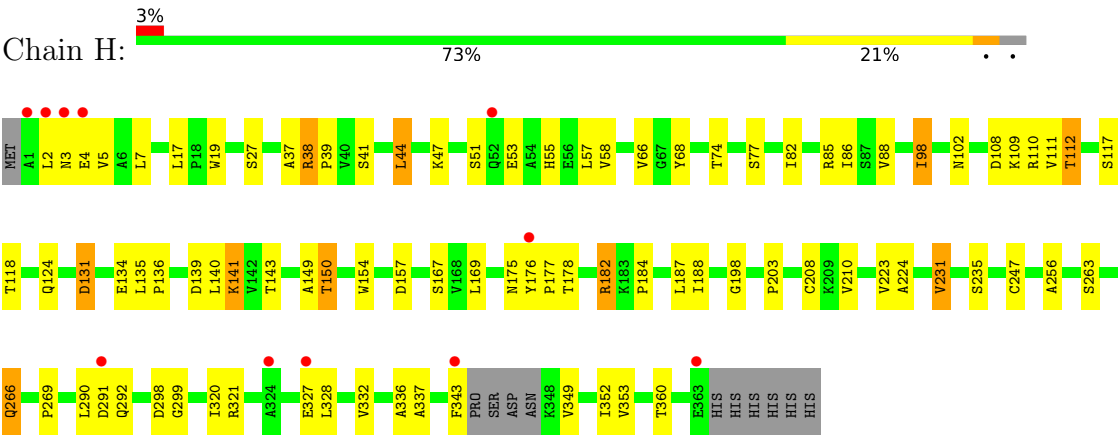
● Molecule 1: Fimbrial subunit CupB6



● Molecule 1: Fimbrial subunit CupB6



● Molecule 1: Fimbrial subunit CupB6



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 358.81Å 88.93Å 172.97Å<br>90.00° 112.94° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 97.29 – 2.77<br>97.29 – 2.77                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.2 (97.29-2.77)<br>96.2 (97.29-2.77)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.89 (at 2.77Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0103                                             | Depositor        |
| R, $R_{free}$                                                           | 0.238 , 0.266<br>0.232 , 0.261                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6115 reflections (4.95%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 58.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.029                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 47.3                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 20981                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$      |
| 1   | A     | 0.94         | 3/2692 (0.1%)   | 1.15        | 24/3671 (0.7%)   |
| 1   | B     | 1.04         | 7/2661 (0.3%)   | 1.22        | 27/3627 (0.7%)   |
| 1   | C     | 1.00         | 6/2619 (0.2%)   | 1.18        | 17/3572 (0.5%)   |
| 1   | D     | 1.00         | 2/2666 (0.1%)   | 1.16        | 24/3640 (0.7%)   |
| 1   | E     | 0.94         | 2/2654 (0.1%)   | 1.13        | 22/3616 (0.6%)   |
| 1   | F     | 0.93         | 2/2491 (0.1%)   | 1.16        | 21/3396 (0.6%)   |
| 1   | G     | 0.92         | 1/2603 (0.0%)   | 1.16        | 21/3555 (0.6%)   |
| 1   | H     | 0.91         | 0/2698          | 1.11        | 12/3673 (0.3%)   |
| All | All   | 0.96         | 23/21084 (0.1%) | 1.16        | 168/28750 (0.6%) |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | B     | 180 | VAL  | C-O   | -7.03 | 1.16        | 1.24     |
| 1   | B     | 86  | ILE  | C-O   | -6.85 | 1.16        | 1.24     |
| 1   | B     | 79  | VAL  | C-O   | -6.66 | 1.17        | 1.24     |
| 1   | C     | 320 | ILE  | C-O   | -6.65 | 1.17        | 1.24     |
| 1   | C     | 215 | GLU  | C-O   | -5.79 | 1.17        | 1.24     |
| 1   | A     | 328 | LEU  | C-O   | -5.74 | 1.17        | 1.23     |
| 1   | A     | 198 | GLY  | C-N   | 5.72  | 1.40        | 1.33     |
| 1   | C     | 322 | ILE  | C-O   | -5.55 | 1.18        | 1.24     |
| 1   | C     | 201 | PRO  | CA-C  | 5.51  | 1.55        | 1.52     |
| 1   | F     | 200 | PRO  | C-N   | 5.49  | 1.38        | 1.33     |
| 1   | B     | 84  | TYR  | C-O   | -5.34 | 1.17        | 1.24     |
| 1   | A     | 189 | GLY  | C-N   | 5.33  | 1.40        | 1.33     |
| 1   | B     | 300 | THR  | C-N   | 5.27  | 1.40        | 1.33     |
| 1   | E     | 200 | PRO  | C-N   | 5.24  | 1.38        | 1.33     |
| 1   | C     | 135 | LEU  | C-N   | 5.16  | 1.39        | 1.33     |
| 1   | G     | 251 | ALA  | N-CA  | -5.15 | 1.39        | 1.45     |
| 1   | C     | 204 | ILE  | CA-C  | -5.12 | 1.48        | 1.53     |
| 1   | B     | 302 | TYR  | C-N   | 5.07  | 1.40        | 1.33     |
| 1   | B     | 173 | ALA  | C-O   | -5.07 | 1.17        | 1.24     |
| 1   | D     | 148 | SER  | C-O   | -5.06 | 1.17        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | E     | 135 | LEU  | C-N   | 5.05 | 1.39        | 1.33     |
| 1   | D     | 135 | LEU  | C-N   | 5.04 | 1.39        | 1.33     |
| 1   | F     | 135 | LEU  | C-N   | 5.03 | 1.39        | 1.33     |

All (168) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 231 | VAL  | N-CA-C | 8.07  | 118.85      | 110.62   |
| 1   | F     | 135 | LEU  | CA-C-N | -7.60 | 112.50      | 120.03   |
| 1   | F     | 135 | LEU  | C-N-CA | -7.60 | 112.50      | 120.03   |
| 1   | H     | 349 | VAL  | N-CA-C | 7.58  | 118.78      | 109.30   |
| 1   | G     | 68  | TYR  | CA-C-N | -7.53 | 113.07      | 120.52   |
| 1   | G     | 68  | TYR  | C-N-CA | -7.53 | 113.07      | 120.52   |
| 1   | F     | 332 | VAL  | N-CA-C | 7.36  | 117.53      | 106.42   |
| 1   | F     | 200 | PRO  | CA-C-N | -7.34 | 114.30      | 119.66   |
| 1   | F     | 200 | PRO  | C-N-CA | -7.34 | 114.30      | 119.66   |
| 1   | C     | 179 | GLY  | N-CA-C | -7.31 | 104.98      | 114.85   |
| 1   | C     | 323 | GLY  | N-CA-C | 7.28  | 124.28      | 111.25   |
| 1   | C     | 135 | LEU  | CA-C-N | -7.21 | 113.25      | 120.31   |
| 1   | C     | 135 | LEU  | C-N-CA | -7.21 | 113.25      | 120.31   |
| 1   | A     | 198 | GLY  | CA-C-N | -7.18 | 112.99      | 120.38   |
| 1   | A     | 198 | GLY  | C-N-CA | -7.18 | 112.99      | 120.38   |
| 1   | D     | 135 | LEU  | CA-C-N | -7.17 | 112.93      | 120.03   |
| 1   | D     | 135 | LEU  | C-N-CA | -7.17 | 112.93      | 120.03   |
| 1   | B     | 174 | ASP  | N-CA-C | 7.09  | 120.12      | 110.55   |
| 1   | C     | 200 | PRO  | CA-C-N | -7.00 | 114.62      | 119.66   |
| 1   | C     | 200 | PRO  | C-N-CA | -7.00 | 114.62      | 119.66   |
| 1   | E     | 135 | LEU  | CA-C-N | -6.99 | 113.11      | 120.03   |
| 1   | E     | 135 | LEU  | C-N-CA | -6.99 | 113.11      | 120.03   |
| 1   | D     | 331 | GLY  | N-CA-C | 6.99  | 122.77      | 111.38   |
| 1   | B     | 300 | THR  | CA-C-N | -6.92 | 112.81      | 120.14   |
| 1   | B     | 300 | THR  | C-N-CA | -6.92 | 112.81      | 120.14   |
| 1   | H     | 135 | LEU  | CA-C-N | -6.91 | 113.19      | 120.03   |
| 1   | H     | 135 | LEU  | C-N-CA | -6.91 | 113.19      | 120.03   |
| 1   | D     | 347 | ASN  | N-CA-C | 6.84  | 120.11      | 111.69   |
| 1   | A     | 47  | LYS  | CA-C-N | -6.83 | 113.62      | 120.31   |
| 1   | A     | 47  | LYS  | C-N-CA | -6.83 | 113.62      | 120.31   |
| 1   | E     | 252 | LYS  | CA-C-N | -6.74 | 113.36      | 120.03   |
| 1   | E     | 252 | LYS  | C-N-CA | -6.74 | 113.36      | 120.03   |
| 1   | F     | 22  | VAL  | N-CA-C | -6.73 | 106.03      | 111.81   |
| 1   | A     | 135 | LEU  | CA-C-N | -6.69 | 113.40      | 120.03   |
| 1   | A     | 135 | LEU  | C-N-CA | -6.69 | 113.40      | 120.03   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 189 | GLY  | CA-C-N | -6.64 | 112.78      | 119.56   |
| 1   | A     | 189 | GLY  | C-N-CA | -6.64 | 112.78      | 119.56   |
| 1   | G     | 98  | ILE  | N-CA-C | -6.62 | 102.46      | 108.95   |
| 1   | B     | 302 | TYR  | CA-C-N | -6.57 | 113.21      | 119.85   |
| 1   | B     | 302 | TYR  | C-N-CA | -6.57 | 113.21      | 119.85   |
| 1   | G     | 135 | LEU  | CA-C-N | -6.54 | 113.24      | 119.85   |
| 1   | G     | 135 | LEU  | C-N-CA | -6.54 | 113.24      | 119.85   |
| 1   | B     | 135 | LEU  | CA-C-N | -6.53 | 113.56      | 120.03   |
| 1   | B     | 135 | LEU  | C-N-CA | -6.53 | 113.56      | 120.03   |
| 1   | B     | 201 | PRO  | CA-C-N | -6.43 | 115.03      | 119.66   |
| 1   | B     | 201 | PRO  | C-N-CA | -6.43 | 115.03      | 119.66   |
| 1   | F     | 183 | LYS  | N-CA-C | 6.42  | 117.88      | 109.93   |
| 1   | A     | 327 | GLU  | N-CA-C | 6.40  | 119.24      | 111.82   |
| 1   | D     | 17  | LEU  | CA-C-N | -6.32 | 114.12      | 120.31   |
| 1   | D     | 17  | LEU  | C-N-CA | -6.32 | 114.12      | 120.31   |
| 1   | A     | 201 | PRO  | CA-C-N | -6.26 | 113.93      | 120.38   |
| 1   | A     | 201 | PRO  | C-N-CA | -6.26 | 113.93      | 120.38   |
| 1   | B     | 183 | LYS  | N-CA-C | 6.26  | 117.96      | 110.07   |
| 1   | A     | 139 | ASP  | N-CA-C | 6.17  | 118.08      | 111.36   |
| 1   | C     | 331 | GLY  | N-CA-C | 6.15  | 118.87      | 110.69   |
| 1   | A     | 201 | PRO  | O-C-N  | 6.11  | 124.12      | 121.31   |
| 1   | A     | 201 | PRO  | N-CA-C | 6.04  | 116.26      | 110.47   |
| 1   | C     | 103 | GLN  | CA-C-N | -6.00 | 114.09      | 120.03   |
| 1   | C     | 103 | GLN  | C-N-CA | -6.00 | 114.09      | 120.03   |
| 1   | B     | 98  | ILE  | CA-C-N | -5.99 | 114.44      | 120.31   |
| 1   | B     | 98  | ILE  | C-N-CA | -5.99 | 114.44      | 120.31   |
| 1   | A     | 202 | PRO  | CA-C-N | -5.97 | 114.46      | 120.31   |
| 1   | A     | 202 | PRO  | C-N-CA | -5.97 | 114.46      | 120.31   |
| 1   | E     | 200 | PRO  | CA-C-N | -5.95 | 115.32      | 119.66   |
| 1   | E     | 200 | PRO  | C-N-CA | -5.95 | 115.32      | 119.66   |
| 1   | B     | 131 | ASP  | CA-C-N | -5.94 | 112.75      | 119.28   |
| 1   | B     | 131 | ASP  | C-N-CA | -5.94 | 112.75      | 119.28   |
| 1   | E     | 290 | LEU  | N-CA-C | 5.93  | 117.55      | 111.14   |
| 1   | E     | 267 | ALA  | N-CA-C | -5.91 | 104.84      | 111.28   |
| 1   | B     | 202 | PRO  | CA-C-N | -5.86 | 114.57      | 120.31   |
| 1   | B     | 202 | PRO  | C-N-CA | -5.86 | 114.57      | 120.31   |
| 1   | B     | 103 | GLN  | CA-C-N | -5.85 | 113.94      | 119.85   |
| 1   | B     | 103 | GLN  | C-N-CA | -5.85 | 113.94      | 119.85   |
| 1   | D     | 174 | ASP  | N-CA-C | 5.83  | 118.43      | 110.55   |
| 1   | C     | 131 | ASP  | CA-C-N | -5.80 | 112.90      | 119.28   |
| 1   | C     | 131 | ASP  | C-N-CA | -5.80 | 112.90      | 119.28   |
| 1   | F     | 290 | LEU  | CA-C-N | 5.79  | 128.04      | 120.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 290 | LEU  | C-N-CA | 5.79  | 128.04      | 120.28   |
| 1   | E     | 131 | ASP  | CA-C-N | -5.79 | 112.91      | 119.28   |
| 1   | E     | 131 | ASP  | C-N-CA | -5.79 | 112.91      | 119.28   |
| 1   | F     | 103 | GLN  | CA-C-N | -5.76 | 114.32      | 120.03   |
| 1   | F     | 103 | GLN  | C-N-CA | -5.76 | 114.32      | 120.03   |
| 1   | E     | 180 | VAL  | N-CA-C | -5.75 | 101.28      | 109.51   |
| 1   | E     | 181 | CYS  | N-CA-C | 5.75  | 118.13      | 108.23   |
| 1   | A     | 325 | GLU  | N-CA-C | 5.74  | 118.00      | 111.11   |
| 1   | B     | 252 | LYS  | CA-C-N | -5.71 | 114.08      | 120.14   |
| 1   | B     | 252 | LYS  | C-N-CA | -5.71 | 114.08      | 120.14   |
| 1   | D     | 103 | GLN  | CA-C-N | -5.70 | 114.39      | 120.03   |
| 1   | D     | 103 | GLN  | C-N-CA | -5.70 | 114.39      | 120.03   |
| 1   | B     | 290 | LEU  | CA-C-N | 5.68  | 127.89      | 120.28   |
| 1   | B     | 290 | LEU  | C-N-CA | 5.68  | 127.89      | 120.28   |
| 1   | F     | 230 | ARG  | N-CA-C | 5.68  | 117.37      | 109.31   |
| 1   | D     | 131 | ASP  | CA-C-N | -5.67 | 112.75      | 119.05   |
| 1   | D     | 131 | ASP  | C-N-CA | -5.67 | 112.75      | 119.05   |
| 1   | D     | 207 | LYS  | N-CA-C | 5.67  | 118.47      | 110.14   |
| 1   | D     | 267 | ALA  | N-CA-C | -5.67 | 105.11      | 111.28   |
| 1   | A     | 68  | TYR  | CA-C-N | -5.66 | 114.76      | 120.31   |
| 1   | A     | 68  | TYR  | C-N-CA | -5.66 | 114.76      | 120.31   |
| 1   | G     | 198 | GLY  | CA-C-N | -5.66 | 114.55      | 120.38   |
| 1   | G     | 198 | GLY  | C-N-CA | -5.66 | 114.55      | 120.38   |
| 1   | F     | 131 | ASP  | CA-C-N | -5.63 | 112.80      | 119.05   |
| 1   | F     | 131 | ASP  | C-N-CA | -5.63 | 112.80      | 119.05   |
| 1   | F     | 252 | LYS  | CA-C-N | -5.61 | 114.81      | 120.31   |
| 1   | F     | 252 | LYS  | C-N-CA | -5.61 | 114.81      | 120.31   |
| 1   | G     | 131 | ASP  | CA-C-N | -5.61 | 112.82      | 119.05   |
| 1   | G     | 131 | ASP  | C-N-CA | -5.61 | 112.82      | 119.05   |
| 1   | G     | 202 | PRO  | N-CA-C | 5.57  | 117.50      | 110.70   |
| 1   | B     | 17  | LEU  | CA-C-N | -5.50 | 114.67      | 120.66   |
| 1   | B     | 17  | LEU  | C-N-CA | -5.50 | 114.67      | 120.66   |
| 1   | D     | 239 | SER  | N-CA-C | 5.49  | 118.57      | 109.46   |
| 1   | D     | 228 | PHE  | CA-C-N | 5.49  | 124.83      | 118.85   |
| 1   | D     | 228 | PHE  | C-N-CA | 5.49  | 124.83      | 118.85   |
| 1   | F     | 4   | GLU  | N-CA-C | 5.48  | 117.60      | 110.53   |
| 1   | G     | 254 | GLU  | N-CA-C | -5.45 | 100.51      | 109.40   |
| 1   | B     | 180 | VAL  | N-CA-C | -5.43 | 102.04      | 109.37   |
| 1   | A     | 204 | ILE  | CA-C-N | -5.41 | 114.35      | 119.76   |
| 1   | A     | 204 | ILE  | C-N-CA | -5.41 | 114.35      | 119.76   |
| 1   | H     | 98  | ILE  | CA-C-N | -5.39 | 115.03      | 120.85   |
| 1   | H     | 98  | ILE  | C-N-CA | -5.39 | 115.03      | 120.85   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 17  | LEU  | CA-C-N | -5.38 | 114.44      | 120.14   |
| 1   | G     | 17  | LEU  | C-N-CA | -5.38 | 114.44      | 120.14   |
| 1   | A     | 331 | GLY  | N-CA-C | 5.37  | 117.44      | 110.45   |
| 1   | D     | 139 | ASP  | N-CA-C | 5.37  | 119.09      | 112.54   |
| 1   | E     | 201 | PRO  | N-CA-C | 5.36  | 115.61      | 110.47   |
| 1   | E     | 47  | LYS  | CA-C-N | -5.35 | 114.47      | 120.14   |
| 1   | E     | 47  | LYS  | C-N-CA | -5.35 | 114.47      | 120.14   |
| 1   | H     | 131 | ASP  | CA-C-N | -5.35 | 113.11      | 119.05   |
| 1   | H     | 131 | ASP  | C-N-CA | -5.35 | 113.11      | 119.05   |
| 1   | B     | 199 | PRO  | CA-C-N | -5.34 | 114.88      | 120.38   |
| 1   | B     | 199 | PRO  | C-N-CA | -5.34 | 114.88      | 120.38   |
| 1   | D     | 68  | TYR  | CA-C-N | -5.32 | 114.76      | 120.03   |
| 1   | D     | 68  | TYR  | C-N-CA | -5.32 | 114.76      | 120.03   |
| 1   | E     | 198 | GLY  | CA-C-N | -5.31 | 114.91      | 120.38   |
| 1   | E     | 198 | GLY  | C-N-CA | -5.31 | 114.91      | 120.38   |
| 1   | E     | 207 | LYS  | N-CA-C | 5.29  | 118.33      | 110.14   |
| 1   | F     | 313 | LEU  | CA-C-N | -5.28 | 114.16      | 120.13   |
| 1   | F     | 313 | LEU  | C-N-CA | -5.28 | 114.16      | 120.13   |
| 1   | G     | 38  | ARG  | CA-C-N | -5.27 | 114.53      | 119.85   |
| 1   | G     | 38  | ARG  | C-N-CA | -5.27 | 114.53      | 119.85   |
| 1   | H     | 263 | SER  | N-CA-C | 5.26  | 117.01      | 111.28   |
| 1   | D     | 204 | ILE  | CA-C-N | -5.23 | 114.53      | 119.76   |
| 1   | D     | 204 | ILE  | C-N-CA | -5.23 | 114.53      | 119.76   |
| 1   | G     | 290 | LEU  | CA-C-N | 5.23  | 127.72      | 120.29   |
| 1   | G     | 290 | LEU  | C-N-CA | 5.23  | 127.72      | 120.29   |
| 1   | E     | 201 | PRO  | CA-C-N | -5.20 | 115.03      | 120.38   |
| 1   | E     | 201 | PRO  | C-N-CA | -5.20 | 115.03      | 120.38   |
| 1   | A     | 252 | LYS  | CA-C-N | -5.17 | 115.24      | 120.31   |
| 1   | A     | 252 | LYS  | C-N-CA | -5.17 | 115.24      | 120.31   |
| 1   | F     | 321 | ARG  | N-CA-C | 5.17  | 117.19      | 108.96   |
| 1   | G     | 47  | LYS  | CA-C-N | -5.16 | 114.67      | 120.14   |
| 1   | G     | 47  | LYS  | C-N-CA | -5.16 | 114.67      | 120.14   |
| 1   | G     | 313 | LEU  | CA-C-N | -5.14 | 114.62      | 119.76   |
| 1   | G     | 313 | LEU  | C-N-CA | -5.14 | 114.62      | 119.76   |
| 1   | E     | 98  | ILE  | CA-C-N | -5.13 | 115.31      | 120.85   |
| 1   | E     | 98  | ILE  | C-N-CA | -5.13 | 115.31      | 120.85   |
| 1   | C     | 91  | GLN  | N-CA-C | -5.13 | 105.87      | 111.82   |
| 1   | C     | 346 | ASP  | N-CA-C | 5.12  | 117.41      | 108.76   |
| 1   | F     | 327 | GLU  | N-CA-C | 5.12  | 117.75      | 111.82   |
| 1   | C     | 17  | LEU  | CA-C-N | -5.09 | 115.11      | 120.66   |
| 1   | C     | 17  | LEU  | C-N-CA | -5.09 | 115.11      | 120.66   |
| 1   | D     | 329 | LYS  | N-CA-C | -5.07 | 101.08      | 108.07   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | H     | 198 | GLY  | CA-C-N | -5.07 | 115.16      | 120.38   |
| 1   | H     | 198 | GLY  | C-N-CA | -5.07 | 115.16      | 120.38   |
| 1   | C     | 302 | TYR  | CA-C-N | -5.04 | 114.76      | 119.85   |
| 1   | C     | 302 | TYR  | C-N-CA | -5.04 | 114.76      | 119.85   |
| 1   | H     | 327 | GLU  | N-CA-C | 5.03  | 117.65      | 111.82   |
| 1   | D     | 47  | LYS  | CA-C-N | -5.02 | 114.57      | 119.99   |
| 1   | D     | 47  | LYS  | C-N-CA | -5.02 | 114.57      | 119.99   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2637  | 0        | 2592     | 105     | 0            |
| 1   | B     | 2608  | 0        | 2565     | 105     | 0            |
| 1   | C     | 2574  | 0        | 2501     | 144     | 0            |
| 1   | D     | 2616  | 0        | 2548     | 165     | 0            |
| 1   | E     | 2602  | 0        | 2573     | 112     | 0            |
| 1   | F     | 2452  | 0        | 2334     | 144     | 0            |
| 1   | G     | 2550  | 0        | 2482     | 159     | 0            |
| 1   | H     | 2644  | 0        | 2628     | 62      | 0            |
| 2   | A     | 39    | 0        | 0        | 1       | 0            |
| 2   | B     | 62    | 0        | 0        | 2       | 0            |
| 2   | C     | 40    | 0        | 0        | 1       | 0            |
| 2   | D     | 68    | 0        | 0        | 0       | 0            |
| 2   | E     | 26    | 0        | 0        | 2       | 0            |
| 2   | F     | 13    | 0        | 0        | 1       | 0            |
| 2   | G     | 9     | 0        | 0        | 0       | 0            |
| 2   | H     | 41    | 0        | 0        | 0       | 0            |
| All | All   | 20981 | 0        | 20223    | 972     | 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 24.

All (972) 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) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:228:PHE:CE2  | 1:G:282:PHE:HE1  | 1.21                     | 1.57              |
| 1:G:325:GLU:HA   | 1:G:328:LEU:CD2  | 1.35                     | 1.55              |
| 1:D:224:ALA:CA   | 1:D:360:THR:HB   | 1.11                     | 1.54              |
| 1:G:279:ALA:CA   | 1:G:330:ALA:HB2  | 1.37                     | 1.52              |
| 1:G:228:PHE:CE2  | 1:G:282:PHE:CE1  | 2.00                     | 1.50              |
| 1:D:224:ALA:HA   | 1:D:360:THR:CB   | 1.42                     | 1.43              |
| 1:G:279:ALA:CB   | 1:G:330:ALA:CB   | 1.98                     | 1.41              |
| 1:G:325:GLU:CA   | 1:G:328:LEU:HD21 | 0.94                     | 1.41              |
| 1:G:324:ALA:O    | 1:G:328:LEU:CD2  | 1.72                     | 1.36              |
| 1:G:325:GLU:CA   | 1:G:328:LEU:CD2  | 1.89                     | 1.35              |
| 1:G:324:ALA:O    | 1:G:328:LEU:HD23 | 1.22                     | 1.34              |
| 1:G:228:PHE:CD2  | 1:G:282:PHE:HE1  | 1.45                     | 1.33              |
| 1:G:279:ALA:HA   | 1:G:330:ALA:CB   | 1.62                     | 1.30              |
| 1:G:279:ALA:CA   | 1:G:330:ALA:CB   | 2.12                     | 1.27              |
| 1:G:228:PHE:HE2  | 1:G:282:PHE:CE1  | 1.40                     | 1.26              |
| 1:C:4:GLU:O      | 1:C:55:HIS:CB    | 1.82                     | 1.25              |
| 1:E:150:THR:CG2  | 1:E:188:ILE:HG12 | 1.66                     | 1.25              |
| 1:G:325:GLU:N    | 1:G:328:LEU:HD21 | 1.51                     | 1.25              |
| 1:C:5:VAL:HG22   | 1:C:55:HIS:CD2   | 1.72                     | 1.25              |
| 1:G:279:ALA:HB2  | 1:G:330:ALA:CB   | 1.61                     | 1.24              |
| 1:F:274:LEU:HD23 | 1:F:333:ALA:CB   | 1.66                     | 1.24              |
| 1:B:4:GLU:O      | 1:B:112:THR:HG21 | 1.08                     | 1.23              |
| 1:G:217:ASN:ND2  | 1:G:354:ASN:OD1  | 1.72                     | 1.21              |
| 1:G:228:PHE:CD2  | 1:G:282:PHE:CE1  | 2.25                     | 1.21              |
| 1:G:279:ALA:CB   | 1:G:330:ALA:HB3  | 1.63                     | 1.21              |
| 1:F:339:PHE:CE1  | 1:F:351:GLY:HA3  | 1.77                     | 1.19              |
| 1:C:7:LEU:HD23   | 1:C:47:LYS:O     | 1.41                     | 1.18              |
| 1:D:224:ALA:CB   | 1:D:360:THR:HB   | 1.75                     | 1.16              |
| 1:D:224:ALA:CA   | 1:D:360:THR:CB   | 2.06                     | 1.15              |
| 1:E:150:THR:HG22 | 1:E:188:ILE:HG12 | 1.19                     | 1.15              |
| 1:C:4:GLU:O      | 1:C:55:HIS:HB2   | 0.97                     | 1.14              |
| 1:G:324:ALA:C    | 1:G:328:LEU:CD2  | 2.18                     | 1.14              |
| 1:F:222:SER:OG   | 1:F:358:ASN:HB2  | 1.45                     | 1.14              |
| 1:C:5:VAL:CG2    | 1:C:55:HIS:HD2   | 1.64                     | 1.11              |
| 1:D:279:ALA:N    | 1:D:331:GLY:O    | 1.84                     | 1.11              |
| 1:D:338:GLU:HG2  | 1:D:352:ILE:CD1  | 1.81                     | 1.10              |
| 1:G:278:GLY:HA2  | 1:G:332:VAL:HG13 | 1.30                     | 1.10              |
| 1:C:292:GLN:NE2  | 1:D:22:VAL:HG11  | 1.66                     | 1.10              |
| 1:B:141:LYS:HG3  | 1:B:203:PRO:HB3  | 1.26                     | 1.10              |
| 1:A:343:PHE:N    | 1:A:344:PRO:HA   | 1.67                     | 1.09              |
| 1:B:4:GLU:O      | 1:B:112:THR:CG2  | 2.00                     | 1.09              |
| 1:D:338:GLU:HG2  | 1:D:352:ILE:HD13 | 1.35                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:325:GLU:HA   | 1:G:328:LEU:CG   | 1.83                     | 1.09              |
| 1:C:5:VAL:CG2    | 1:C:55:HIS:CD2   | 2.36                     | 1.08              |
| 1:G:278:GLY:CA   | 1:G:332:VAL:HG13 | 1.84                     | 1.06              |
| 1:G:325:GLU:C    | 1:G:328:LEU:HD21 | 1.80                     | 1.06              |
| 1:D:224:ALA:HA   | 1:D:360:THR:CA   | 1.85                     | 1.06              |
| 1:B:4:GLU:C      | 1:B:112:THR:HG21 | 1.79                     | 1.05              |
| 1:G:279:ALA:HB1  | 1:G:330:ALA:HB3  | 1.39                     | 1.05              |
| 1:G:328:LEU:HD23 | 1:G:328:LEU:H    | 1.17                     | 1.04              |
| 1:D:234:THR:HG23 | 1:D:320:ILE:HD12 | 1.36                     | 1.04              |
| 1:B:34:VAL:CG2   | 1:B:85:ARG:NH2   | 2.21                     | 1.04              |
| 1:F:138:GLY:O    | 1:F:206:LYS:NZ   | 1.91                     | 1.04              |
| 1:B:34:VAL:CG2   | 1:B:85:ARG:HH21  | 1.70                     | 1.04              |
| 1:A:88:VAL:HG12  | 1:A:122:TYR:CE1  | 1.93                     | 1.03              |
| 1:C:343:PHE:N    | 1:C:344:PRO:HA   | 1.70                     | 1.02              |
| 1:E:41:SER:OG    | 1:E:121:ASP:OD1  | 1.76                     | 1.02              |
| 1:G:278:GLY:HA2  | 1:G:332:VAL:CG1  | 1.87                     | 1.02              |
| 1:G:325:GLU:C    | 1:G:328:LEU:CD2  | 2.31                     | 1.02              |
| 1:E:141:LYS:HG3  | 1:E:203:PRO:HB3  | 1.40                     | 1.02              |
| 1:F:110:ARG:NH1  | 1:F:119:THR:O    | 1.91                     | 1.02              |
| 1:F:274:LEU:HD23 | 1:F:333:ALA:HB1  | 1.05                     | 1.02              |
| 1:C:41:SER:OG    | 1:C:121:ASP:OD1  | 1.76                     | 1.01              |
| 1:E:157:ASP:O    | 1:E:182:ARG:NH2  | 1.94                     | 1.01              |
| 1:G:279:ALA:HB2  | 1:G:330:ALA:HB1  | 1.34                     | 1.01              |
| 1:G:229:PRO:HG2  | 1:G:233:ASP:OD2  | 1.58                     | 1.01              |
| 1:C:224:ALA:HA   | 1:C:360:THR:O    | 1.60                     | 1.01              |
| 1:F:222:SER:HA   | 1:F:358:ASN:O    | 1.60                     | 1.00              |
| 1:C:292:GLN:HE21 | 1:D:22:VAL:HG11  | 1.19                     | 1.00              |
| 1:C:6:ALA:HB1    | 1:C:46:TYR:CD2   | 1.95                     | 1.00              |
| 1:C:55:HIS:CE1   | 1:C:159:LEU:HD23 | 1.96                     | 1.00              |
| 1:C:292:GLN:NE2  | 1:D:22:VAL:CG1   | 2.23                     | 1.00              |
| 1:D:223:VAL:O    | 1:D:360:THR:N    | 1.93                     | 1.00              |
| 1:A:88:VAL:HG12  | 1:A:122:TYR:CD1  | 1.96                     | 1.00              |
| 1:C:55:HIS:HE1   | 1:C:159:LEU:HD23 | 1.23                     | 0.99              |
| 1:C:5:VAL:HG22   | 1:C:55:HIS:HD2   | 0.83                     | 0.99              |
| 1:D:224:ALA:N    | 1:D:360:THR:HB   | 1.76                     | 0.99              |
| 1:F:285:VAL:HG11 | 1:F:294:ARG:HH11 | 1.24                     | 0.98              |
| 1:H:157:ASP:O    | 1:H:182:ARG:NH2  | 1.96                     | 0.98              |
| 1:D:224:ALA:HB2  | 1:D:360:THR:CG2  | 1.94                     | 0.98              |
| 1:D:274:LEU:HD12 | 1:D:274:LEU:H    | 1.29                     | 0.98              |
| 1:H:231:VAL:O    | 1:H:321:ARG:O    | 1.82                     | 0.97              |
| 1:D:278:GLY:HA2  | 1:D:332:VAL:HB   | 1.44                     | 0.97              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:110:ARG:NH2  | 1:E:119:THR:O    | 1.98                     | 0.96              |
| 1:G:325:GLU:O    | 1:G:328:LEU:HG   | 1.64                     | 0.96              |
| 1:C:130:VAL:CG1  | 1:C:134:GLU:HB2  | 1.96                     | 0.96              |
| 1:D:110:ARG:NH2  | 1:D:119:THR:O    | 1.98                     | 0.95              |
| 1:D:109:LYS:HG3  | 1:D:165:ILE:HD11 | 1.48                     | 0.95              |
| 1:A:258:ARG:NH2  | 1:A:298:ASP:O    | 2.00                     | 0.94              |
| 1:B:34:VAL:HG22  | 1:B:85:ARG:HH21  | 1.29                     | 0.94              |
| 1:H:4:GLU:OE2    | 1:H:4:GLU:N      | 2.01                     | 0.94              |
| 1:B:34:VAL:HG22  | 1:B:85:ARG:NH2   | 1.83                     | 0.93              |
| 1:E:210:VAL:HG12 | 1:E:211:GLU:H    | 1.30                     | 0.93              |
| 1:H:150:THR:CG2  | 1:H:188:ILE:HG12 | 1.98                     | 0.93              |
| 1:F:231:VAL:O    | 1:F:232:ASN:HB2  | 1.67                     | 0.93              |
| 1:D:278:GLY:C    | 1:D:331:GLY:O    | 2.11                     | 0.93              |
| 1:F:6:ALA:C      | 1:F:7:LEU:HD12   | 1.93                     | 0.93              |
| 1:F:274:LEU:CD2  | 1:F:333:ALA:HB1  | 1.96                     | 0.93              |
| 1:E:4:GLU:HB2    | 1:E:112:THR:HG23 | 1.51                     | 0.93              |
| 1:E:175:ASN:HD21 | 1:E:179:GLY:H    | 1.12                     | 0.93              |
| 1:F:260:LYS:CE   | 1:F:260:LYS:CG   | 2.47                     | 0.92              |
| 1:E:32:GLY:HA3   | 1:E:72:TYR:CE2   | 2.04                     | 0.92              |
| 1:E:150:THR:HG21 | 1:E:188:ILE:HG12 | 1.51                     | 0.91              |
| 1:C:7:LEU:CD2    | 1:C:47:LYS:O     | 2.18                     | 0.91              |
| 1:E:77:SER:OG    | 1:E:82:ILE:O     | 1.87                     | 0.91              |
| 1:C:84:TYR:OH    | 1:C:124:GLN:NE2  | 2.04                     | 0.91              |
| 1:C:89:ASP:OD1   | 1:C:95:LYS:HE3   | 1.71                     | 0.90              |
| 1:G:7:LEU:HD23   | 1:G:180:VAL:HA   | 1.50                     | 0.90              |
| 1:C:7:LEU:HD23   | 1:C:7:LEU:H      | 1.37                     | 0.90              |
| 1:A:48:PRO:HG2   | 1:A:114:PHE:O    | 1.71                     | 0.90              |
| 1:A:26:THR:HG22  | 1:A:28:GLY:H     | 1.37                     | 0.90              |
| 1:F:285:VAL:HG11 | 1:F:294:ARG:NH1  | 1.86                     | 0.90              |
| 1:A:150:THR:HG22 | 1:A:188:ILE:HG23 | 1.52                     | 0.89              |
| 1:D:224:ALA:HB2  | 1:D:360:THR:HG21 | 1.52                     | 0.89              |
| 1:F:249:ALA:O    | 1:F:250:LEU:HB2  | 1.73                     | 0.89              |
| 1:C:92:ASP:O     | 1:D:230:ARG:NH2  | 2.06                     | 0.89              |
| 1:B:207:LYS:HG3  | 1:B:343:PHE:CZ   | 2.08                     | 0.88              |
| 1:C:6:ALA:CB     | 1:C:46:TYR:CD2   | 2.56                     | 0.88              |
| 1:G:229:PRO:CG   | 1:G:233:ASP:OD2  | 2.20                     | 0.88              |
| 1:F:47:LYS:CD    | 1:F:47:LYS:CB    | 2.51                     | 0.88              |
| 1:E:175:ASN:O    | 1:E:175:ASN:ND2  | 2.06                     | 0.88              |
| 1:G:206:LYS:HA   | 1:G:251:ALA:HB2  | 1.56                     | 0.88              |
| 1:C:130:VAL:HG12 | 1:C:134:GLU:HB2  | 1.55                     | 0.87              |
| 1:E:7:LEU:HD23   | 1:E:180:VAL:HA   | 1.57                     | 0.87              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:86:ILE:HG23  | 1:A:98:ILE:HD12  | 1.55                     | 0.87              |
| 1:G:229:PRO:HD2  | 1:G:233:ASP:OD2  | 1.75                     | 0.87              |
| 1:B:227:ASN:O    | 1:B:229:PRO:HD3  | 1.75                     | 0.86              |
| 1:A:141:LYS:HG3  | 1:A:203:PRO:HB3  | 1.57                     | 0.86              |
| 1:G:338:GLU:HB3  | 1:G:352:ILE:HD13 | 1.56                     | 0.86              |
| 1:E:361:GLU:O    | 2:E:401:HOH:O    | 1.93                     | 0.86              |
| 1:C:172:PRO:HB2  | 1:C:182:ARG:HH11 | 1.39                     | 0.86              |
| 1:H:108:ASP:OD2  | 1:H:110:ARG:NH1  | 2.09                     | 0.86              |
| 1:C:208:CYS:H    | 1:C:343:PHE:HE2  | 1.25                     | 0.85              |
| 1:C:292:GLN:HE21 | 1:D:22:VAL:CG1   | 1.86                     | 0.85              |
| 1:D:7:LEU:HD23   | 1:D:180:VAL:HA   | 1.56                     | 0.85              |
| 1:D:342:THR:O    | 1:D:342:THR:HG22 | 1.75                     | 0.85              |
| 1:G:229:PRO:CD   | 1:G:233:ASP:OD2  | 2.25                     | 0.85              |
| 1:G:227:ASN:O    | 1:G:229:PRO:HD3  | 1.75                     | 0.85              |
| 1:F:244:LEU:O    | 1:F:310:SER:OG   | 1.95                     | 0.85              |
| 1:F:231:VAL:CG1  | 1:F:322:ILE:CB   | 2.55                     | 0.84              |
| 1:G:325:GLU:HA   | 1:G:328:LEU:CD1  | 2.06                     | 0.84              |
| 1:F:224:ALA:HB2  | 1:F:360:THR:HG22 | 1.58                     | 0.84              |
| 1:A:175:ASN:ND2  | 1:A:175:ASN:O    | 2.10                     | 0.84              |
| 1:B:7:LEU:HD23   | 1:B:180:VAL:HA   | 1.60                     | 0.84              |
| 1:F:226:LYS:O    | 1:F:228:PHE:N    | 2.10                     | 0.84              |
| 1:D:342:THR:O    | 1:D:342:THR:CG2  | 2.25                     | 0.84              |
| 1:F:339:PHE:CD1  | 1:F:351:GLY:HA3  | 2.13                     | 0.83              |
| 1:D:278:GLY:CA   | 1:D:332:VAL:HB   | 2.06                     | 0.83              |
| 1:A:343:PHE:N    | 1:A:344:PRO:CA   | 2.41                     | 0.83              |
| 1:H:224:ALA:HA   | 1:H:360:THR:O    | 1.78                     | 0.83              |
| 1:G:231:VAL:HA   | 1:G:321:ARG:HD3  | 1.58                     | 0.83              |
| 1:F:222:SER:CB   | 1:F:358:ASN:HB2  | 2.08                     | 0.83              |
| 1:C:131:ASP:HB2  | 1:C:134:GLU:HG3  | 1.59                     | 0.82              |
| 1:D:224:ALA:CB   | 1:D:360:THR:CG2  | 2.57                     | 0.82              |
| 1:A:5:VAL:HG22   | 1:A:55:HIS:CD2   | 2.14                     | 0.82              |
| 1:F:5:VAL:HG12   | 1:F:7:LEU:HD11   | 1.60                     | 0.82              |
| 1:C:4:GLU:C      | 1:C:55:HIS:HB2   | 2.03                     | 0.82              |
| 1:C:172:PRO:HB2  | 1:C:182:ARG:NH1  | 1.94                     | 0.82              |
| 1:C:88:VAL:HG22  | 1:C:122:TYR:CE1  | 2.16                     | 0.81              |
| 1:F:274:LEU:HD11 | 1:F:283:GLY:HA2  | 1.63                     | 0.81              |
| 1:B:5:VAL:HB     | 1:B:55:HIS:CD2   | 2.15                     | 0.81              |
| 1:B:231:VAL:O    | 1:B:232:ASN:HB2  | 1.80                     | 0.81              |
| 1:F:222:SER:OG   | 1:F:358:ASN:CB   | 2.29                     | 0.81              |
| 1:G:324:ALA:O    | 1:G:328:LEU:HD22 | 1.77                     | 0.80              |
| 1:B:4:GLU:HG2    | 1:B:112:THR:HG22 | 1.61                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:154:TRP:CH2  | 1:C:184:PRO:HG3  | 2.17                     | 0.80              |
| 1:F:274:LEU:HD12 | 1:F:274:LEU:N    | 1.95                     | 0.80              |
| 1:B:110:ARG:NH1  | 1:B:119:THR:O    | 2.14                     | 0.80              |
| 1:D:237:GLU:OE1  | 1:D:316:SER:OG   | 1.99                     | 0.80              |
| 1:F:331:GLY:H    | 1:F:359:ILE:HB   | 1.45                     | 0.80              |
| 1:G:7:LEU:CD2    | 1:G:180:VAL:HA   | 2.12                     | 0.80              |
| 1:D:343:PHE:N    | 1:D:344:PRO:HA   | 1.95                     | 0.79              |
| 1:E:17:LEU:O     | 1:E:38:ARG:HD2   | 1.83                     | 0.79              |
| 1:D:77:SER:OG    | 1:D:82:ILE:O     | 2.00                     | 0.79              |
| 1:G:228:PHE:HD2  | 1:G:282:PHE:CE1  | 1.93                     | 0.79              |
| 1:H:150:THR:HG21 | 1:H:188:ILE:HG12 | 1.62                     | 0.79              |
| 1:D:87:SER:HB3   | 1:D:97:VAL:HA    | 1.64                     | 0.79              |
| 1:F:288:ASN:ND2  | 1:F:313:LEU:HD11 | 1.98                     | 0.79              |
| 1:C:91:GLN:NE2   | 1:C:91:GLN:CG    | 2.45                     | 0.79              |
| 1:D:274:LEU:HD23 | 1:D:333:ALA:HB1  | 1.63                     | 0.79              |
| 1:G:157:ASP:O    | 1:G:182:ARG:NH2  | 2.16                     | 0.79              |
| 1:C:154:TRP:CD2  | 1:C:184:PRO:HB3  | 2.18                     | 0.78              |
| 1:F:20:ARG:NH1   | 1:F:20:ARG:NH2   | 2.30                     | 0.78              |
| 1:D:360:THR:HG22 | 1:D:361:GLU:CD   | 2.08                     | 0.78              |
| 1:A:341:PHE:O    | 1:A:346:ASP:HB3  | 1.84                     | 0.78              |
| 1:F:5:VAL:HG12   | 1:F:7:LEU:CD1    | 2.13                     | 0.78              |
| 1:G:5:VAL:HG23   | 1:G:51:SER:HB3   | 1.65                     | 0.78              |
| 1:A:141:LYS:CG   | 1:A:203:PRO:HB3  | 2.14                     | 0.77              |
| 1:D:224:ALA:HA   | 1:D:360:THR:HB   | 0.77                     | 0.77              |
| 1:D:224:ALA:CB   | 1:D:360:THR:CB   | 2.47                     | 0.77              |
| 1:H:66:VAL:CG2   | 1:H:149:ALA:HB2  | 2.14                     | 0.77              |
| 1:C:141:LYS:CD   | 1:C:141:LYS:NZ   | 2.47                     | 0.77              |
| 1:E:7:LEU:CD2    | 1:E:180:VAL:HA   | 2.15                     | 0.77              |
| 1:E:141:LYS:CG   | 1:E:203:PRO:HB3  | 2.14                     | 0.77              |
| 1:G:325:GLU:HA   | 1:G:328:LEU:HD21 | 0.76                     | 0.76              |
| 1:A:53:GLU:N     | 1:A:53:GLU:OE1   | 2.18                     | 0.76              |
| 1:F:47:LYS:CD    | 1:F:47:LYS:NZ    | 2.49                     | 0.76              |
| 1:B:228:PHE:HE1  | 1:B:234:THR:HA   | 1.51                     | 0.76              |
| 1:D:234:THR:HG22 | 1:D:319:TYR:O    | 1.85                     | 0.76              |
| 1:G:324:ALA:C    | 1:G:328:LEU:HD22 | 2.11                     | 0.76              |
| 1:D:279:ALA:CA   | 1:D:331:GLY:O    | 2.34                     | 0.75              |
| 1:G:260:LYS:O    | 1:G:260:LYS:HD3  | 1.85                     | 0.75              |
| 1:A:26:THR:HG22  | 1:A:28:GLY:N     | 2.01                     | 0.75              |
| 1:D:209:LYS:HB3  | 1:D:245:SER:O    | 1.86                     | 0.75              |
| 1:F:225:LEU:HD22 | 1:F:225:LEU:H    | 1.52                     | 0.75              |
| 1:E:150:THR:HG22 | 1:E:188:ILE:CG1  | 2.09                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:177:PRO:HD2  | 1:A:180:VAL:HG22 | 1.68                     | 0.75              |
| 1:C:329:LYS:NZ   | 1:C:329:LYS:CD   | 2.50                     | 0.75              |
| 1:D:224:ALA:HB2  | 1:D:360:THR:CB   | 2.15                     | 0.75              |
| 1:F:41:SER:OG    | 1:F:121:ASP:OD1  | 2.04                     | 0.74              |
| 1:F:222:SER:HG   | 1:F:358:ASN:HB2  | 1.52                     | 0.74              |
| 1:D:87:SER:CB    | 1:D:97:VAL:HA    | 2.17                     | 0.74              |
| 1:A:342:THR:C    | 1:A:344:PRO:HA   | 2.12                     | 0.74              |
| 1:F:231:VAL:O    | 1:F:232:ASN:CB   | 2.34                     | 0.74              |
| 1:H:86:ILE:HG23  | 1:H:98:ILE:HD12  | 1.68                     | 0.74              |
| 1:D:279:ALA:HB3  | 1:D:333:ALA:HB2  | 1.69                     | 0.73              |
| 1:D:141:LYS:HG3  | 1:D:203:PRO:HB3  | 1.68                     | 0.73              |
| 1:E:210:VAL:HG12 | 1:E:211:GLU:N    | 2.02                     | 0.73              |
| 1:D:274:LEU:CD2  | 1:D:333:ALA:HB1  | 2.17                     | 0.73              |
| 1:G:228:PHE:CD2  | 1:G:282:PHE:CZ   | 2.76                     | 0.73              |
| 1:D:274:LEU:HD12 | 1:D:274:LEU:N    | 2.01                     | 0.73              |
| 1:B:86:ILE:HG23  | 1:B:98:ILE:HD12  | 1.70                     | 0.73              |
| 1:D:227:ASN:O    | 1:D:229:PRO:HD3  | 1.88                     | 0.73              |
| 1:B:34:VAL:HG21  | 1:B:85:ARG:HH21  | 1.54                     | 0.72              |
| 1:C:154:TRP:CE2  | 1:C:184:PRO:HB3  | 2.25                     | 0.72              |
| 1:D:108:ASP:OD2  | 1:D:110:ARG:NH1  | 2.22                     | 0.72              |
| 1:F:231:VAL:HG12 | 1:F:322:ILE:CB   | 2.18                     | 0.72              |
| 1:A:180:VAL:HG11 | 1:A:182:ARG:CZ   | 2.19                     | 0.72              |
| 1:C:207:LYS:HE2  | 1:C:345:SER:OG   | 1.89                     | 0.72              |
| 1:D:222:SER:HA   | 1:D:358:ASN:O    | 1.89                     | 0.72              |
| 1:E:340:THR:HG23 | 1:E:348:LYS:O    | 1.90                     | 0.72              |
| 1:G:325:GLU:HA   | 1:G:328:LEU:HD11 | 1.72                     | 0.72              |
| 1:G:101:ASP:OD1  | 1:G:102:ASN:N    | 2.23                     | 0.72              |
| 1:B:7:LEU:CD2    | 1:B:180:VAL:HA   | 2.19                     | 0.71              |
| 1:C:55:HIS:HE1   | 1:C:159:LEU:CD2  | 2.03                     | 0.71              |
| 1:F:285:VAL:CG1  | 1:F:294:ARG:HH11 | 2.00                     | 0.71              |
| 1:B:226:LYS:NZ   | 1:B:226:LYS:CD   | 2.54                     | 0.71              |
| 1:B:324:ALA:O    | 1:B:328:LEU:HD13 | 1.91                     | 0.71              |
| 1:F:91:GLN:CG    | 1:F:110:ARG:HH21 | 2.02                     | 0.71              |
| 1:H:110:ARG:HG2  | 1:H:118:THR:OG1  | 1.89                     | 0.71              |
| 1:E:336:ALA:HB1  | 1:E:352:ILE:HD11 | 1.70                     | 0.71              |
| 1:F:222:SER:HA   | 1:F:358:ASN:C    | 2.15                     | 0.71              |
| 1:C:130:VAL:HG11 | 1:C:134:GLU:HB2  | 1.71                     | 0.71              |
| 1:E:4:GLU:O      | 1:E:112:THR:HG21 | 1.91                     | 0.71              |
| 1:G:228:PHE:HE2  | 1:G:282:PHE:CD1  | 2.06                     | 0.71              |
| 1:G:110:ARG:HH11 | 1:G:110:ARG:CG   | 2.04                     | 0.70              |
| 1:G:222:SER:HA   | 1:G:358:ASN:O    | 1.91                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:157:ASP:O    | 1:A:182:ARG:NH2  | 2.24                     | 0.70              |
| 1:D:265:GLN:NE2  | 1:D:269:PRO:HG3  | 2.06                     | 0.70              |
| 1:A:48:PRO:CG    | 1:A:114:PHE:O    | 2.39                     | 0.70              |
| 1:D:66:VAL:CG2   | 1:D:149:ALA:HB2  | 2.22                     | 0.70              |
| 1:A:88:VAL:CG1   | 1:A:122:TYR:CE1  | 2.74                     | 0.70              |
| 1:B:3:ASN:HA     | 1:B:112:THR:HB   | 1.74                     | 0.70              |
| 1:D:210:VAL:HG12 | 1:D:211:GLU:N    | 2.06                     | 0.70              |
| 1:D:274:LEU:HD11 | 1:D:282:PHE:O    | 1.91                     | 0.70              |
| 1:G:321:ARG:HH11 | 1:G:324:ALA:HA   | 1.56                     | 0.70              |
| 1:B:234:THR:CG2  | 1:B:320:ILE:HD12 | 2.22                     | 0.70              |
| 1:B:319:TYR:OH   | 1:B:333:ALA:O    | 2.10                     | 0.70              |
| 1:D:227:ASN:O    | 1:D:229:PRO:CD   | 2.40                     | 0.70              |
| 1:F:274:LEU:CD2  | 1:F:333:ALA:CB   | 2.60                     | 0.70              |
| 1:F:66:VAL:CG2   | 1:F:149:ALA:HB2  | 2.23                     | 0.69              |
| 1:G:92:ASP:OD1   | 1:G:92:ASP:N     | 2.19                     | 0.69              |
| 1:D:138:GLY:O    | 1:D:206:LYS:HE3  | 1.92                     | 0.69              |
| 1:F:339:PHE:CE1  | 1:F:351:GLY:CA   | 2.69                     | 0.69              |
| 1:G:328:LEU:CD2  | 1:G:328:LEU:H    | 1.98                     | 0.69              |
| 1:B:229:PRO:HD2  | 1:B:233:ASP:OD2  | 1.92                     | 0.69              |
| 1:B:207:LYS:HG3  | 1:B:343:PHE:CE1  | 2.27                     | 0.69              |
| 1:H:336:ALA:HB1  | 1:H:352:ILE:HD11 | 1.75                     | 0.69              |
| 1:A:87:SER:HB3   | 1:A:97:VAL:HA    | 1.75                     | 0.69              |
| 1:D:283:GLY:C    | 1:D:320:ILE:HG22 | 2.18                     | 0.68              |
| 1:F:296:ARG:HD2  | 2:F:412:HOH:O    | 1.92                     | 0.68              |
| 1:A:341:PHE:O    | 1:A:346:ASP:CB   | 2.40                     | 0.68              |
| 1:G:278:GLY:HA3  | 1:G:332:VAL:HG13 | 1.76                     | 0.68              |
| 1:A:150:THR:CG2  | 1:A:188:ILE:HG23 | 2.21                     | 0.68              |
| 1:C:91:GLN:CG    | 1:C:91:GLN:OE1   | 2.41                     | 0.68              |
| 1:C:91:GLN:NE2   | 1:C:91:GLN:OE1   | 2.26                     | 0.68              |
| 1:F:78:ASP:OD2   | 1:F:143:THR:HB   | 1.92                     | 0.68              |
| 1:G:279:ALA:HA   | 1:G:330:ALA:HB2  | 0.70                     | 0.68              |
| 1:G:325:GLU:O    | 1:G:328:LEU:CG   | 2.40                     | 0.68              |
| 1:C:44:LEU:HB3   | 1:C:118:THR:HG23 | 1.75                     | 0.68              |
| 1:F:139:ASP:OD2  | 1:F:141:LYS:HG2  | 1.94                     | 0.68              |
| 1:G:231:VAL:O    | 1:G:232:ASN:HB2  | 1.91                     | 0.68              |
| 1:D:206:LYS:C    | 1:D:251:ALA:HB2  | 2.18                     | 0.68              |
| 1:H:44:LEU:HB3   | 1:H:118:THR:CG2  | 2.24                     | 0.67              |
| 1:B:141:LYS:CG   | 1:B:203:PRO:HB3  | 2.17                     | 0.67              |
| 1:C:225:LEU:HD23 | 1:C:225:LEU:O    | 1.94                     | 0.67              |
| 1:F:5:VAL:CG1    | 1:F:7:LEU:HD11   | 2.24                     | 0.67              |
| 1:E:32:GLY:CA    | 1:E:72:TYR:CE2   | 2.76                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:225:LEU:N    | 1:D:360:THR:O    | 2.15                     | 0.67              |
| 1:E:4:GLU:HG3    | 1:E:112:THR:HG21 | 1.75                     | 0.67              |
| 1:F:53:GLU:N     | 1:F:53:GLU:OE1   | 2.26                     | 0.67              |
| 1:F:91:GLN:HG2   | 1:F:110:ARG:HH21 | 1.59                     | 0.67              |
| 1:F:36:PHE:CE1   | 1:F:202:PRO:HG2  | 2.30                     | 0.67              |
| 1:F:222:SER:OG   | 1:F:358:ASN:ND2  | 2.27                     | 0.67              |
| 1:H:3:ASN:ND2    | 1:H:111:VAL:HG13 | 2.10                     | 0.67              |
| 1:A:241:ASP:OD1  | 1:A:312:ASP:HB2  | 1.95                     | 0.67              |
| 1:B:327:GLU:OE2  | 1:B:327:GLU:HA   | 1.93                     | 0.67              |
| 1:D:210:VAL:HG22 | 1:D:244:LEU:HD22 | 1.76                     | 0.67              |
| 1:A:258:ARG:CZ   | 1:A:298:ASP:O    | 2.42                     | 0.67              |
| 1:B:141:LYS:HG3  | 1:B:203:PRO:CB   | 2.15                     | 0.67              |
| 1:D:234:THR:HG23 | 1:D:320:ILE:CD1  | 2.18                     | 0.67              |
| 1:H:4:GLU:H      | 1:H:4:GLU:CD     | 2.01                     | 0.67              |
| 1:D:328:LEU:HD12 | 1:D:328:LEU:N    | 2.10                     | 0.66              |
| 1:G:221:GLY:O    | 1:G:358:ASN:N    | 2.26                     | 0.66              |
| 1:A:48:PRO:HG2   | 1:A:114:PHE:HA   | 1.78                     | 0.66              |
| 1:G:319:TYR:OH   | 1:G:333:ALA:HB3  | 1.95                     | 0.66              |
| 1:F:59:ILE:HA    | 1:F:154:TRP:O    | 1.95                     | 0.66              |
| 1:H:3:ASN:HD21   | 1:H:111:VAL:HG13 | 1.60                     | 0.66              |
| 1:E:4:GLU:CB     | 1:E:112:THR:HG23 | 2.25                     | 0.66              |
| 1:B:139:ASP:O    | 1:B:140:LEU:HB2  | 1.95                     | 0.66              |
| 1:F:13:ASN:ND2   | 1:F:197:GLY:N    | 2.43                     | 0.66              |
| 1:G:5:VAL:CG2    | 1:G:51:SER:HB3   | 2.25                     | 0.66              |
| 1:C:130:VAL:CG1  | 1:C:134:GLU:CB   | 2.71                     | 0.66              |
| 1:F:22:VAL:O     | 1:F:23:ASN:ND2   | 2.29                     | 0.66              |
| 1:D:241:ASP:OD2  | 1:D:243:SER:OG   | 2.14                     | 0.66              |
| 1:E:175:ASN:O    | 1:E:178:THR:HA   | 1.96                     | 0.66              |
| 1:G:6:ALA:O      | 1:G:7:LEU:HD23   | 1.96                     | 0.66              |
| 1:A:5:VAL:CG2    | 1:A:51:SER:HB2   | 2.26                     | 0.66              |
| 1:G:139:ASP:O    | 1:G:140:LEU:HB2  | 1.96                     | 0.66              |
| 1:G:338:GLU:HB3  | 1:G:352:ILE:CD1  | 2.25                     | 0.66              |
| 1:G:63:TRP:HB2   | 1:G:100:VAL:HA   | 1.78                     | 0.65              |
| 1:E:4:GLU:CG     | 1:E:112:THR:CG2  | 2.74                     | 0.65              |
| 1:G:324:ALA:C    | 1:G:328:LEU:HD21 | 1.97                     | 0.65              |
| 1:F:225:LEU:H    | 1:F:225:LEU:CD2  | 2.10                     | 0.65              |
| 1:G:228:PHE:HD2  | 1:G:282:PHE:CZ   | 2.14                     | 0.65              |
| 1:H:141:LYS:HG3  | 1:H:203:PRO:HB3  | 1.78                     | 0.65              |
| 1:A:231:VAL:O    | 1:A:232:ASN:HB2  | 1.96                     | 0.65              |
| 1:D:339:PHE:CZ   | 1:D:351:GLY:HA3  | 2.31                     | 0.65              |
| 1:E:10:SER:O     | 1:E:44:LEU:HD12  | 1.97                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:225:LEU:HD22 | 1:F:225:LEU:N    | 2.11                     | 0.65              |
| 1:E:175:ASN:HD22 | 1:E:175:ASN:C    | 2.04                     | 0.64              |
| 1:C:86:ILE:HG23  | 1:C:98:ILE:HD12  | 1.80                     | 0.64              |
| 1:C:88:VAL:HG22  | 1:C:122:TYR:CD1  | 2.33                     | 0.64              |
| 1:D:265:GLN:HE22 | 1:D:269:PRO:HG3  | 1.61                     | 0.64              |
| 1:B:334:ASP:OD1  | 1:B:356:SER:HA   | 1.97                     | 0.64              |
| 1:G:71:PRO:O     | 1:G:74:THR:OG1   | 2.14                     | 0.64              |
| 1:A:177:PRO:O    | 1:A:180:VAL:HG23 | 1.98                     | 0.64              |
| 1:C:7:LEU:HD23   | 1:C:7:LEU:N      | 2.11                     | 0.64              |
| 1:F:223:VAL:O    | 1:F:360:THR:N    | 2.29                     | 0.64              |
| 1:B:235:SER:HG   | 1:B:319:TYR:H    | 1.45                     | 0.64              |
| 1:E:175:ASN:ND2  | 1:E:179:GLY:H    | 1.91                     | 0.64              |
| 1:G:283:GLY:C    | 1:G:320:ILE:HG22 | 2.22                     | 0.64              |
| 1:C:6:ALA:HB1    | 1:C:46:TYR:HD2   | 1.57                     | 0.64              |
| 1:D:210:VAL:HG12 | 1:D:211:GLU:H    | 1.63                     | 0.63              |
| 1:E:176:TYR:HA   | 1:E:177:PRO:C    | 2.23                     | 0.63              |
| 1:C:154:TRP:CZ3  | 1:C:184:PRO:HD3  | 2.33                     | 0.63              |
| 1:C:343:PHE:N    | 1:C:344:PRO:CA   | 2.56                     | 0.63              |
| 1:E:56:GLU:HG3   | 1:E:160:LYS:HG3  | 1.80                     | 0.63              |
| 1:G:343:PHE:HB2  | 1:G:344:PRO:C    | 2.23                     | 0.63              |
| 1:B:34:VAL:HG21  | 1:B:85:ARG:NH2   | 2.09                     | 0.63              |
| 1:C:176:TYR:CA   | 1:C:177:PRO:O    | 2.47                     | 0.62              |
| 1:F:3:ASN:HB2    | 1:F:112:THR:O    | 1.98                     | 0.62              |
| 1:B:6:ALA:O      | 1:B:7:LEU:HD23   | 1.98                     | 0.62              |
| 1:D:274:LEU:HA   | 1:D:334:ASP:O    | 1.99                     | 0.62              |
| 1:D:265:GLN:HE22 | 1:D:269:PRO:CG   | 2.11                     | 0.62              |
| 1:E:48:PRO:HG2   | 1:E:114:PHE:O    | 1.99                     | 0.62              |
| 1:E:62:ASN:HD22  | 1:E:103:GLN:C    | 2.07                     | 0.62              |
| 1:H:291:ASP:O    | 1:H:292:GLN:HB2  | 1.98                     | 0.62              |
| 1:D:231:VAL:O    | 1:D:232:ASN:HB2  | 1.99                     | 0.62              |
| 1:G:175:ASN:HD21 | 1:G:179:GLY:H    | 1.48                     | 0.62              |
| 1:D:234:THR:CG2  | 1:D:320:ILE:HD12 | 2.21                     | 0.62              |
| 1:G:86:ILE:HG23  | 1:G:98:ILE:HD12  | 1.81                     | 0.62              |
| 1:A:3:ASN:ND2    | 1:A:160:LYS:HE3  | 2.15                     | 0.62              |
| 1:C:292:GLN:HE22 | 1:D:22:VAL:CG1   | 2.12                     | 0.62              |
| 1:E:4:GLU:HG3    | 1:E:112:THR:CG2  | 2.29                     | 0.62              |
| 1:C:231:VAL:HG12 | 1:C:232:ASN:OD1  | 2.00                     | 0.62              |
| 1:F:224:ALA:CB   | 1:F:360:THR:HG22 | 2.30                     | 0.62              |
| 1:E:139:ASP:O    | 1:E:140:LEU:HB2  | 2.00                     | 0.62              |
| 1:A:6:ALA:C      | 1:A:7:LEU:HD23   | 2.25                     | 0.61              |
| 1:D:338:GLU:CG   | 1:D:352:ILE:HD13 | 2.22                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:204:ILE:HD12 | 1:D:204:ILE:N    | 2.16                     | 0.61              |
| 1:G:260:LYS:HD3  | 1:G:260:LYS:C    | 2.25                     | 0.61              |
| 1:G:329:LYS:O    | 1:G:330:ALA:HB3  | 2.00                     | 0.61              |
| 1:A:48:PRO:HG2   | 1:A:114:PHE:C    | 2.26                     | 0.61              |
| 1:B:68:TYR:CD2   | 1:D:72:TYR:HA    | 2.35                     | 0.61              |
| 1:B:139:ASP:OD1  | 1:B:140:LEU:N    | 2.34                     | 0.61              |
| 1:D:44:LEU:HD21  | 1:D:57:LEU:HD21  | 1.82                     | 0.61              |
| 1:D:338:GLU:HG2  | 1:D:352:ILE:HD11 | 1.78                     | 0.61              |
| 1:E:17:LEU:HD12  | 1:E:39:PRO:HG2   | 1.83                     | 0.61              |
| 1:E:5:VAL:HG22   | 1:E:55:HIS:CG    | 2.36                     | 0.61              |
| 1:F:92:ASP:OD1   | 1:F:92:ASP:N     | 2.27                     | 0.61              |
| 1:B:108:ASP:OD2  | 1:B:110:ARG:NH2  | 2.31                     | 0.61              |
| 1:D:279:ALA:CB   | 1:D:333:ALA:HB2  | 2.31                     | 0.61              |
| 1:F:289:GLY:HA3  | 1:F:314:PRO:HG2  | 1.83                     | 0.61              |
| 1:B:235:SER:OG   | 1:B:319:TYR:HB2  | 2.01                     | 0.60              |
| 1:H:74:THR:HG22  | 1:H:85:ARG:HB3   | 1.81                     | 0.60              |
| 1:C:130:VAL:HG12 | 1:C:131:ASP:N    | 2.15                     | 0.60              |
| 1:B:157:ASP:O    | 1:B:182:ARG:NH2  | 2.35                     | 0.60              |
| 1:D:228:PHE:CD2  | 1:D:282:PHE:HE2  | 2.20                     | 0.60              |
| 1:H:44:LEU:HB3   | 1:H:118:THR:HG23 | 1.83                     | 0.60              |
| 1:E:141:LYS:HG3  | 1:E:203:PRO:CB   | 2.25                     | 0.60              |
| 1:A:38:ARG:HH21  | 1:A:38:ARG:HB3   | 1.66                     | 0.60              |
| 1:B:227:ASN:O    | 1:B:229:PRO:CD   | 2.48                     | 0.60              |
| 1:G:321:ARG:NH1  | 1:G:324:ALA:HA   | 2.16                     | 0.60              |
| 1:C:291:ASP:O    | 1:C:292:GLN:HB2  | 2.01                     | 0.60              |
| 1:D:224:ALA:N    | 1:D:360:THR:CB   | 2.50                     | 0.60              |
| 1:G:343:PHE:N    | 1:G:344:PRO:HA   | 2.16                     | 0.60              |
| 1:A:177:PRO:HD2  | 1:A:180:VAL:CG2  | 2.32                     | 0.60              |
| 1:G:16:GLY:C     | 1:G:17:LEU:HD23  | 2.27                     | 0.60              |
| 1:D:298:ASP:OD1  | 1:D:298:ASP:N    | 2.34                     | 0.60              |
| 1:C:44:LEU:HB3   | 1:C:118:THR:CG2  | 2.32                     | 0.59              |
| 1:C:342:THR:C    | 1:C:344:PRO:HA   | 2.26                     | 0.59              |
| 1:G:96:ARG:NH1   | 1:G:107:LEU:O    | 2.35                     | 0.59              |
| 1:A:55:HIS:O     | 1:A:112:THR:OG1  | 2.20                     | 0.59              |
| 1:D:224:ALA:HA   | 1:D:360:THR:N    | 2.17                     | 0.59              |
| 1:E:142:VAL:O    | 1:E:201:PRO:HD2  | 2.02                     | 0.59              |
| 1:H:154:TRP:CE3  | 1:H:184:PRO:HB3  | 2.37                     | 0.59              |
| 1:C:92:ASP:C     | 1:D:230:ARG:HH21 | 2.04                     | 0.59              |
| 1:H:131:ASP:HB2  | 1:H:134:GLU:HG3  | 1.84                     | 0.59              |
| 1:B:44:LEU:HB3   | 1:B:118:THR:HG23 | 1.84                     | 0.59              |
| 1:C:176:TYR:HA   | 1:C:177:PRO:C    | 2.27                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:280:ALA:HB3  | 1:B:329:LYS:HB3  | 1.84                     | 0.59              |
| 1:F:62:ASN:HB3   | 1:F:104:PRO:HA   | 1.85                     | 0.59              |
| 1:F:223:VAL:N    | 1:F:358:ASN:O    | 2.33                     | 0.59              |
| 1:C:5:VAL:HG23   | 1:C:55:HIS:CD2   | 2.36                     | 0.59              |
| 1:F:224:ALA:HA   | 1:F:360:THR:O    | 2.03                     | 0.59              |
| 1:A:48:PRO:CG    | 1:A:114:PHE:HA   | 2.32                     | 0.59              |
| 1:D:254:GLU:HB2  | 1:D:342:THR:HG22 | 1.84                     | 0.59              |
| 1:E:91:GLN:HG3   | 1:E:110:ARG:NH1  | 2.18                     | 0.59              |
| 1:H:58:VAL:HG11  | 1:H:169:LEU:HD13 | 1.84                     | 0.59              |
| 1:B:131:ASP:HB2  | 1:B:134:GLU:HG3  | 1.84                     | 0.58              |
| 1:G:175:ASN:O    | 1:G:175:ASN:ND2  | 2.35                     | 0.58              |
| 1:C:6:ALA:HB2    | 1:C:46:TYR:CD2   | 2.37                     | 0.58              |
| 1:F:274:LEU:N    | 1:F:274:LEU:CD1  | 2.66                     | 0.58              |
| 1:H:139:ASP:O    | 1:H:140:LEU:HB2  | 2.03                     | 0.58              |
| 1:F:327:GLU:N    | 1:F:327:GLU:OE1  | 2.36                     | 0.58              |
| 1:A:176:TYR:HA   | 1:A:177:PRO:C    | 2.27                     | 0.58              |
| 1:C:92:ASP:C     | 1:D:230:ARG:NH2  | 2.61                     | 0.58              |
| 1:D:45:ASN:OD1   | 1:D:45:ASN:N     | 2.34                     | 0.58              |
| 1:E:66:VAL:HG22  | 1:E:149:ALA:HB2  | 1.84                     | 0.58              |
| 1:E:210:VAL:HG22 | 1:E:244:LEU:HD22 | 1.86                     | 0.58              |
| 1:G:10:SER:O     | 1:G:44:LEU:HD12  | 2.04                     | 0.58              |
| 1:C:130:VAL:HG13 | 1:C:134:GLU:OE1  | 2.04                     | 0.58              |
| 1:G:17:LEU:O     | 1:G:38:ARG:HD2   | 2.04                     | 0.58              |
| 1:G:139:ASP:N    | 1:G:139:ASP:OD1  | 2.36                     | 0.58              |
| 1:A:5:VAL:HG23   | 1:A:51:SER:HB2   | 1.86                     | 0.58              |
| 1:B:228:PHE:HE1  | 1:B:234:THR:CA   | 2.16                     | 0.58              |
| 1:C:292:GLN:HG3  | 1:D:34:VAL:HG21  | 1.86                     | 0.58              |
| 1:D:339:PHE:CE1  | 1:D:351:GLY:HA3  | 2.39                     | 0.58              |
| 1:F:91:GLN:HG3   | 1:F:110:ARG:HE   | 1.68                     | 0.58              |
| 1:F:222:SER:HG   | 1:F:358:ASN:HD22 | 1.52                     | 0.58              |
| 1:G:325:GLU:C    | 1:G:328:LEU:HD23 | 2.26                     | 0.58              |
| 1:A:48:PRO:HG2   | 1:A:114:PHE:CA   | 2.34                     | 0.58              |
| 1:D:306:ARG:HD2  | 1:D:311:ALA:HB2  | 1.85                     | 0.58              |
| 1:A:306:ARG:HD2  | 1:A:311:ALA:HB2  | 1.85                     | 0.57              |
| 1:E:181:CYS:HA   | 1:E:183:LYS:NZ   | 2.19                     | 0.57              |
| 1:E:291:ASP:O    | 1:E:292:GLN:HB2  | 2.04                     | 0.57              |
| 1:A:139:ASP:O    | 1:A:140:LEU:HB2  | 2.03                     | 0.57              |
| 1:B:41:SER:OG    | 1:B:121:ASP:OD1  | 2.16                     | 0.57              |
| 1:C:227:ASN:HD22 | 1:C:227:ASN:N    | 2.00                     | 0.57              |
| 1:F:7:LEU:HD12   | 1:F:7:LEU:N      | 2.18                     | 0.57              |
| 1:A:62:ASN:HB3   | 1:A:104:PRO:HA   | 1.87                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:6:ALA:CB     | 1:C:46:TYR:HD2   | 2.09                     | 0.57              |
| 1:D:17:LEU:O     | 1:D:38:ARG:HD2   | 2.05                     | 0.57              |
| 1:G:212:VAL:HG12 | 1:G:213:GLY:N    | 2.19                     | 0.57              |
| 1:H:5:VAL:HG23   | 1:H:51:SER:HB2   | 1.86                     | 0.57              |
| 1:C:157:ASP:O    | 1:C:182:ARG:NH2  | 2.38                     | 0.57              |
| 1:G:78:ASP:OD1   | 1:G:79:VAL:N     | 2.38                     | 0.57              |
| 1:H:139:ASP:OD1  | 1:H:140:LEU:N    | 2.37                     | 0.57              |
| 1:D:86:ILE:HG23  | 1:D:98:ILE:HD12  | 1.87                     | 0.57              |
| 1:D:12:ASP:OD2   | 1:D:45:ASN:ND2   | 2.37                     | 0.57              |
| 1:G:222:SER:OG   | 1:G:358:ASN:HB2  | 2.04                     | 0.57              |
| 1:C:150:THR:CG2  | 1:C:188:ILE:HG22 | 2.35                     | 0.57              |
| 1:F:272:LEU:HB3  | 1:F:284:ILE:HG13 | 1.84                     | 0.56              |
| 1:G:41:SER:OG    | 1:G:121:ASP:OD1  | 2.13                     | 0.56              |
| 1:C:46:TYR:N     | 1:C:46:TYR:CD1   | 2.72                     | 0.56              |
| 1:F:176:TYR:HA   | 1:F:177:PRO:C    | 2.29                     | 0.56              |
| 1:F:224:ALA:HB2  | 1:F:360:THR:CG2  | 2.33                     | 0.56              |
| 1:G:139:ASP:OD2  | 1:G:141:LYS:HD2  | 2.04                     | 0.56              |
| 1:A:158:ARG:HH21 | 1:A:163:ALA:HB2  | 1.69                     | 0.56              |
| 1:C:141:LYS:NZ   | 1:C:201:PRO:O    | 2.38                     | 0.56              |
| 1:C:231:VAL:O    | 1:C:232:ASN:HB2  | 2.03                     | 0.56              |
| 1:F:231:VAL:HG13 | 1:F:322:ILE:CB   | 2.35                     | 0.56              |
| 1:B:288:ASN:CG   | 1:B:291:ASP:HB2  | 2.29                     | 0.56              |
| 1:G:212:VAL:CG1  | 1:G:213:GLY:N    | 2.69                     | 0.56              |
| 1:G:272:LEU:HD11 | 1:G:337:ALA:HB2  | 1.88                     | 0.56              |
| 1:A:175:ASN:C    | 1:A:175:ASN:HD22 | 2.11                     | 0.56              |
| 1:E:175:ASN:ND2  | 1:E:178:THR:HA   | 2.20                     | 0.56              |
| 1:H:7:LEU:HD23   | 1:H:178:THR:O    | 2.06                     | 0.56              |
| 1:B:88:VAL:HG12  | 1:B:122:TYR:CE2  | 2.41                     | 0.56              |
| 1:E:4:GLU:O      | 1:E:4:GLU:HG3    | 2.04                     | 0.56              |
| 1:F:60:GLY:O     | 1:F:154:TRP:HD1  | 1.88                     | 0.56              |
| 1:H:19:TRP:HA    | 1:H:38:ARG:HG3   | 1.87                     | 0.56              |
| 1:A:4:GLU:O      | 1:A:112:THR:HG21 | 2.05                     | 0.56              |
| 1:B:7:LEU:HD22   | 1:B:180:VAL:N    | 2.21                     | 0.56              |
| 1:C:139:ASP:O    | 1:C:140:LEU:HB2  | 2.06                     | 0.56              |
| 1:E:9:CYS:HA     | 1:E:45:ASN:O     | 2.06                     | 0.56              |
| 1:F:335:GLY:N    | 1:F:355:PHE:O    | 2.39                     | 0.56              |
| 1:G:237:GLU:HB3  | 1:G:316:SER:OG   | 2.05                     | 0.56              |
| 1:B:10:SER:O     | 1:B:44:LEU:HD12  | 2.06                     | 0.56              |
| 1:C:159:LEU:HD12 | 1:C:162:GLU:OE2  | 2.05                     | 0.56              |
| 1:E:231:VAL:O    | 1:E:232:ASN:HB2  | 2.05                     | 0.56              |
| 1:B:300:THR:HG23 | 1:C:65:GLY:O     | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:210:VAL:CG1  | 1:E:211:GLU:H    | 2.11                     | 0.55              |
| 1:H:17:LEU:O     | 1:H:38:ARG:HD3   | 2.07                     | 0.55              |
| 1:B:207:LYS:HG3  | 1:B:343:PHE:CE2  | 2.41                     | 0.55              |
| 1:C:24:GLU:OE2   | 1:C:24:GLU:HA    | 2.06                     | 0.55              |
| 1:E:86:ILE:HG23  | 1:E:98:ILE:HD12  | 1.89                     | 0.55              |
| 1:E:225:LEU:HD23 | 1:E:359:ILE:CG2  | 2.36                     | 0.55              |
| 1:F:222:SER:CA   | 1:F:358:ASN:O    | 2.43                     | 0.55              |
| 1:G:227:ASN:O    | 1:G:229:PRO:CD   | 2.49                     | 0.55              |
| 1:D:44:LEU:CD2   | 1:D:57:LEU:HD21  | 2.37                     | 0.55              |
| 1:F:86:ILE:HG23  | 1:F:98:ILE:HD12  | 1.89                     | 0.55              |
| 1:C:74:THR:HG22  | 1:C:85:ARG:HB2   | 1.89                     | 0.55              |
| 1:C:88:VAL:HG22  | 1:C:122:TYR:HE1  | 1.68                     | 0.55              |
| 1:D:141:LYS:CG   | 1:D:203:PRO:HB3  | 2.36                     | 0.55              |
| 1:G:231:VAL:HA   | 1:G:321:ARG:CD   | 2.32                     | 0.55              |
| 1:B:88:VAL:HG12  | 1:B:122:TYR:CD2  | 2.42                     | 0.55              |
| 1:B:192:SER:O    | 1:B:195:ILE:HG22 | 2.06                     | 0.55              |
| 1:F:10:SER:O     | 1:F:44:LEU:HD12  | 2.06                     | 0.55              |
| 1:F:72:TYR:HA    | 1:H:68:TYR:CD2   | 2.41                     | 0.55              |
| 1:F:235:SER:OG   | 1:F:319:TYR:HB2  | 2.06                     | 0.55              |
| 1:F:331:GLY:N    | 1:F:359:ILE:HB   | 2.19                     | 0.55              |
| 1:F:61:GLY:O     | 1:F:99:PRO:HD2   | 2.07                     | 0.55              |
| 1:A:343:PHE:H    | 1:A:345:SER:N    | 2.05                     | 0.55              |
| 1:B:322:ILE:HG22 | 1:B:322:ILE:O    | 2.07                     | 0.55              |
| 1:C:130:VAL:HG11 | 1:C:134:GLU:CB   | 2.34                     | 0.55              |
| 1:D:110:ARG:HD2  | 1:D:118:THR:OG1  | 2.05                     | 0.55              |
| 1:D:208:CYS:O    | 1:D:210:VAL:HG23 | 2.07                     | 0.55              |
| 1:G:38:ARG:NH1   | 1:G:197:GLY:O    | 2.39                     | 0.55              |
| 1:C:234:THR:HG22 | 1:C:320:ILE:HG13 | 1.89                     | 0.55              |
| 1:D:140:LEU:HB2  | 1:D:204:ILE:HD13 | 1.89                     | 0.55              |
| 1:G:131:ASP:HB2  | 1:G:134:GLU:HG3  | 1.89                     | 0.55              |
| 1:H:154:TRP:CD2  | 1:H:184:PRO:HB3  | 2.42                     | 0.55              |
| 1:F:283:GLY:O    | 1:F:320:ILE:HG22 | 2.07                     | 0.54              |
| 1:H:150:THR:HG22 | 1:H:187:LEU:O    | 2.07                     | 0.54              |
| 1:F:176:TYR:C    | 1:F:176:TYR:CD1  | 2.86                     | 0.54              |
| 1:G:7:LEU:CD2    | 1:G:180:VAL:CA   | 2.86                     | 0.54              |
| 1:B:231:VAL:O    | 1:B:232:ASN:CB   | 2.53                     | 0.54              |
| 1:G:206:LYS:CA   | 1:G:251:ALA:HB2  | 2.34                     | 0.54              |
| 1:A:6:ALA:O      | 1:A:7:LEU:HD22   | 2.07                     | 0.54              |
| 1:C:176:TYR:HA   | 1:C:177:PRO:O    | 2.08                     | 0.54              |
| 1:A:269:PRO:HD2  | 1:D:102:ASN:HB2  | 1.90                     | 0.54              |
| 1:G:56:GLU:HG3   | 1:G:160:LYS:HG3  | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:2:LEU:O      | 1:H:3:ASN:HB2    | 2.08                     | 0.54              |
| 1:E:245:SER:C    | 1:E:246:GLU:HG2  | 2.33                     | 0.54              |
| 1:B:300:THR:HG23 | 1:C:65:GLY:C     | 2.32                     | 0.53              |
| 1:F:7:LEU:HD23   | 1:F:178:THR:O    | 2.08                     | 0.53              |
| 1:G:110:ARG:HH11 | 1:G:110:ARG:HG2  | 1.73                     | 0.53              |
| 1:A:21:VAL:HG22  | 1:A:36:PHE:CE1   | 2.43                     | 0.53              |
| 1:F:56:GLU:HG3   | 1:F:160:LYS:HG3  | 1.90                     | 0.53              |
| 1:C:62:ASN:HB3   | 1:C:104:PRO:HA   | 1.88                     | 0.53              |
| 1:E:48:PRO:HG2   | 1:E:114:PHE:HA   | 1.90                     | 0.53              |
| 1:E:75:VAL:HG12  | 1:E:145:VAL:HG13 | 1.91                     | 0.53              |
| 1:F:288:ASN:CG   | 1:F:291:ASP:HB2  | 2.33                     | 0.53              |
| 2:B:440:HOH:O    | 1:E:237:GLU:HG3  | 2.07                     | 0.53              |
| 1:G:325:GLU:C    | 1:G:328:LEU:CG   | 2.82                     | 0.53              |
| 1:B:268:ASP:OD1  | 1:B:270:THR:OG1  | 2.23                     | 0.53              |
| 1:D:223:VAL:O    | 1:D:359:ILE:HA   | 2.09                     | 0.53              |
| 1:G:339:PHE:CE2  | 1:G:353:VAL:HG23 | 2.42                     | 0.53              |
| 1:D:328:LEU:H    | 1:D:328:LEU:CD1  | 2.22                     | 0.53              |
| 1:E:6:ALA:O      | 1:E:7:LEU:HD23   | 2.09                     | 0.53              |
| 1:G:247:CYS:O    | 1:G:309:ASP:OD1  | 2.27                     | 0.52              |
| 1:G:328:LEU:HD23 | 1:G:328:LEU:N    | 2.02                     | 0.52              |
| 1:A:26:THR:CG2   | 1:A:28:GLY:H     | 2.18                     | 0.52              |
| 1:B:7:LEU:CD2    | 1:B:180:VAL:CA   | 2.85                     | 0.52              |
| 1:E:32:GLY:CA    | 1:E:72:TYR:CZ    | 2.92                     | 0.52              |
| 1:F:220:LEU:HD11 | 1:F:355:PHE:HB3  | 1.91                     | 0.52              |
| 1:H:109:LYS:O    | 1:H:110:ARG:HD2  | 2.08                     | 0.52              |
| 1:C:89:ASP:CG    | 1:C:95:LYS:HE3   | 2.34                     | 0.52              |
| 1:H:44:LEU:HB3   | 1:H:118:THR:HG22 | 1.92                     | 0.52              |
| 1:A:128:LEU:HD11 | 1:A:130:VAL:O    | 2.10                     | 0.52              |
| 1:F:319:TYR:OH   | 1:F:357:GLY:HA3  | 2.10                     | 0.52              |
| 1:E:4:GLU:HB2    | 1:E:112:THR:CG2  | 2.30                     | 0.52              |
| 1:A:338:GLU:HG2  | 1:A:352:ILE:HD13 | 1.92                     | 0.52              |
| 1:B:215:GLU:HA   | 1:B:352:ILE:O    | 2.09                     | 0.52              |
| 1:C:334:ASP:OD1  | 1:C:356:SER:HA   | 2.09                     | 0.52              |
| 1:D:274:LEU:H    | 1:D:274:LEU:CD1  | 2.13                     | 0.52              |
| 1:A:25:LEU:CD2   | 1:A:204:ILE:HD13 | 2.40                     | 0.52              |
| 1:B:174:ASP:O    | 1:B:182:ARG:HD2  | 2.10                     | 0.52              |
| 1:D:288:ASN:HB3  | 1:D:291:ASP:OD1  | 2.10                     | 0.52              |
| 1:E:334:ASP:OD1  | 1:E:356:SER:HA   | 2.10                     | 0.52              |
| 1:G:325:GLU:O    | 1:G:328:LEU:CD2  | 2.54                     | 0.52              |
| 1:C:136:PRO:HD2  | 1:C:140:LEU:CD2  | 2.40                     | 0.52              |
| 1:F:288:ASN:HD21 | 1:F:313:LEU:HD11 | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:334:ASP:OD1  | 1:A:356:SER:HA   | 2.10                     | 0.52              |
| 1:D:210:VAL:CG1  | 1:D:211:GLU:N    | 2.73                     | 0.52              |
| 1:F:60:GLY:HA2   | 1:F:105:HIS:O    | 2.10                     | 0.52              |
| 1:A:180:VAL:HG11 | 1:A:182:ARG:NH2  | 2.25                     | 0.51              |
| 1:G:244:LEU:O    | 1:G:310:SER:HB2  | 2.10                     | 0.51              |
| 1:B:224:ALA:HA   | 1:B:360:THR:O    | 2.09                     | 0.51              |
| 1:C:172:PRO:CB   | 1:C:182:ARG:NH1  | 2.70                     | 0.51              |
| 1:C:342:THR:HB   | 1:C:344:PRO:HB3  | 1.92                     | 0.51              |
| 1:F:7:LEU:HG     | 1:F:180:VAL:HA   | 1.91                     | 0.51              |
| 1:G:319:TYR:OH   | 1:G:333:ALA:CB   | 2.58                     | 0.51              |
| 1:D:321:ARG:O    | 1:D:321:ARG:HG3  | 2.10                     | 0.51              |
| 1:H:266:GLN:NE2  | 1:H:269:PRO:HA   | 2.25                     | 0.51              |
| 1:B:5:VAL:HG12   | 1:B:49:GLN:O     | 2.11                     | 0.51              |
| 1:B:17:LEU:O     | 1:B:38:ARG:HD2   | 2.09                     | 0.51              |
| 1:C:336:ALA:HB1  | 1:C:352:ILE:HD11 | 1.92                     | 0.51              |
| 1:E:209:LYS:CB   | 1:E:246:GLU:HG3  | 2.40                     | 0.51              |
| 1:F:36:PHE:CE1   | 1:F:202:PRO:CG   | 2.94                     | 0.51              |
| 1:G:339:PHE:HE2  | 1:G:353:VAL:HG23 | 1.75                     | 0.51              |
| 1:H:337:ALA:O    | 1:H:352:ILE:HG13 | 2.10                     | 0.51              |
| 1:A:95:LYS:HE2   | 1:A:123:LEU:HD22 | 1.93                     | 0.51              |
| 1:B:25:LEU:HD23  | 1:B:204:ILE:HD13 | 1.93                     | 0.51              |
| 1:E:40:VAL:HG23  | 1:E:122:TYR:HB2  | 1.91                     | 0.51              |
| 1:E:58:VAL:HG11  | 1:E:169:LEU:HD13 | 1.92                     | 0.51              |
| 1:E:181:CYS:HA   | 1:E:183:LYS:HZ1  | 1.75                     | 0.51              |
| 1:B:55:HIS:CE1   | 1:B:159:LEU:HD23 | 2.46                     | 0.51              |
| 1:F:139:ASP:CG   | 1:F:141:LYS:HG2  | 2.36                     | 0.51              |
| 1:A:4:GLU:OE2    | 1:A:113:SER:HA   | 2.11                     | 0.51              |
| 1:C:130:VAL:CG1  | 1:C:131:ASP:N    | 2.73                     | 0.51              |
| 1:G:223:VAL:N    | 1:G:358:ASN:O    | 2.35                     | 0.51              |
| 1:D:328:LEU:HD12 | 1:D:328:LEU:H    | 1.75                     | 0.51              |
| 1:D:328:LEU:N    | 1:D:328:LEU:CD1  | 2.73                     | 0.51              |
| 1:B:63:TRP:HB2   | 1:B:100:VAL:HA   | 1.92                     | 0.50              |
| 1:D:155:ALA:O    | 1:D:181:CYS:HB3  | 2.12                     | 0.50              |
| 1:E:136:PRO:O    | 1:E:140:LEU:HD21 | 2.12                     | 0.50              |
| 1:A:77:SER:HB3   | 1:A:82:ILE:O     | 2.11                     | 0.50              |
| 1:E:132:PRO:HA   | 1:E:135:LEU:HD12 | 1.93                     | 0.50              |
| 1:F:144:SER:OG   | 1:F:145:VAL:N    | 2.44                     | 0.50              |
| 1:D:223:VAL:N    | 1:D:358:ASN:O    | 2.43                     | 0.50              |
| 1:G:338:GLU:CB   | 1:G:352:ILE:HD13 | 2.35                     | 0.50              |
| 1:A:343:PHE:H    | 1:A:344:PRO:HA   | 1.67                     | 0.50              |
| 1:B:25:LEU:CD2   | 1:B:204:ILE:HD13 | 2.42                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:265:GLN:OE1  | 1:B:265:GLN:HA   | 2.12                     | 0.50              |
| 1:E:31:LYS:HB3   | 1:E:72:TYR:OH    | 2.11                     | 0.50              |
| 1:F:13:ASN:HD21  | 1:F:197:GLY:N    | 2.10                     | 0.50              |
| 1:D:210:VAL:CG1  | 1:D:211:GLU:H    | 2.24                     | 0.50              |
| 1:B:7:LEU:HD22   | 1:B:180:VAL:CA   | 2.41                     | 0.50              |
| 1:D:228:PHE:O    | 1:D:321:ARG:NH1  | 2.43                     | 0.50              |
| 1:D:265:GLN:OE1  | 1:D:298:ASP:HB3  | 2.12                     | 0.50              |
| 1:F:265:GLN:HA   | 1:F:265:GLN:NE2  | 2.26                     | 0.50              |
| 1:F:285:VAL:HG21 | 1:F:294:ARG:NH1  | 2.26                     | 0.50              |
| 1:F:268:ASP:OD1  | 1:F:270:THR:OG1  | 2.28                     | 0.50              |
| 1:C:66:VAL:HG22  | 1:C:149:ALA:HB2  | 1.93                     | 0.50              |
| 1:C:175:ASN:O    | 1:C:178:THR:HA   | 2.11                     | 0.50              |
| 1:D:136:PRO:O    | 1:D:140:LEU:HD21 | 2.12                     | 0.50              |
| 1:E:208:CYS:HA   | 1:E:247:CYS:HA   | 1.93                     | 0.50              |
| 1:D:259:ASP:OD2  | 1:D:272:LEU:HD12 | 2.11                     | 0.50              |
| 1:E:208:CYS:O    | 1:E:210:VAL:HG23 | 2.12                     | 0.50              |
| 1:G:144:SER:OG   | 1:G:145:VAL:N    | 2.45                     | 0.50              |
| 1:G:255:ILE:HG23 | 1:G:255:ILE:O    | 2.11                     | 0.50              |
| 1:A:6:ALA:C      | 1:A:7:LEU:CD2    | 2.85                     | 0.49              |
| 1:G:110:ARG:HH11 | 1:G:110:ARG:HG3  | 1.74                     | 0.49              |
| 1:A:21:VAL:HG22  | 1:A:36:PHE:HE1   | 1.78                     | 0.49              |
| 1:B:69:PRO:HG3   | 1:B:100:VAL:HB   | 1.93                     | 0.49              |
| 1:D:63:TRP:HB2   | 1:D:100:VAL:HA   | 1.93                     | 0.49              |
| 1:D:222:SER:CA   | 1:D:358:ASN:O    | 2.59                     | 0.49              |
| 1:G:66:VAL:HG22  | 1:G:149:ALA:HB2  | 1.94                     | 0.49              |
| 1:F:66:VAL:HG22  | 1:F:149:ALA:HB2  | 1.93                     | 0.49              |
| 1:C:7:LEU:CD2    | 1:C:7:LEU:N      | 2.76                     | 0.49              |
| 1:E:241:ASP:OD2  | 1:E:312:ASP:OD2  | 2.30                     | 0.49              |
| 1:F:222:SER:CA   | 1:F:358:ASN:HB2  | 2.41                     | 0.49              |
| 1:G:176:TYR:CD1  | 1:G:177:PRO:HA   | 2.47                     | 0.49              |
| 1:B:307:VAL:O    | 1:B:308:GLY:C    | 2.54                     | 0.49              |
| 1:C:229:PRO:HD2  | 1:C:233:ASP:OD2  | 2.12                     | 0.49              |
| 1:E:150:THR:HG21 | 1:E:188:ILE:CG1  | 2.34                     | 0.49              |
| 1:G:325:GLU:CA   | 1:G:328:LEU:CG   | 2.63                     | 0.49              |
| 1:E:20:ARG:HG3   | 1:E:37:ALA:O     | 2.12                     | 0.49              |
| 1:F:228:PHE:N    | 1:F:229:PRO:CD   | 2.75                     | 0.49              |
| 1:D:4:GLU:O      | 1:D:55:HIS:HB2   | 2.12                     | 0.49              |
| 1:F:278:GLY:HA3  | 1:F:332:VAL:O    | 2.12                     | 0.49              |
| 1:C:260:LYS:HD3  | 1:C:261:TYR:CZ   | 2.48                     | 0.49              |
| 1:D:227:ASN:O    | 1:D:229:PRO:HD2  | 2.13                     | 0.49              |
| 1:F:91:GLN:HG3   | 1:F:110:ARG:HH21 | 1.77                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:37:ALA:HA    | 1:A:124:GLN:O    | 2.13                     | 0.49              |
| 1:F:5:VAL:HG12   | 1:F:7:LEU:HD12   | 1.94                     | 0.49              |
| 1:B:85:ARG:NE    | 1:B:125:GLU:OE1  | 2.46                     | 0.48              |
| 1:B:115:SER:HB3  | 1:H:41:SER:OG    | 2.13                     | 0.48              |
| 1:C:10:SER:O     | 1:C:44:LEU:HD12  | 2.13                     | 0.48              |
| 1:C:128:LEU:HD11 | 1:C:130:VAL:O    | 2.13                     | 0.48              |
| 1:C:224:ALA:HB3  | 1:C:227:ASN:ND2  | 2.28                     | 0.48              |
| 1:D:228:PHE:CB   | 1:D:321:ARG:HD3  | 2.43                     | 0.48              |
| 1:G:96:ARG:CZ    | 1:G:165:ILE:HG21 | 2.43                     | 0.48              |
| 1:A:72:TYR:HA    | 1:C:68:TYR:CD2   | 2.49                     | 0.48              |
| 1:B:91:GLN:NE2   | 1:B:91:GLN:CA    | 2.76                     | 0.48              |
| 1:D:228:PHE:HB3  | 1:D:321:ARG:HD3  | 1.96                     | 0.48              |
| 1:E:74:THR:HG22  | 1:E:85:ARG:HB2   | 1.94                     | 0.48              |
| 1:D:224:ALA:HA   | 1:D:360:THR:C    | 2.37                     | 0.48              |
| 1:A:6:ALA:O      | 1:A:7:LEU:CD2    | 2.62                     | 0.48              |
| 1:D:7:LEU:HD23   | 1:D:180:VAL:CA   | 2.38                     | 0.48              |
| 1:D:209:LYS:NZ   | 1:D:209:LYS:CD   | 2.76                     | 0.48              |
| 1:F:167:SER:OG   | 1:H:167:SER:OG   | 2.31                     | 0.48              |
| 1:G:206:LYS:C    | 1:G:251:ALA:CB   | 2.87                     | 0.48              |
| 1:H:139:ASP:O    | 1:H:140:LEU:CB   | 2.61                     | 0.48              |
| 1:D:158:ARG:NH2  | 1:D:162:GLU:OE1  | 2.46                     | 0.48              |
| 1:G:44:LEU:HB3   | 1:G:118:THR:HG23 | 1.95                     | 0.48              |
| 1:G:291:ASP:O    | 1:G:292:GLN:HB2  | 2.13                     | 0.48              |
| 1:A:78:ASP:OD2   | 1:A:143:THR:OG1  | 2.29                     | 0.48              |
| 1:A:86:ILE:CG2   | 1:A:98:ILE:HD12  | 2.34                     | 0.48              |
| 1:E:46:TYR:OH    | 2:E:402:HOH:O    | 2.20                     | 0.48              |
| 1:G:343:PHE:N    | 1:G:344:PRO:CA   | 2.76                     | 0.48              |
| 1:A:180:VAL:CG1  | 1:A:182:ARG:CZ   | 2.91                     | 0.48              |
| 1:C:7:LEU:HB2    | 1:C:179:GLY:C    | 2.38                     | 0.48              |
| 1:C:342:THR:HG22 | 1:C:346:ASP:O    | 2.14                     | 0.48              |
| 1:E:4:GLU:CG     | 1:E:112:THR:HG23 | 2.44                     | 0.48              |
| 1:F:61:GLY:C     | 1:F:98:ILE:HG23  | 2.39                     | 0.48              |
| 1:G:218:VAL:O    | 1:G:355:PHE:HA   | 2.14                     | 0.48              |
| 1:A:19:TRP:HA    | 1:A:38:ARG:HG3   | 1.94                     | 0.48              |
| 1:B:235:SER:OG   | 1:B:319:TYR:N    | 2.44                     | 0.48              |
| 1:C:292:GLN:CG   | 1:D:34:VAL:HG21  | 2.44                     | 0.48              |
| 1:F:225:LEU:HD22 | 1:F:360:THR:O    | 2.13                     | 0.48              |
| 1:A:343:PHE:H    | 1:A:345:SER:H    | 1.63                     | 0.47              |
| 1:C:150:THR:HB   | 1:C:188:ILE:HG22 | 1.96                     | 0.47              |
| 1:C:342:THR:HB   | 1:C:344:PRO:CB   | 2.44                     | 0.47              |
| 1:G:3:ASN:C      | 1:G:4:GLU:HG2    | 2.39                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:66:VAL:HG22  | 1:H:149:ALA:HB2  | 1.94                     | 0.47              |
| 1:C:187:LEU:N    | 1:C:187:LEU:HD12 | 2.29                     | 0.47              |
| 1:D:66:VAL:CG2   | 1:D:149:ALA:CB   | 2.91                     | 0.47              |
| 1:F:340:THR:HG22 | 1:F:341:PHE:N    | 2.29                     | 0.47              |
| 1:G:16:GLY:O     | 1:G:17:LEU:HD23  | 2.14                     | 0.47              |
| 1:E:4:GLU:CB     | 1:E:112:THR:CG2  | 2.92                     | 0.47              |
| 1:A:211:GLU:CD   | 1:A:214:ARG:HD3  | 2.39                     | 0.47              |
| 1:B:207:LYS:CG   | 1:B:343:PHE:CE1  | 2.97                     | 0.47              |
| 1:D:206:LYS:C    | 1:D:251:ALA:CB   | 2.87                     | 0.47              |
| 1:G:37:ALA:HA    | 1:G:124:GLN:O    | 2.14                     | 0.47              |
| 1:G:58:VAL:HG11  | 1:G:169:LEU:HD13 | 1.95                     | 0.47              |
| 1:A:26:THR:O     | 1:A:132:PRO:HG2  | 2.15                     | 0.47              |
| 1:A:53:GLU:N     | 1:A:53:GLU:CD    | 2.73                     | 0.47              |
| 1:A:222:SER:OG   | 1:A:358:ASN:HB2  | 2.14                     | 0.47              |
| 1:F:220:LEU:CD1  | 1:F:355:PHE:HB3  | 2.45                     | 0.47              |
| 1:F:247:CYS:HB2  | 1:F:309:ASP:O    | 2.15                     | 0.47              |
| 1:G:110:ARG:CG   | 1:G:110:ARG:NH1  | 2.72                     | 0.47              |
| 1:C:227:ASN:O    | 1:C:229:PRO:HD3  | 2.14                     | 0.47              |
| 1:C:280:ALA:HB3  | 1:C:329:LYS:HB2  | 1.96                     | 0.47              |
| 1:D:31:LYS:HD3   | 1:D:130:VAL:HA   | 1.97                     | 0.47              |
| 1:G:278:GLY:HA2  | 1:G:332:VAL:HG11 | 1.89                     | 0.47              |
| 1:B:5:VAL:CG1    | 1:B:49:GLN:O     | 2.63                     | 0.47              |
| 1:D:244:LEU:HD21 | 1:D:341:PHE:CE2  | 2.49                     | 0.47              |
| 1:F:63:TRP:HB2   | 1:F:100:VAL:HA   | 1.97                     | 0.47              |
| 1:F:286:VAL:HA   | 1:F:316:SER:O    | 2.15                     | 0.47              |
| 1:D:274:LEU:CA   | 1:D:334:ASP:O    | 2.63                     | 0.47              |
| 1:D:360:THR:CG2  | 1:D:361:GLU:CD   | 2.86                     | 0.47              |
| 1:E:48:PRO:CG    | 1:E:114:PHE:HA   | 2.45                     | 0.47              |
| 1:E:131:ASP:HB2  | 1:E:134:GLU:HG3  | 1.97                     | 0.47              |
| 1:A:150:THR:HG22 | 1:A:188:ILE:CG2  | 2.35                     | 0.46              |
| 1:A:258:ARG:NH2  | 1:A:298:ASP:C    | 2.72                     | 0.46              |
| 1:B:77:SER:OG    | 1:B:82:ILE:O     | 2.28                     | 0.46              |
| 1:D:234:THR:CG2  | 1:D:320:ILE:CD1  | 2.89                     | 0.46              |
| 1:G:174:ASP:O    | 1:G:182:ARG:HD2  | 2.15                     | 0.46              |
| 1:B:92:ASP:OD1   | 1:B:92:ASP:N     | 2.46                     | 0.46              |
| 1:F:136:PRO:O    | 1:F:140:LEU:HD21 | 2.15                     | 0.46              |
| 1:F:320:ILE:HG12 | 1:F:321:ARG:N    | 2.29                     | 0.46              |
| 1:H:208:CYS:HA   | 1:H:247:CYS:HA   | 1.96                     | 0.46              |
| 1:A:341:PHE:O    | 1:A:346:ASP:HB2  | 2.14                     | 0.46              |
| 1:C:150:THR:HG22 | 1:C:188:ILE:HG22 | 1.96                     | 0.46              |
| 1:D:283:GLY:O    | 1:D:320:ILE:HG22 | 2.15                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:77:SER:O     | 1:E:146:SER:HB3  | 2.16                     | 0.46              |
| 1:E:92:ASP:OD1   | 1:E:92:ASP:N     | 2.43                     | 0.46              |
| 1:G:63:TRP:CE2   | 1:G:151:LEU:HD13 | 2.50                     | 0.46              |
| 1:E:156:VAL:HA   | 1:E:181:CYS:O    | 2.15                     | 0.46              |
| 1:G:283:GLY:O    | 1:G:320:ILE:HG22 | 2.16                     | 0.46              |
| 1:E:32:GLY:HA3   | 1:E:72:TYR:CZ    | 2.48                     | 0.46              |
| 1:E:88:VAL:HG22  | 1:E:122:TYR:CE2  | 2.51                     | 0.46              |
| 1:F:60:GLY:O     | 1:F:154:TRP:CD1  | 2.67                     | 0.46              |
| 1:G:234:THR:HA   | 1:G:319:TYR:O    | 2.16                     | 0.46              |
| 1:A:66:VAL:HG23  | 1:A:149:ALA:HB2  | 1.98                     | 0.46              |
| 1:A:175:ASN:HD21 | 1:A:179:GLY:H    | 1.63                     | 0.46              |
| 1:A:229:PRO:O    | 1:A:321:ARG:NH1  | 2.48                     | 0.46              |
| 1:B:4:GLU:CA     | 1:B:112:THR:HG21 | 2.44                     | 0.46              |
| 1:B:207:LYS:CG   | 1:B:343:PHE:CZ   | 2.90                     | 0.46              |
| 1:F:66:VAL:CG2   | 1:F:149:ALA:CB   | 2.94                     | 0.46              |
| 1:G:128:LEU:HG   | 1:G:130:VAL:O    | 2.16                     | 0.46              |
| 1:A:58:VAL:HG11  | 1:A:169:LEU:HD13 | 1.98                     | 0.45              |
| 1:D:90:ALA:HB3   | 1:D:92:ASP:OD1   | 2.16                     | 0.45              |
| 1:D:172:PRO:HG2  | 1:D:182:ARG:CZ   | 2.46                     | 0.45              |
| 1:D:279:ALA:HB2  | 1:D:331:GLY:O    | 2.16                     | 0.45              |
| 1:C:77:SER:OG    | 1:C:82:ILE:O     | 2.27                     | 0.45              |
| 1:G:206:LYS:O    | 1:G:251:ALA:HB1  | 2.17                     | 0.45              |
| 1:D:157:ASP:C    | 1:D:158:ARG:HG2  | 2.42                     | 0.45              |
| 1:D:361:GLU:OE1  | 1:D:361:GLU:N    | 2.49                     | 0.45              |
| 1:G:279:ALA:HB2  | 1:G:330:ALA:HB3  | 1.49                     | 0.45              |
| 1:F:91:GLN:CG    | 1:F:110:ARG:NH2  | 2.76                     | 0.45              |
| 1:B:209:LYS:O    | 1:B:209:LYS:HG3  | 2.16                     | 0.45              |
| 1:C:6:ALA:HB1    | 1:C:46:TYR:CG    | 2.49                     | 0.45              |
| 1:D:7:LEU:CD2    | 1:D:180:VAL:HA   | 2.38                     | 0.45              |
| 1:D:279:ALA:CB   | 1:D:331:GLY:O    | 2.65                     | 0.45              |
| 1:E:183:LYS:H    | 1:E:183:LYS:HD2  | 1.81                     | 0.45              |
| 1:G:241:ASP:OD1  | 1:G:242:ILE:N    | 2.50                     | 0.45              |
| 1:H:223:VAL:HG11 | 1:H:235:SER:HB2  | 1.99                     | 0.45              |
| 1:D:332:VAL:HG12 | 1:D:332:VAL:O    | 2.16                     | 0.45              |
| 1:F:225:LEU:CD2  | 1:F:225:LEU:N    | 2.76                     | 0.45              |
| 1:D:74:THR:HG22  | 1:D:85:ARG:HB3   | 1.97                     | 0.45              |
| 1:E:81:GLY:HA3   | 1:E:130:VAL:HG22 | 1.98                     | 0.45              |
| 1:H:136:PRO:O    | 1:H:140:LEU:HD21 | 2.17                     | 0.45              |
| 1:A:17:LEU:O     | 1:A:38:ARG:HD3   | 2.17                     | 0.45              |
| 1:A:25:LEU:HD23  | 1:A:204:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:229:PRO:CD   | 1:B:233:ASP:OD2  | 2.62                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:229:PRO:HG2  | 1:B:233:ASP:OD2  | 2.16                     | 0.45              |
| 1:H:5:VAL:HG22   | 1:H:55:HIS:CD2   | 2.51                     | 0.45              |
| 1:A:259:ASP:OD2  | 1:A:273:SER:HB3  | 2.15                     | 0.45              |
| 1:C:234:THR:CG2  | 1:C:320:ILE:HG13 | 2.47                     | 0.45              |
| 1:C:291:ASP:O    | 1:C:292:GLN:CB   | 2.65                     | 0.45              |
| 1:D:280:ALA:O    | 1:D:282:PHE:HD1  | 2.00                     | 0.45              |
| 1:F:31:LYS:HB3   | 1:F:72:TYR:OH    | 2.16                     | 0.44              |
| 1:F:283:GLY:O    | 1:F:320:ILE:N    | 2.40                     | 0.44              |
| 1:A:157:ASP:C    | 1:A:158:ARG:HG2  | 2.42                     | 0.44              |
| 1:C:227:ASN:N    | 1:C:227:ASN:ND2  | 2.65                     | 0.44              |
| 1:D:283:GLY:O    | 1:D:320:ILE:N    | 2.30                     | 0.44              |
| 1:H:3:ASN:N      | 1:H:4:GLU:OE2    | 2.51                     | 0.44              |
| 1:H:3:ASN:HA     | 1:H:112:THR:OG1  | 2.18                     | 0.44              |
| 1:D:360:THR:HG22 | 1:D:361:GLU:OE1  | 2.17                     | 0.44              |
| 1:G:329:LYS:O    | 1:G:330:ALA:CB   | 2.65                     | 0.44              |
| 1:C:62:ASN:ND2   | 1:C:154:TRP:HE1  | 2.15                     | 0.44              |
| 1:C:131:ASP:HB3  | 2:C:439:HOH:O    | 2.17                     | 0.44              |
| 1:D:225:LEU:CD1  | 1:D:282:PHE:HZ   | 2.31                     | 0.44              |
| 1:G:269:PRO:HD3  | 1:H:102:ASN:O    | 2.17                     | 0.44              |
| 1:B:58:VAL:HG11  | 1:B:169:LEU:HD13 | 2.00                     | 0.44              |
| 1:E:62:ASN:HD22  | 1:E:104:PRO:N    | 2.15                     | 0.44              |
| 1:E:269:PRO:HD3  | 1:F:102:ASN:O    | 2.17                     | 0.44              |
| 1:G:228:PHE:CE2  | 1:G:282:PHE:CD1  | 2.88                     | 0.44              |
| 1:A:139:ASP:OD1  | 1:A:140:LEU:N    | 2.51                     | 0.44              |
| 1:E:175:ASN:HD21 | 1:E:179:GLY:N    | 1.96                     | 0.44              |
| 1:B:85:ARG:HG3   | 1:B:125:GLU:HB2  | 2.00                     | 0.44              |
| 1:C:225:LEU:HD23 | 1:C:225:LEU:C    | 2.42                     | 0.44              |
| 1:D:204:ILE:N    | 1:D:204:ILE:CD1  | 2.80                     | 0.44              |
| 1:H:154:TRP:CZ3  | 1:H:184:PRO:HB3  | 2.53                     | 0.44              |
| 1:B:60:GLY:HA2   | 1:B:105:HIS:O    | 2.18                     | 0.44              |
| 1:B:266:GLN:O    | 1:B:267:ALA:C    | 2.61                     | 0.44              |
| 1:C:13:ASN:OD1   | 1:C:196:GLY:HA2  | 2.18                     | 0.44              |
| 1:D:44:LEU:CD2   | 1:D:57:LEU:CD2   | 2.96                     | 0.44              |
| 1:G:206:LYS:C    | 1:G:251:ALA:HB1  | 2.43                     | 0.44              |
| 1:C:141:LYS:NZ   | 1:C:141:LYS:CG   | 2.81                     | 0.44              |
| 1:C:145:VAL:CG1  | 1:C:149:ALA:HB3  | 2.48                     | 0.44              |
| 1:B:4:GLU:O      | 1:B:112:THR:CB   | 2.64                     | 0.43              |
| 1:C:66:VAL:CG2   | 1:C:149:ALA:HB2  | 2.48                     | 0.43              |
| 1:D:138:GLY:O    | 1:D:206:LYS:HG3  | 2.17                     | 0.43              |
| 1:E:5:VAL:HG22   | 1:E:55:HIS:CD2   | 2.52                     | 0.43              |
| 1:F:56:GLU:CG    | 1:F:160:LYS:HG3  | 2.47                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:75:VAL:HG12  | 1:F:145:VAL:CG2  | 2.48                     | 0.43              |
| 1:A:74:THR:HG22  | 1:A:85:ARG:HB2   | 2.01                     | 0.43              |
| 1:C:207:LYS:HG2  | 1:C:343:PHE:CD2  | 2.52                     | 0.43              |
| 1:E:25:LEU:HD21  | 1:E:250:LEU:HD11 | 2.00                     | 0.43              |
| 1:E:48:PRO:HG2   | 1:E:114:PHE:C    | 2.43                     | 0.43              |
| 1:E:244:LEU:O    | 1:E:310:SER:HB3  | 2.18                     | 0.43              |
| 1:F:225:LEU:CD2  | 1:F:361:GLU:HA   | 2.48                     | 0.43              |
| 1:B:91:GLN:NE2   | 1:B:91:GLN:HA    | 2.32                     | 0.43              |
| 1:C:6:ALA:HB2    | 1:C:46:TYR:CE2   | 2.53                     | 0.43              |
| 1:E:81:GLY:HA3   | 1:E:130:VAL:CG2  | 2.48                     | 0.43              |
| 1:D:66:VAL:HG21  | 1:D:149:ALA:HB2  | 1.97                     | 0.43              |
| 1:G:325:GLU:CA   | 1:G:328:LEU:HD11 | 2.46                     | 0.43              |
| 1:A:92:ASP:OD1   | 1:A:92:ASP:N     | 2.44                     | 0.43              |
| 1:D:208:CYS:HA   | 1:D:247:CYS:HA   | 2.00                     | 0.43              |
| 1:D:266:GLN:OE1  | 1:D:266:GLN:N    | 2.38                     | 0.43              |
| 1:F:64:SER:O     | 1:F:149:ALA:HA   | 2.18                     | 0.43              |
| 1:D:56:GLU:HG3   | 1:D:160:LYS:HG3  | 2.01                     | 0.43              |
| 1:A:79:VAL:HG21  | 1:A:140:LEU:O    | 2.19                     | 0.43              |
| 1:B:66:VAL:HG13  | 1:B:100:VAL:CG1  | 2.48                     | 0.43              |
| 1:B:234:THR:HG22 | 1:B:320:ILE:HD12 | 2.00                     | 0.43              |
| 1:C:336:ALA:HB1  | 1:C:352:ILE:CD1  | 2.49                     | 0.43              |
| 1:C:260:LYS:HD3  | 1:C:261:TYR:CE1  | 2.54                     | 0.43              |
| 1:E:68:TYR:CG    | 1:G:72:TYR:HA    | 2.53                     | 0.43              |
| 1:F:225:LEU:HD23 | 1:F:361:GLU:HA   | 2.01                     | 0.43              |
| 1:B:114:PHE:CE2  | 1:H:41:SER:HB2   | 2.52                     | 0.43              |
| 1:F:307:VAL:O    | 1:F:308:GLY:C    | 2.61                     | 0.43              |
| 1:G:202:PRO:HA   | 1:G:203:PRO:HD3  | 1.88                     | 0.43              |
| 1:B:243:SER:HB2  | 1:B:312:ASP:HB3  | 2.01                     | 0.43              |
| 1:E:68:TYR:CD2   | 1:G:72:TYR:HA    | 2.54                     | 0.43              |
| 1:E:244:LEU:O    | 1:E:310:SER:CB   | 2.67                     | 0.43              |
| 1:F:265:GLN:HA   | 1:F:265:GLN:HE21 | 1.84                     | 0.43              |
| 1:G:176:TYR:HA   | 1:G:177:PRO:C    | 2.43                     | 0.43              |
| 1:G:330:ALA:O    | 1:G:359:ILE:O    | 2.36                     | 0.43              |
| 1:B:5:VAL:HB     | 1:B:55:HIS:HD2   | 1.79                     | 0.42              |
| 1:C:282:PHE:CD2  | 1:C:359:ILE:CD1  | 3.02                     | 0.42              |
| 1:D:60:GLY:HA2   | 1:D:105:HIS:O    | 2.18                     | 0.42              |
| 1:E:66:VAL:HG22  | 1:E:149:ALA:CB   | 2.48                     | 0.42              |
| 1:F:283:GLY:C    | 1:F:320:ILE:HG22 | 2.44                     | 0.42              |
| 1:B:291:ASP:O    | 1:B:292:GLN:HB2  | 2.19                     | 0.42              |
| 1:D:228:PHE:CE2  | 1:D:282:PHE:HE2  | 2.37                     | 0.42              |
| 1:A:175:ASN:ND2  | 1:A:175:ASN:C    | 2.73                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:342:THR:HG23 | 2:A:419:HOH:O    | 2.18                     | 0.42              |
| 1:D:62:ASN:HB3   | 1:D:104:PRO:HA   | 2.01                     | 0.42              |
| 1:E:57:LEU:HD12  | 1:E:57:LEU:HA    | 1.76                     | 0.42              |
| 1:B:91:GLN:HE21  | 1:B:91:GLN:N     | 2.16                     | 0.42              |
| 1:C:319:TYR:CE1  | 1:C:333:ALA:HB1  | 2.54                     | 0.42              |
| 1:E:63:TRP:HB2   | 1:E:100:VAL:HA   | 2.01                     | 0.42              |
| 1:E:230:ARG:CZ   | 1:E:230:ARG:HB2  | 2.49                     | 0.42              |
| 1:H:321:ARG:CZ   | 1:H:328:LEU:HD11 | 2.49                     | 0.42              |
| 1:C:225:LEU:HD21 | 1:C:328:LEU:HD12 | 2.02                     | 0.42              |
| 1:C:288:ASN:ND2  | 1:C:313:LEU:HD11 | 2.35                     | 0.42              |
| 1:E:62:ASN:ND2   | 1:E:104:PRO:N    | 2.67                     | 0.42              |
| 1:F:139:ASP:OD1  | 1:F:140:LEU:N    | 2.53                     | 0.42              |
| 1:G:223:VAL:HB   | 1:G:359:ILE:HD13 | 2.01                     | 0.42              |
| 1:G:247:CYS:HB2  | 1:G:309:ASP:O    | 2.20                     | 0.42              |
| 1:A:139:ASP:O    | 1:A:140:LEU:CB   | 2.68                     | 0.42              |
| 1:C:7:LEU:HB2    | 1:C:179:GLY:O    | 2.20                     | 0.42              |
| 1:C:17:LEU:HD23  | 1:C:17:LEU:HA    | 1.85                     | 0.42              |
| 1:D:210:VAL:HG21 | 1:D:343:PHE:HZ   | 1.83                     | 0.42              |
| 1:D:360:THR:HG22 | 1:D:361:GLU:OE2  | 2.19                     | 0.42              |
| 1:F:269:PRO:O    | 1:F:297:PHE:HD1  | 2.02                     | 0.42              |
| 1:G:21:VAL:HG22  | 1:G:36:PHE:CE1   | 2.54                     | 0.42              |
| 1:H:66:VAL:CG2   | 1:H:149:ALA:CB   | 2.92                     | 0.42              |
| 1:C:154:TRP:CH2  | 1:C:184:PRO:CG   | 2.98                     | 0.42              |
| 1:D:288:ASN:ND2  | 1:D:313:LEU:HD11 | 2.35                     | 0.42              |
| 1:E:81:GLY:HA2   | 1:E:130:VAL:HG13 | 2.01                     | 0.42              |
| 1:C:222:SER:HA   | 1:C:358:ASN:O    | 2.19                     | 0.42              |
| 1:D:274:LEU:HD22 | 1:D:333:ALA:HB1  | 1.99                     | 0.42              |
| 1:D:291:ASP:O    | 1:D:292:GLN:HB2  | 2.20                     | 0.42              |
| 1:C:157:ASP:O    | 1:C:158:ARG:HG2  | 2.19                     | 0.42              |
| 1:E:139:ASP:OD1  | 1:E:140:LEU:N    | 2.53                     | 0.42              |
| 1:G:7:LEU:HD22   | 1:G:180:VAL:CA   | 2.49                     | 0.42              |
| 1:C:7:LEU:O      | 1:C:8:ASN:HB2    | 2.20                     | 0.42              |
| 1:C:141:LYS:NZ   | 1:C:141:LYS:HG2  | 2.35                     | 0.42              |
| 1:C:231:VAL:HA   | 1:C:321:ARG:HG2  | 2.01                     | 0.42              |
| 1:H:175:ASN:O    | 1:H:178:THR:HA   | 2.20                     | 0.42              |
| 1:H:298:ASP:OD1  | 1:H:299:GLY:N    | 2.53                     | 0.42              |
| 1:A:23:ASN:HD21  | 1:B:290:LEU:HA   | 1.85                     | 0.41              |
| 1:B:4:GLU:N      | 1:B:112:THR:CG2  | 2.83                     | 0.41              |
| 1:B:306:ARG:HD2  | 1:B:311:ALA:HB2  | 2.02                     | 0.41              |
| 1:F:222:SER:HA   | 1:F:358:ASN:HB2  | 2.01                     | 0.41              |
| 1:G:288:ASN:ND2  | 1:G:313:LEU:HD11 | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:90:ALA:HB1   | 1:A:92:ASP:OD1   | 2.20                     | 0.41              |
| 1:A:254:GLU:HG2  | 1:A:303:PRO:HA   | 2.01                     | 0.41              |
| 1:D:206:LYS:O    | 1:D:251:ALA:CB   | 2.68                     | 0.41              |
| 1:E:140:LEU:HB2  | 1:E:204:ILE:CD1  | 2.50                     | 0.41              |
| 1:E:218:VAL:O    | 1:E:355:PHE:HA   | 2.20                     | 0.41              |
| 1:F:26:THR:O     | 1:F:132:PRO:HG2  | 2.19                     | 0.41              |
| 1:G:268:ASP:OD1  | 1:G:270:THR:OG1  | 2.32                     | 0.41              |
| 1:A:157:ASP:O    | 1:A:158:ARG:HG2  | 2.19                     | 0.41              |
| 1:C:136:PRO:HD2  | 1:C:140:LEU:HD21 | 2.01                     | 0.41              |
| 1:C:181:CYS:C    | 1:C:182:ARG:CD   | 2.93                     | 0.41              |
| 1:E:5:VAL:HG23   | 1:E:51:SER:HB2   | 2.02                     | 0.41              |
| 1:E:140:LEU:CB   | 1:E:204:ILE:HD13 | 2.50                     | 0.41              |
| 1:H:57:LEU:HD12  | 1:H:57:LEU:HA    | 1.82                     | 0.41              |
| 1:A:4:GLU:O      | 1:A:55:HIS:HB2   | 2.20                     | 0.41              |
| 1:B:57:LEU:HD12  | 1:B:57:LEU:HA    | 1.87                     | 0.41              |
| 1:B:91:GLN:CA    | 1:B:91:GLN:HE21  | 2.33                     | 0.41              |
| 1:D:104:PRO:HB3  | 1:D:154:TRP:NE1  | 2.36                     | 0.41              |
| 1:G:296:ARG:HB3  | 1:G:298:ASP:OD1  | 2.21                     | 0.41              |
| 1:G:305:ARG:O    | 1:G:311:ALA:HA   | 2.20                     | 0.41              |
| 1:G:338:GLU:H    | 1:G:338:GLU:HG2  | 1.60                     | 0.41              |
| 1:C:154:TRP:CE3  | 1:C:184:PRO:HB3  | 2.54                     | 0.41              |
| 1:D:224:ALA:CB   | 1:D:360:THR:HG22 | 2.48                     | 0.41              |
| 1:H:17:LEU:HD12  | 1:H:39:PRO:HG2   | 2.02                     | 0.41              |
| 1:D:44:LEU:HD21  | 1:D:57:LEU:CD2   | 2.50                     | 0.41              |
| 1:E:60:GLY:HA2   | 1:E:105:HIS:O    | 2.20                     | 0.41              |
| 1:E:179:GLY:O    | 1:E:180:VAL:C    | 2.63                     | 0.41              |
| 1:F:53:GLU:N     | 1:F:53:GLU:CD    | 2.78                     | 0.41              |
| 1:F:156:VAL:HA   | 1:F:181:CYS:O    | 2.21                     | 0.41              |
| 1:F:222:SER:HA   | 1:F:358:ASN:CA   | 2.50                     | 0.41              |
| 1:H:66:VAL:HG21  | 1:H:149:ALA:HB2  | 2.01                     | 0.41              |
| 1:C:89:ASP:HB2   | 1:C:121:ASP:HB3  | 2.02                     | 0.41              |
| 1:F:132:PRO:O    | 1:F:135:LEU:HB2  | 2.20                     | 0.41              |
| 1:F:258:ARG:HA   | 1:F:297:PHE:O    | 2.21                     | 0.41              |
| 1:F:321:ARG:O    | 1:F:322:ILE:CB   | 2.68                     | 0.41              |
| 1:H:256:ALA:HB1  | 1:H:299:GLY:O    | 2.21                     | 0.41              |
| 1:A:19:TRP:CE2   | 1:A:201:PRO:HG3  | 2.56                     | 0.41              |
| 1:H:320:ILE:HG12 | 1:H:321:ARG:N    | 2.36                     | 0.41              |
| 1:A:38:ARG:HB3   | 1:A:38:ARG:NH2   | 2.33                     | 0.41              |
| 1:A:56:GLU:HG3   | 1:A:160:LYS:CG   | 2.51                     | 0.41              |
| 1:A:150:THR:HG22 | 1:A:188:ILE:HG12 | 2.01                     | 0.41              |
| 1:B:111:VAL:HA   | 2:B:414:HOH:O    | 2.21                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:237:GLU:HG2  | 1:B:318:ALA:HB2  | 2.03                     | 0.41              |
| 1:D:110:ARG:CD   | 1:D:118:THR:OG1  | 2.68                     | 0.41              |
| 1:D:265:GLN:HE22 | 1:D:269:PRO:HG2  | 1.83                     | 0.41              |
| 1:E:4:GLU:CD     | 1:E:112:THR:CG2  | 2.94                     | 0.41              |
| 1:E:72:TYR:O     | 1:E:74:THR:HG23  | 2.21                     | 0.41              |
| 1:F:18:PRO:HA    | 1:F:199:PRO:HG2  | 2.03                     | 0.41              |
| 1:F:183:LYS:H    | 1:F:183:LYS:HG3  | 1.60                     | 0.41              |
| 1:F:222:SER:HG   | 1:F:358:ASN:ND2  | 2.15                     | 0.41              |
| 1:D:269:PRO:O    | 1:D:297:PHE:HD1  | 2.04                     | 0.41              |
| 1:G:96:ARG:NH2   | 1:G:165:ILE:HG21 | 2.36                     | 0.41              |
| 1:A:111:VAL:O    | 1:A:111:VAL:HG23 | 2.20                     | 0.40              |
| 1:A:154:TRP:CE2  | 1:A:184:PRO:HB3  | 2.56                     | 0.40              |
| 1:C:54:ALA:O     | 1:C:55:HIS:ND1   | 2.50                     | 0.40              |
| 1:B:207:LYS:HA   | 1:B:343:PHE:CE2  | 2.57                     | 0.40              |
| 1:C:244:LEU:O    | 1:C:310:SER:HB2  | 2.20                     | 0.40              |
| 1:F:317:ALA:CB   | 1:F:355:PHE:HE2  | 2.34                     | 0.40              |
| 1:H:77:SER:OG    | 1:H:82:ILE:O     | 2.29                     | 0.40              |
| 1:F:19:TRP:CE2   | 1:F:201:PRO:HG3  | 2.57                     | 0.40              |
| 1:H:176:TYR:HA   | 1:H:177:PRO:C    | 2.45                     | 0.40              |
| 1:D:360:THR:O    | 1:D:361:GLU:HB2  | 2.22                     | 0.40              |
| 1:F:305:ARG:O    | 1:F:311:ALA:HA   | 2.22                     | 0.40              |
| 1:G:138:GLY:O    | 1:G:206:LYS:HG3  | 2.22                     | 0.40              |
| 1:G:325:GLU:N    | 1:G:328:LEU:CD2  | 2.26                     | 0.40              |
| 1:H:5:VAL:HG23   | 1:H:51:SER:CB    | 2.52                     | 0.40              |
| 1:A:40:VAL:HG13  | 1:A:196:GLY:HA3  | 2.03                     | 0.40              |
| 1:C:4:GLU:O      | 1:C:55:HIS:HB3   | 2.03                     | 0.40              |
| 1:C:4:GLU:HG2    | 1:C:112:THR:HB   | 2.03                     | 0.40              |
| 1:H:37:ALA:HA    | 1:H:124:GLN:O    | 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 359/370 (97%)   | 349 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 1   | B     | 351/370 (95%)   | 343 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 1   | C     | 343/370 (93%)   | 339 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | D     | 355/370 (96%)   | 343 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 1   | E     | 351/370 (95%)   | 348 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 1   | F     | 324/370 (88%)   | 318 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 1   | G     | 345/370 (93%)   | 341 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 1   | H     | 355/370 (96%)   | 348 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| All | All   | 2783/2960 (94%) | 2729 (98%) | 54 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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     | 278/297 (94%)   | 259 (93%)  | 19 (7%)  | 14          | 38 |
| 1   | B     | 274/297 (92%)   | 245 (89%)  | 29 (11%) | 6           | 19 |
| 1   | C     | 267/297 (90%)   | 242 (91%)  | 25 (9%)  | 8           | 24 |
| 1   | D     | 272/297 (92%)   | 248 (91%)  | 24 (9%)  | 9           | 27 |
| 1   | E     | 275/297 (93%)   | 252 (92%)  | 23 (8%)  | 10          | 29 |
| 1   | F     | 249/297 (84%)   | 220 (88%)  | 29 (12%) | 5           | 16 |
| 1   | G     | 265/297 (89%)   | 243 (92%)  | 22 (8%)  | 10          | 29 |
| 1   | H     | 280/297 (94%)   | 262 (94%)  | 18 (6%)  | 16          | 41 |
| All | All   | 2160/2376 (91%) | 1971 (91%) | 189 (9%) | 9           | 27 |

All (189) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | VAL  |
| 1   | A     | 7   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 24  | GLU  |
| 1   | A     | 26  | THR  |
| 1   | A     | 27  | SER  |
| 1   | A     | 38  | ARG  |
| 1   | A     | 109 | LYS  |
| 1   | A     | 112 | THR  |
| 1   | A     | 117 | SER  |
| 1   | A     | 134 | GLU  |
| 1   | A     | 146 | SER  |
| 1   | A     | 164 | SER  |
| 1   | A     | 182 | ARG  |
| 1   | A     | 195 | ILE  |
| 1   | A     | 250 | LEU  |
| 1   | A     | 273 | SER  |
| 1   | A     | 296 | ARG  |
| 1   | A     | 307 | VAL  |
| 1   | A     | 348 | LYS  |
| 1   | B     | 2   | LEU  |
| 1   | B     | 4   | GLU  |
| 1   | B     | 5   | VAL  |
| 1   | B     | 27  | SER  |
| 1   | B     | 41  | SER  |
| 1   | B     | 75  | VAL  |
| 1   | B     | 88  | VAL  |
| 1   | B     | 89  | ASP  |
| 1   | B     | 91  | GLN  |
| 1   | B     | 146 | SER  |
| 1   | B     | 148 | SER  |
| 1   | B     | 150 | THR  |
| 1   | B     | 164 | SER  |
| 1   | B     | 182 | ARG  |
| 1   | B     | 188 | ILE  |
| 1   | B     | 210 | VAL  |
| 1   | B     | 212 | VAL  |
| 1   | B     | 214 | ARG  |
| 1   | B     | 223 | VAL  |
| 1   | B     | 225 | LEU  |
| 1   | B     | 235 | SER  |
| 1   | B     | 243 | SER  |
| 1   | B     | 286 | VAL  |
| 1   | B     | 296 | ARG  |
| 1   | B     | 320 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 327 | GLU  |
| 1   | B     | 332 | VAL  |
| 1   | B     | 353 | VAL  |
| 1   | B     | 361 | GLU  |
| 1   | C     | 7   | LEU  |
| 1   | C     | 24  | GLU  |
| 1   | C     | 27  | SER  |
| 1   | C     | 41  | SER  |
| 1   | C     | 44  | LEU  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 66  | VAL  |
| 1   | C     | 112 | THR  |
| 1   | C     | 115 | SER  |
| 1   | C     | 120 | SER  |
| 1   | C     | 139 | ASP  |
| 1   | C     | 145 | VAL  |
| 1   | C     | 148 | SER  |
| 1   | C     | 150 | THR  |
| 1   | C     | 178 | THR  |
| 1   | C     | 182 | ARG  |
| 1   | C     | 195 | ILE  |
| 1   | C     | 215 | GLU  |
| 1   | C     | 223 | VAL  |
| 1   | C     | 290 | LEU  |
| 1   | C     | 309 | ASP  |
| 1   | C     | 320 | ILE  |
| 1   | C     | 321 | ARG  |
| 1   | C     | 332 | VAL  |
| 1   | C     | 352 | ILE  |
| 1   | D     | 2   | LEU  |
| 1   | D     | 27  | SER  |
| 1   | D     | 31  | LYS  |
| 1   | D     | 45  | ASN  |
| 1   | D     | 53  | GLU  |
| 1   | D     | 89  | ASP  |
| 1   | D     | 134 | GLU  |
| 1   | D     | 146 | SER  |
| 1   | D     | 159 | LEU  |
| 1   | D     | 183 | LYS  |
| 1   | D     | 230 | ARG  |
| 1   | D     | 234 | THR  |
| 1   | D     | 243 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 274 | LEU  |
| 1   | D     | 276 | SER  |
| 1   | D     | 296 | ARG  |
| 1   | D     | 298 | ASP  |
| 1   | D     | 310 | SER  |
| 1   | D     | 321 | ARG  |
| 1   | D     | 342 | THR  |
| 1   | D     | 346 | ASP  |
| 1   | D     | 349 | VAL  |
| 1   | D     | 353 | VAL  |
| 1   | D     | 361 | GLU  |
| 1   | E     | 20  | ARG  |
| 1   | E     | 27  | SER  |
| 1   | E     | 31  | LYS  |
| 1   | E     | 41  | SER  |
| 1   | E     | 66  | VAL  |
| 1   | E     | 77  | SER  |
| 1   | E     | 109 | LYS  |
| 1   | E     | 110 | ARG  |
| 1   | E     | 111 | VAL  |
| 1   | E     | 164 | SER  |
| 1   | E     | 182 | ARG  |
| 1   | E     | 183 | LYS  |
| 1   | E     | 211 | GLU  |
| 1   | E     | 214 | ARG  |
| 1   | E     | 246 | GLU  |
| 1   | E     | 263 | SER  |
| 1   | E     | 272 | LEU  |
| 1   | E     | 291 | ASP  |
| 1   | E     | 306 | ARG  |
| 1   | E     | 310 | SER  |
| 1   | E     | 348 | LYS  |
| 1   | E     | 353 | VAL  |
| 1   | E     | 356 | SER  |
| 1   | F     | 4   | GLU  |
| 1   | F     | 24  | GLU  |
| 1   | F     | 27  | SER  |
| 1   | F     | 31  | LYS  |
| 1   | F     | 41  | SER  |
| 1   | F     | 53  | GLU  |
| 1   | F     | 66  | VAL  |
| 1   | F     | 88  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 92  | ASP  |
| 1   | F     | 134 | GLU  |
| 1   | F     | 150 | THR  |
| 1   | F     | 176 | TYR  |
| 1   | F     | 182 | ARG  |
| 1   | F     | 183 | LYS  |
| 1   | F     | 188 | ILE  |
| 1   | F     | 204 | ILE  |
| 1   | F     | 206 | LYS  |
| 1   | F     | 225 | LEU  |
| 1   | F     | 231 | VAL  |
| 1   | F     | 236 | THR  |
| 1   | F     | 263 | SER  |
| 1   | F     | 272 | LEU  |
| 1   | F     | 274 | LEU  |
| 1   | F     | 284 | ILE  |
| 1   | F     | 291 | ASP  |
| 1   | F     | 310 | SER  |
| 1   | F     | 327 | GLU  |
| 1   | F     | 342 | THR  |
| 1   | F     | 360 | THR  |
| 1   | G     | 2   | LEU  |
| 1   | G     | 27  | SER  |
| 1   | G     | 41  | SER  |
| 1   | G     | 66  | VAL  |
| 1   | G     | 88  | VAL  |
| 1   | G     | 92  | ASP  |
| 1   | G     | 95  | LYS  |
| 1   | G     | 109 | LYS  |
| 1   | G     | 110 | ARG  |
| 1   | G     | 148 | SER  |
| 1   | G     | 150 | THR  |
| 1   | G     | 182 | ARG  |
| 1   | G     | 210 | VAL  |
| 1   | G     | 223 | VAL  |
| 1   | G     | 225 | LEU  |
| 1   | G     | 236 | THR  |
| 1   | G     | 260 | LYS  |
| 1   | G     | 272 | LEU  |
| 1   | G     | 296 | ARG  |
| 1   | G     | 328 | LEU  |
| 1   | G     | 332 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 354 | ASN  |
| 1   | H     | 27  | SER  |
| 1   | H     | 38  | ARG  |
| 1   | H     | 44  | LEU  |
| 1   | H     | 47  | LYS  |
| 1   | H     | 53  | GLU  |
| 1   | H     | 88  | VAL  |
| 1   | H     | 112 | THR  |
| 1   | H     | 117 | SER  |
| 1   | H     | 141 | LYS  |
| 1   | H     | 143 | THR  |
| 1   | H     | 150 | THR  |
| 1   | H     | 182 | ARG  |
| 1   | H     | 210 | VAL  |
| 1   | H     | 266 | GLN  |
| 1   | H     | 290 | LEU  |
| 1   | H     | 332 | VAL  |
| 1   | H     | 343 | PHE  |
| 1   | H     | 353 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 3   | ASN  |
| 1   | A     | 23  | ASN  |
| 1   | A     | 55  | HIS  |
| 1   | A     | 175 | ASN  |
| 1   | B     | 55  | HIS  |
| 1   | B     | 91  | GLN  |
| 1   | B     | 103 | GLN  |
| 1   | B     | 217 | ASN  |
| 1   | B     | 358 | ASN  |
| 1   | C     | 23  | ASN  |
| 1   | C     | 62  | ASN  |
| 1   | C     | 227 | ASN  |
| 1   | C     | 292 | GLN  |
| 1   | C     | 358 | ASN  |
| 1   | D     | 8   | ASN  |
| 1   | D     | 23  | ASN  |
| 1   | D     | 55  | HIS  |
| 1   | D     | 91  | GLN  |
| 1   | D     | 103 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 175 | ASN  |
| 1   | E     | 62  | ASN  |
| 1   | E     | 103 | GLN  |
| 1   | E     | 152 | ASN  |
| 1   | E     | 175 | ASN  |
| 1   | E     | 358 | ASN  |
| 1   | F     | 13  | ASN  |
| 1   | F     | 103 | GLN  |
| 1   | F     | 265 | GLN  |
| 1   | F     | 292 | GLN  |
| 1   | F     | 354 | ASN  |
| 1   | G     | 3   | ASN  |
| 1   | G     | 49  | GLN  |
| 1   | G     | 55  | HIS  |
| 1   | G     | 91  | GLN  |
| 1   | G     | 175 | ASN  |
| 1   | G     | 292 | GLN  |
| 1   | G     | 293 | GLN  |
| 1   | H     | 3   | ASN  |
| 1   | H     | 23  | ASN  |
| 1   | H     | 175 | ASN  |
| 1   | H     | 266 | GLN  |
| 1   | H     | 358 | 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1   | A     | 361/370 (97%)   | 0.27   | 11 (3%) 52 45  | 26, 50, 83, 129       | 0     |
| 1   | B     | 355/370 (95%)   | 0.39   | 23 (6%) 25 20  | 26, 46, 79, 105       | 0     |
| 1   | C     | 353/370 (95%)   | 0.72   | 45 (12%) 8 6   | 23, 55, 92, 109       | 0     |
| 1   | D     | 359/370 (97%)   | 0.57   | 48 (13%) 7 6   | 18, 42, 98, 128       | 0     |
| 1   | E     | 355/370 (95%)   | 0.33   | 21 (5%) 28 23  | 29, 56, 82, 102       | 0     |
| 1   | F     | 342/370 (92%)   | 0.93   | 54 (15%) 5 4   | 28, 65, 102, 124      | 0     |
| 1   | G     | 353/370 (95%)   | 0.89   | 46 (13%) 7 6   | 26, 69, 98, 117       | 0     |
| 1   | H     | 359/370 (97%)   | 0.16   | 11 (3%) 51 44  | 34, 56, 83, 112       | 0     |
| All | All   | 2837/2960 (95%) | 0.53   | 259 (9%) 15 12 | 18, 56, 94, 129       | 0     |

All (259) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 176 | TYR  | 8.1  |
| 1   | F     | 333 | ALA  | 7.6  |
| 1   | D     | 10  | SER  | 7.3  |
| 1   | F     | 322 | ILE  | 7.1  |
| 1   | C     | 213 | GLY  | 6.3  |
| 1   | C     | 50  | ALA  | 6.1  |
| 1   | H     | 3   | ASN  | 5.9  |
| 1   | B     | 228 | PHE  | 5.8  |
| 1   | D     | 325 | GLU  | 5.8  |
| 1   | D     | 347 | ASN  | 5.8  |
| 1   | G     | 325 | GLU  | 5.7  |
| 1   | C     | 178 | THR  | 5.7  |
| 1   | C     | 212 | VAL  | 5.6  |
| 1   | G     | 344 | PRO  | 5.5  |
| 1   | F     | 261 | TYR  | 5.5  |
| 1   | B     | 360 | THR  | 5.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 336 | ALA  | 5.1  |
| 1   | D     | 322 | ILE  | 5.1  |
| 1   | F     | 197 | GLY  | 5.0  |
| 1   | F     | 361 | GLU  | 4.9  |
| 1   | G     | 359 | ILE  | 4.9  |
| 1   | C     | 291 | ASP  | 4.8  |
| 1   | G     | 330 | ALA  | 4.7  |
| 1   | D     | 228 | PHE  | 4.6  |
| 1   | C     | 343 | PHE  | 4.6  |
| 1   | G     | 332 | VAL  | 4.5  |
| 1   | D     | 327 | GLU  | 4.5  |
| 1   | B     | 1   | ALA  | 4.4  |
| 1   | F     | 335 | GLY  | 4.4  |
| 1   | F     | 275 | LYS  | 4.4  |
| 1   | F     | 357 | GLY  | 4.4  |
| 1   | H     | 2   | LEU  | 4.3  |
| 1   | C     | 94  | VAL  | 4.3  |
| 1   | E     | 210 | VAL  | 4.3  |
| 1   | B     | 227 | ASN  | 4.2  |
| 1   | B     | 85  | ARG  | 4.2  |
| 1   | D     | 210 | VAL  | 4.2  |
| 1   | C     | 17  | LEU  | 4.2  |
| 1   | D     | 227 | ASN  | 4.1  |
| 1   | D     | 359 | ILE  | 4.1  |
| 1   | F     | 220 | LEU  | 4.1  |
| 1   | C     | 325 | GLU  | 4.1  |
| 1   | F     | 228 | PHE  | 4.1  |
| 1   | A     | 347 | ASN  | 4.0  |
| 1   | C     | 54  | ALA  | 4.0  |
| 1   | G     | 229 | PRO  | 3.9  |
| 1   | B     | 324 | ALA  | 3.9  |
| 1   | H     | 1   | ALA  | 3.9  |
| 1   | D     | 209 | LYS  | 3.9  |
| 1   | C     | 15  | LYS  | 3.8  |
| 1   | G     | 224 | ALA  | 3.8  |
| 1   | B     | 343 | PHE  | 3.8  |
| 1   | H     | 343 | PHE  | 3.8  |
| 1   | G     | 324 | ALA  | 3.8  |
| 1   | D     | 262 | VAL  | 3.8  |
| 1   | D     | 211 | GLU  | 3.7  |
| 1   | D     | 217 | ASN  | 3.7  |
| 1   | G     | 329 | LYS  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 214 | ARG  | 3.7  |
| 1   | D     | 328 | LEU  | 3.7  |
| 1   | C     | 179 | GLY  | 3.7  |
| 1   | A     | 111 | VAL  | 3.6  |
| 1   | D     | 330 | ALA  | 3.6  |
| 1   | F     | 326 | GLY  | 3.6  |
| 1   | F     | 8   | ASN  | 3.5  |
| 1   | D     | 348 | LYS  | 3.5  |
| 1   | G     | 223 | VAL  | 3.5  |
| 1   | H     | 4   | GLU  | 3.4  |
| 1   | D     | 343 | PHE  | 3.4  |
| 1   | F     | 195 | ILE  | 3.4  |
| 1   | E     | 208 | CYS  | 3.4  |
| 1   | E     | 363 | GLU  | 3.4  |
| 1   | G     | 279 | ALA  | 3.4  |
| 1   | H     | 291 | ASP  | 3.4  |
| 1   | C     | 346 | ASP  | 3.4  |
| 1   | F     | 260 | LYS  | 3.3  |
| 1   | F     | 262 | VAL  | 3.3  |
| 1   | D     | 342 | THR  | 3.3  |
| 1   | B     | 10  | SER  | 3.3  |
| 1   | B     | 224 | ALA  | 3.3  |
| 1   | C     | 110 | ARG  | 3.2  |
| 1   | D     | 224 | ALA  | 3.2  |
| 1   | F     | 223 | VAL  | 3.2  |
| 1   | C     | 143 | THR  | 3.2  |
| 1   | F     | 236 | THR  | 3.1  |
| 1   | D     | 332 | VAL  | 3.1  |
| 1   | F     | 332 | VAL  | 3.1  |
| 1   | C     | 347 | ASN  | 3.1  |
| 1   | C     | 327 | GLU  | 3.1  |
| 1   | B     | 361 | GLU  | 3.1  |
| 1   | C     | 8   | ASN  | 3.1  |
| 1   | D     | 45  | ASN  | 3.1  |
| 1   | G     | 227 | ASN  | 3.1  |
| 1   | D     | 279 | ALA  | 3.1  |
| 1   | F     | 321 | ARG  | 3.1  |
| 1   | D     | 243 | SER  | 3.1  |
| 1   | F     | 4   | GLU  | 3.0  |
| 1   | D     | 352 | ILE  | 3.0  |
| 1   | F     | 337 | ALA  | 3.0  |
| 1   | B     | 358 | ASN  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 114 | PHE  | 3.0  |
| 1   | G     | 360 | THR  | 2.9  |
| 1   | C     | 130 | VAL  | 2.9  |
| 1   | D     | 9   | CYS  | 2.9  |
| 1   | F     | 343 | PHE  | 2.9  |
| 1   | D     | 333 | ALA  | 2.9  |
| 1   | F     | 231 | VAL  | 2.9  |
| 1   | D     | 344 | PRO  | 2.9  |
| 1   | D     | 208 | CYS  | 2.9  |
| 1   | C     | 196 | GLY  | 2.8  |
| 1   | G     | 161 | GLY  | 2.8  |
| 1   | C     | 360 | THR  | 2.8  |
| 1   | E     | 9   | CYS  | 2.8  |
| 1   | F     | 230 | ARG  | 2.8  |
| 1   | F     | 225 | LEU  | 2.8  |
| 1   | C     | 177 | PRO  | 2.8  |
| 1   | E     | 222 | SER  | 2.8  |
| 1   | G     | 273 | SER  | 2.8  |
| 1   | A     | 8   | ASN  | 2.8  |
| 1   | C     | 111 | VAL  | 2.8  |
| 1   | C     | 114 | PHE  | 2.8  |
| 1   | F     | 282 | PHE  | 2.8  |
| 1   | E     | 72  | TYR  | 2.8  |
| 1   | A     | 362 | LEU  | 2.7  |
| 1   | B     | 332 | VAL  | 2.7  |
| 1   | G     | 231 | VAL  | 2.7  |
| 1   | H     | 327 | GLU  | 2.7  |
| 1   | D     | 346 | ASP  | 2.7  |
| 1   | F     | 360 | THR  | 2.7  |
| 1   | G     | 220 | LEU  | 2.7  |
| 1   | G     | 178 | THR  | 2.7  |
| 1   | F     | 328 | LEU  | 2.6  |
| 1   | G     | 214 | ARG  | 2.6  |
| 1   | F     | 226 | LYS  | 2.6  |
| 1   | B     | 267 | ALA  | 2.6  |
| 1   | F     | 224 | ALA  | 2.6  |
| 1   | G     | 236 | THR  | 2.6  |
| 1   | C     | 7   | LEU  | 2.6  |
| 1   | C     | 194 | ALA  | 2.6  |
| 1   | D     | 212 | VAL  | 2.6  |
| 1   | D     | 349 | VAL  | 2.6  |
| 1   | G     | 216 | ILE  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 363 | GLU  | 2.6  |
| 1   | F     | 358 | ASN  | 2.6  |
| 1   | D     | 52  | GLN  | 2.6  |
| 1   | F     | 52  | GLN  | 2.6  |
| 1   | D     | 261 | TYR  | 2.6  |
| 1   | D     | 223 | VAL  | 2.6  |
| 1   | G     | 228 | PHE  | 2.6  |
| 1   | E     | 209 | LYS  | 2.5  |
| 1   | C     | 161 | GLY  | 2.5  |
| 1   | A     | 114 | PHE  | 2.5  |
| 1   | G     | 334 | ASP  | 2.5  |
| 1   | F     | 352 | ILE  | 2.5  |
| 1   | F     | 329 | LYS  | 2.5  |
| 1   | G     | 225 | LEU  | 2.5  |
| 1   | C     | 52  | GLN  | 2.5  |
| 1   | A     | 53  | GLU  | 2.5  |
| 1   | F     | 176 | TYR  | 2.5  |
| 1   | A     | 161 | GLY  | 2.5  |
| 1   | E     | 54  | ALA  | 2.5  |
| 1   | G     | 337 | ALA  | 2.5  |
| 1   | E     | 291 | ASP  | 2.5  |
| 1   | B     | 223 | VAL  | 2.5  |
| 1   | C     | 43  | PHE  | 2.5  |
| 1   | E     | 50  | ALA  | 2.5  |
| 1   | F     | 238 | ARG  | 2.4  |
| 1   | F     | 222 | SER  | 2.4  |
| 1   | G     | 258 | ARG  | 2.4  |
| 1   | E     | 10  | SER  | 2.4  |
| 1   | E     | 130 | VAL  | 2.4  |
| 1   | F     | 130 | VAL  | 2.4  |
| 1   | H     | 176 | TYR  | 2.4  |
| 1   | B     | 2   | LEU  | 2.4  |
| 1   | D     | 360 | THR  | 2.4  |
| 1   | G     | 322 | ILE  | 2.4  |
| 1   | G     | 175 | ASN  | 2.4  |
| 1   | D     | 351 | GLY  | 2.4  |
| 1   | G     | 5   | VAL  | 2.4  |
| 1   | E     | 181 | CYS  | 2.4  |
| 1   | F     | 229 | PRO  | 2.4  |
| 1   | F     | 330 | ALA  | 2.4  |
| 1   | B     | 329 | LYS  | 2.3  |
| 1   | E     | 183 | LYS  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 232 | ASN  | 2.3  |
| 1   | C     | 10  | SER  | 2.3  |
| 1   | C     | 210 | VAL  | 2.3  |
| 1   | G     | 212 | VAL  | 2.3  |
| 1   | D     | 225 | LEU  | 2.3  |
| 1   | F     | 284 | ILE  | 2.3  |
| 1   | C     | 348 | LYS  | 2.3  |
| 1   | C     | 91  | GLN  | 2.3  |
| 1   | D     | 265 | GLN  | 2.3  |
| 1   | E     | 197 | GLY  | 2.3  |
| 1   | F     | 212 | VAL  | 2.3  |
| 1   | F     | 209 | LYS  | 2.3  |
| 1   | G     | 356 | SER  | 2.3  |
| 1   | D     | 331 | GLY  | 2.3  |
| 1   | G     | 323 | GLY  | 2.3  |
| 1   | D     | 282 | PHE  | 2.3  |
| 1   | C     | 163 | ALA  | 2.2  |
| 1   | D     | 321 | ARG  | 2.2  |
| 1   | E     | 263 | SER  | 2.2  |
| 1   | C     | 140 | LEU  | 2.2  |
| 1   | F     | 218 | VAL  | 2.2  |
| 1   | G     | 94  | VAL  | 2.2  |
| 1   | D     | 264 | ALA  | 2.2  |
| 1   | D     | 361 | GLU  | 2.2  |
| 1   | B     | 175 | ASN  | 2.2  |
| 1   | G     | 328 | LEU  | 2.2  |
| 1   | C     | 6   | ALA  | 2.2  |
| 1   | F     | 280 | ALA  | 2.2  |
| 1   | A     | 363 | GLU  | 2.2  |
| 1   | E     | 56  | GLU  | 2.2  |
| 1   | F     | 338 | GLU  | 2.2  |
| 1   | F     | 342 | THR  | 2.2  |
| 1   | D     | 213 | GLY  | 2.2  |
| 1   | D     | 326 | GLY  | 2.2  |
| 1   | E     | 179 | GLY  | 2.2  |
| 1   | A     | 3   | ASN  | 2.2  |
| 1   | E     | 8   | ASN  | 2.2  |
| 1   | G     | 326 | GLY  | 2.2  |
| 1   | C     | 180 | VAL  | 2.2  |
| 1   | C     | 90  | ALA  | 2.1  |
| 1   | H     | 324 | ALA  | 2.1  |
| 1   | C     | 329 | LYS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 345 | SER  | 2.1  |
| 1   | G     | 211 | GLU  | 2.1  |
| 1   | C     | 214 | ARG  | 2.1  |
| 1   | F     | 214 | ARG  | 2.1  |
| 1   | G     | 230 | ARG  | 2.1  |
| 1   | E     | 342 | THR  | 2.1  |
| 1   | B     | 3   | ASN  | 2.1  |
| 1   | F     | 265 | GLN  | 2.1  |
| 1   | G     | 8   | ASN  | 2.1  |
| 1   | G     | 232 | ASN  | 2.1  |
| 1   | H     | 52  | GLN  | 2.1  |
| 1   | B     | 176 | TYR  | 2.1  |
| 1   | G     | 253 | PRO  | 2.1  |
| 1   | A     | 345 | SER  | 2.1  |
| 1   | D     | 1   | ALA  | 2.1  |
| 1   | G     | 51  | SER  | 2.1  |
| 1   | E     | 4   | GLU  | 2.1  |
| 1   | F     | 296 | ARG  | 2.1  |
| 1   | G     | 246 | GLU  | 2.1  |
| 1   | C     | 141 | LYS  | 2.1  |
| 1   | B     | 177 | PRO  | 2.1  |
| 1   | C     | 48  | PRO  | 2.1  |
| 1   | B     | 197 | GLY  | 2.1  |
| 1   | C     | 133 | GLY  | 2.1  |
| 1   | B     | 359 | ILE  | 2.1  |
| 1   | C     | 211 | GLU  | 2.0  |
| 1   | A     | 195 | ILE  | 2.0  |
| 1   | F     | 359 | ILE  | 2.0  |
| 1   | G     | 213 | GLY  | 2.0  |
| 1   | F     | 194 | ALA  | 2.0  |
| 1   | G     | 1   | ALA  | 2.0  |
| 1   | G     | 196 | GLY  | 2.0  |
| 1   | G     | 210 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.