



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 2QMH / pdb\_00002qmh  
Title : structure of V267F mutant HprK/P  
Authors : Chaptal, V.; Vincent, F.; Gueguen-Chaignon, V.; Poncet, S.; Deutscher, J.;  
Nessler, S.; Morera, S.  
Deposited on : 2007-07-16  
Resolution : 2.60 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                                                             |

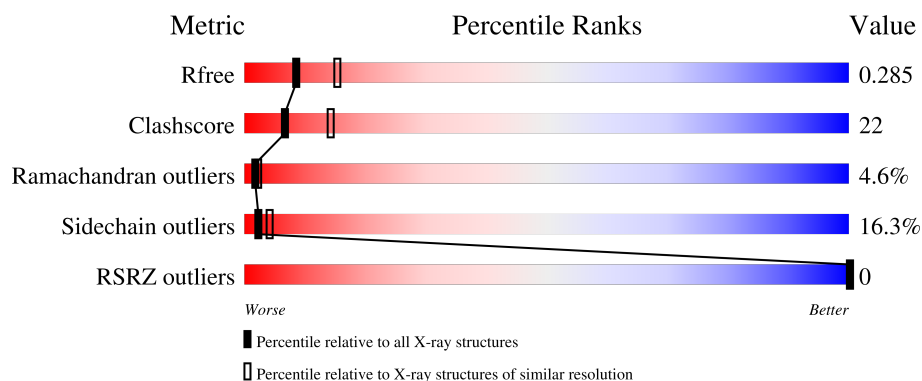
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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                      | 4008 (2.60-2.60)                                      |
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

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     | 205    |                  |
| 1   | B     | 205    |                  |
| 1   | C     | 205    |                  |
| 1   | D     | 205    |                  |
| 1   | E     | 205    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 205    |                  |
| 1   | G     | 205    |                  |
| 1   | H     | 205    |                  |
| 1   | I     | 205    |                  |
| 1   | J     | 205    |                  |
| 1   | K     | 205    |                  |
| 1   | L     | 205    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15591 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 HPr kinase/phosphorylase.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1242  | 787 | 218 | 233 | 4 |         |         |       |
| 1   | B     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1405  | 887 | 245 | 269 | 4 |         |         |       |
| 1   | C     | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 806 | 223 | 236 | 4 |         |         |       |
| 1   | D     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1405  | 887 | 245 | 269 | 4 |         |         |       |
| 1   | E     | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1265  | 799 | 222 | 240 | 4 |         |         |       |
| 1   | F     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1235  | 783 | 215 | 233 | 4 |         |         |       |
| 1   | G     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1238  | 785 | 217 | 232 | 4 |         |         |       |
| 1   | H     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1380  | 872 | 241 | 263 | 4 |         |         |       |
| 1   | I     | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1238  | 785 | 217 | 232 | 4 |         |         |       |
| 1   | J     | 178      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 873 | 241 | 265 | 4 |         |         |       |
| 1   | K     | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 791 | 220 | 235 | 4 |         |         |       |
| 1   | L     | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1246  | 789 | 219 | 234 | 4 |         |         |       |

There are 168 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 115     | MET      | -      | expression tag | UNP Q9RE09 |
| A     | 116     | ARG      | -      | expression tag | UNP Q9RE09 |
| A     | 117     | GLY      | -      | expression tag | UNP Q9RE09 |
| A     | 118     | SER      | -      | expression tag | UNP Q9RE09 |
| A     | 119     | HIS      | -      | expression tag | UNP Q9RE09 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| A     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| A     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| A     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| A     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| A     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| A     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| A     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| A     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| B     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| B     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| B     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| B     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| B     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| B     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| B     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| B     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| B     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| C     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| C     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| C     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| C     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| C     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| C     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| C     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| C     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| C     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| D     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| D     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| D     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| D     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| D     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| D     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| D     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| D     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| D     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| D     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| D     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| D     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| D     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| D     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| E     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| E     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| E     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| E     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| E     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| E     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| E     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| E     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| E     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| F     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| F     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| F     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| F     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| F     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| F     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| F     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| F     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| F     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| G     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| G     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| G     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| G     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| G     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| G     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| G     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| G     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| G     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| G     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| G     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| G     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| G     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| G     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| H     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| H     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| H     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| H     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| H     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| H     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| H     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| H     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| H     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| I     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| I     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| I     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| I     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| I     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| I     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| I     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| I     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| I     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| J     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| J     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| J     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| J     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| J     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |

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| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| J     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| J     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| J     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| J     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| J     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| J     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| J     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| J     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| J     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| K     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| K     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| K     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| K     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| K     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| K     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| K     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| K     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| K     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |
| L     | 115     | MET      | -      | expression tag      | UNP Q9RE09 |
| L     | 116     | ARG      | -      | expression tag      | UNP Q9RE09 |
| L     | 117     | GLY      | -      | expression tag      | UNP Q9RE09 |
| L     | 118     | SER      | -      | expression tag      | UNP Q9RE09 |
| L     | 119     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 120     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 121     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 122     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 123     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 124     | HIS      | -      | expression tag      | UNP Q9RE09 |
| L     | 125     | GLY      | -      | expression tag      | UNP Q9RE09 |
| L     | 126     | SER      | -      | expression tag      | UNP Q9RE09 |
| L     | 127     | MET      | -      | expression tag      | UNP Q9RE09 |
| L     | 267     | PHE      | VAL    | engineered mutation | UNP Q9RE09 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 2   | A     | 1        | Total O<br>1 1 | 0       | 0       |

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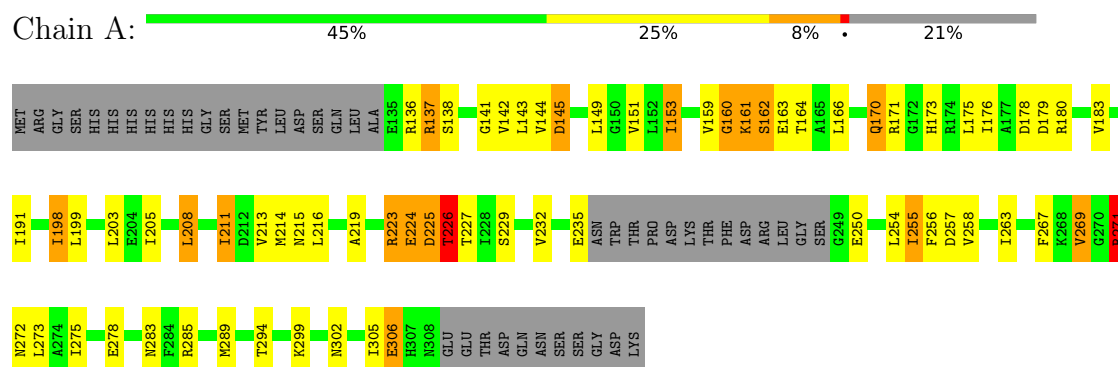
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | B     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 2   | C     | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 2   | D     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 2   | F     | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 2   | G     | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 2   | H     | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 2   | I     | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 2   | K     | 1        | Total<br>1  | O<br>1  | 0       | 0       |
| 2   | L     | 3        | Total<br>3  | O<br>3  | 0       | 0       |

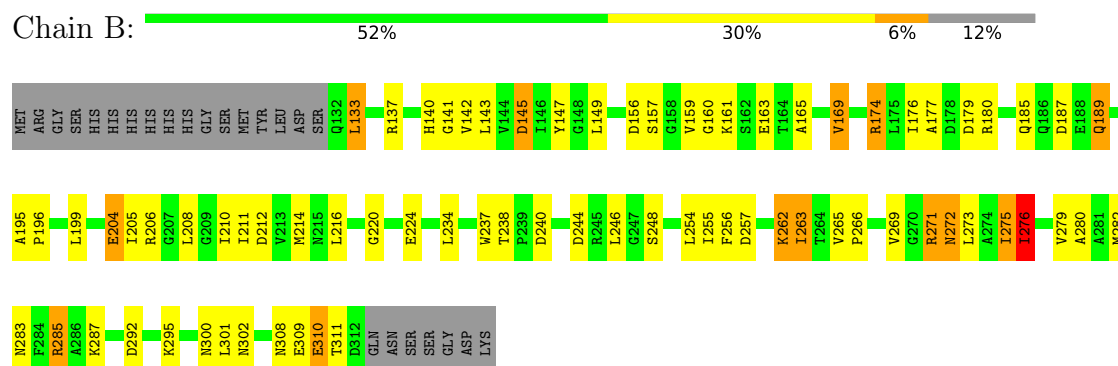
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

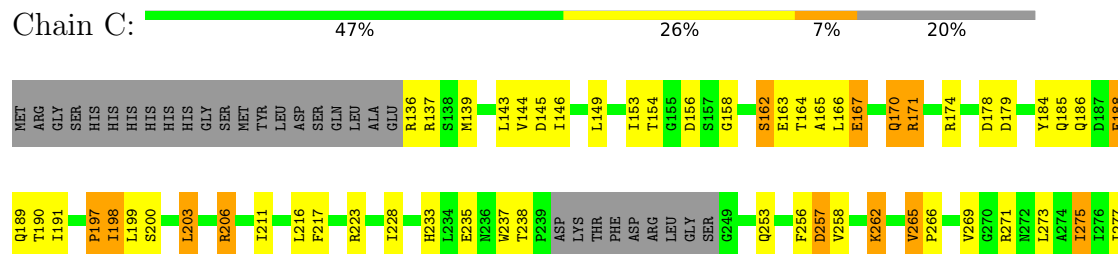
#### • Molecule 1: HPr kinase/phosphorylase



#### • Molecule 1: HPr kinase/phosphorylase

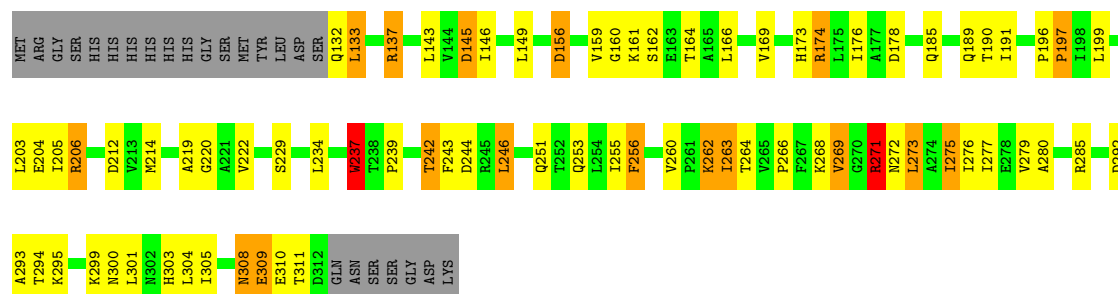


#### • Molecule 1: HPr kinase/phosphorylase

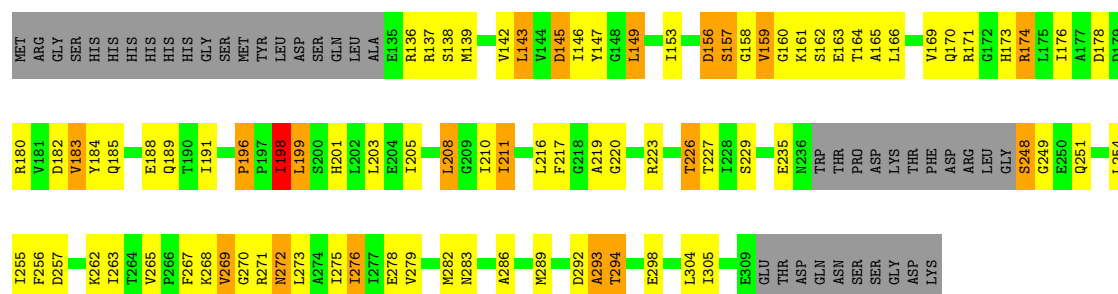




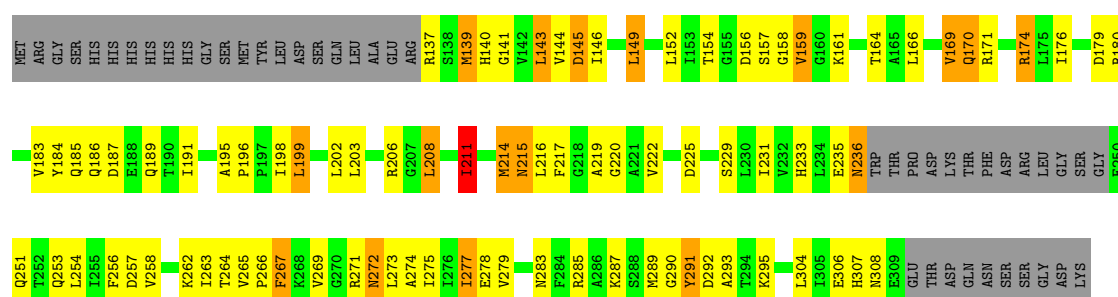
- Molecule 1: HPr kinase/phosphorylase



- Molecule 1: HPr kinase/phosphorylase

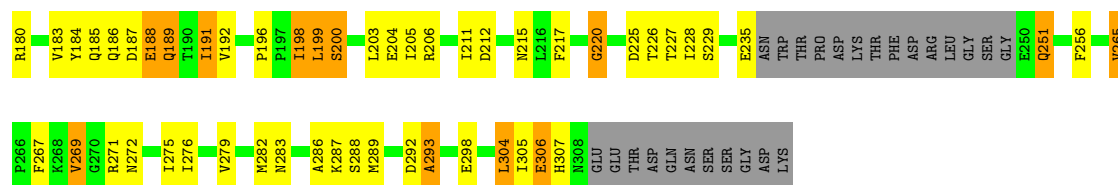


- Molecule 1: HPr kinase/phosphorylase

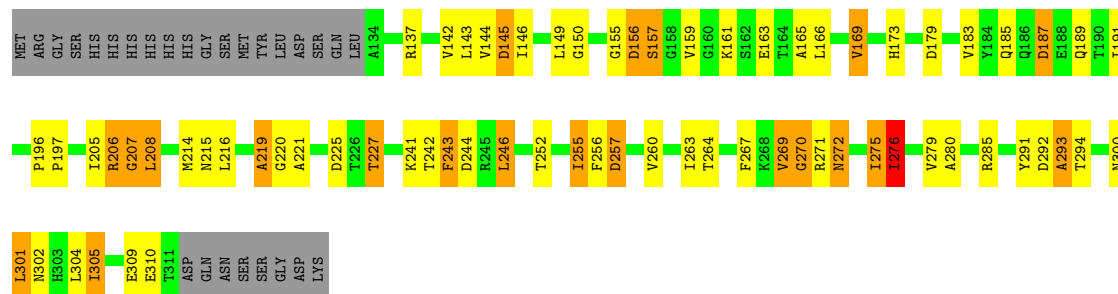


- Molecule 1: HPr kinase/phosphorylase

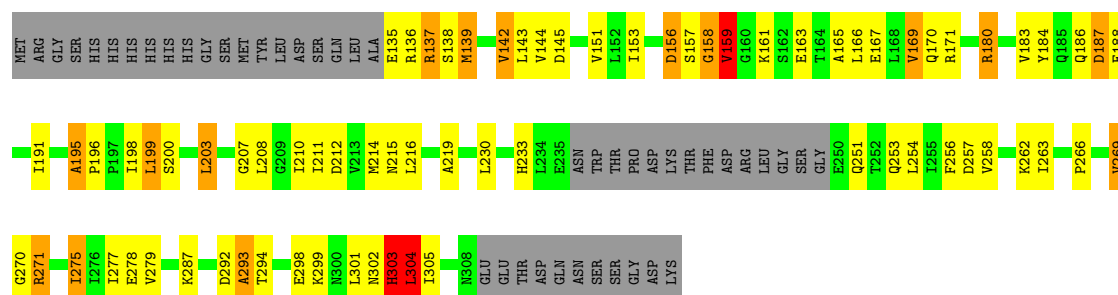




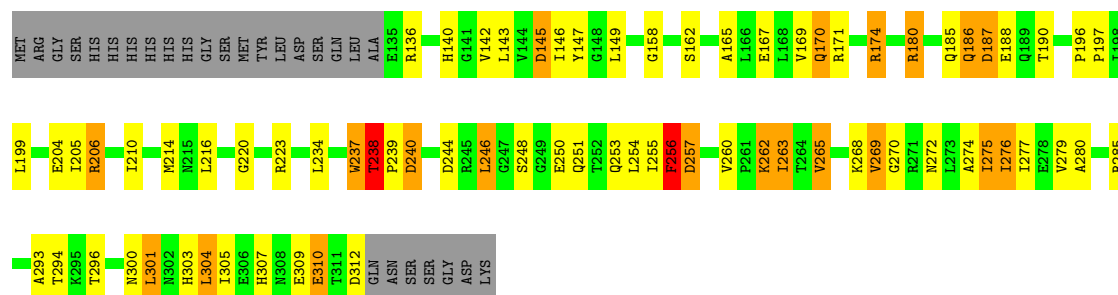
• Molecule 1: HPr kinase/phosphorylase



• Molecule 1: HPr kinase/phosphorylase

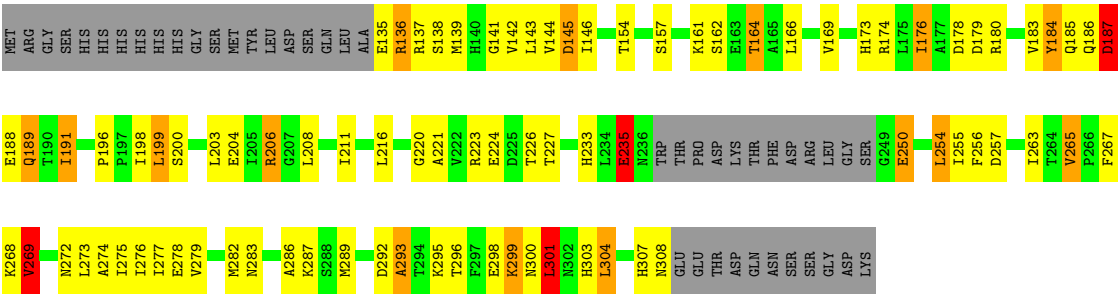


• Molecule 1: HPr kinase/phosphorylase

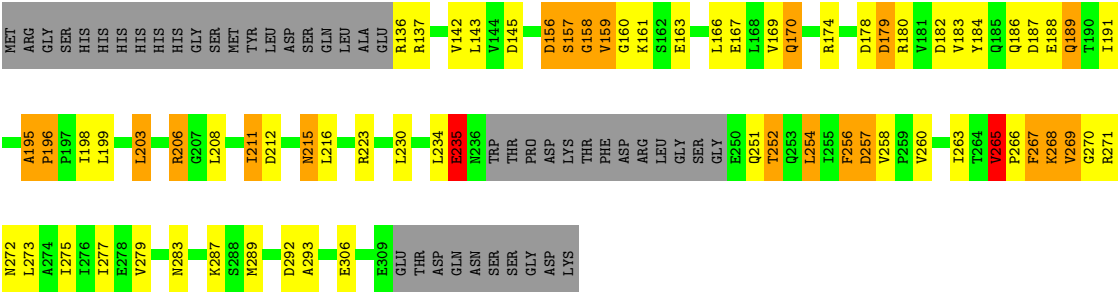


• Molecule 1: HPr kinase/phosphorylase





• Molecule 1: HPr kinase/phosphorylase



## 4 Data and refinement statistics

| Property                                                                | Value                                                                                                                                                                                                                                           | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                                                                                                                                                                                                             | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 69.06Å 106.37Å 106.49Å<br>119.50° 90.02° 89.96°                                                                                                                                                                                                 | Depositor        |
| Resolution (Å)                                                          | 19.43 – 2.60<br>19.43 – 2.60                                                                                                                                                                                                                    | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.3 (19.43-2.60)<br>99.0 (19.43-2.60)                                                                                                                                                                                                          | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.14                                                                                                                                                                                                                                            | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                                                                                                                                                                                                 | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.87 (at 2.59Å)                                                                                                                                                                                                                                 | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                                                                                                                                                                                                                 | Depositor        |
| R, $R_{free}$                                                           | 0.221 , 0.298<br>0.212 , 0.285                                                                                                                                                                                                                  | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 4029 reflections (4.98%)                                                                                                                                                                                                                        | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 55.7                                                                                                                                                                                                                                            | Xtriage          |
| Anisotropy                                                              | 0.026                                                                                                                                                                                                                                           | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 18.8                                                                                                                                                                                                                                     | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$                                                                                                                                                                                     | Xtriage          |
| Estimated twinning fraction                                             | 0.019 for h,-l,k+l<br>0.019 for h,k+l,-k<br>0.019 for h,-k-l,k<br>0.019 for h,l,-k-l<br>0.469 for h,-k,-l<br>0.020 for -h,k,-k-l<br>0.019 for -h,-k-l,l<br>0.469 for -h,-l,-k<br>0.467 for -h,l,k<br>0.019 for -h,-k,k+l<br>0.019 for -h,k+l,-l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                                                                                                                                                                                                            | EDS              |
| Total number of atoms                                                   | 15591                                                                                                                                                                                                                                           | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 53.0                                                                                                                                                                                                                                            | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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     | 1.12         | 0/1259          | 1.30        | 7/1703 (0.4%)   |
| 1   | B     | 1.15         | 4/1427 (0.3%)   | 1.23        | 4/1934 (0.2%)   |
| 1   | C     | 1.07         | 1/1289 (0.1%)   | 1.22        | 5/1747 (0.3%)   |
| 1   | D     | 1.18         | 1/1427 (0.1%)   | 1.27        | 6/1934 (0.3%)   |
| 1   | E     | 1.07         | 3/1282 (0.2%)   | 1.26        | 9/1734 (0.5%)   |
| 1   | F     | 1.05         | 3/1252 (0.2%)   | 1.20        | 6/1695 (0.4%)   |
| 1   | G     | 1.12         | 1/1255 (0.1%)   | 1.24        | 4/1698 (0.2%)   |
| 1   | H     | 1.17         | 1/1402 (0.1%)   | 1.23        | 7/1900 (0.4%)   |
| 1   | I     | 0.98         | 0/1255          | 1.23        | 5/1698 (0.3%)   |
| 1   | J     | 1.17         | 1/1405 (0.1%)   | 1.27        | 10/1904 (0.5%)  |
| 1   | K     | 1.09         | 2/1267 (0.2%)   | 1.20        | 5/1714 (0.3%)   |
| 1   | L     | 1.06         | 1/1263 (0.1%)   | 1.29        | 8/1709 (0.5%)   |
| All | All   | 1.11         | 18/15783 (0.1%) | 1.25        | 76/21370 (0.4%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | K     | 0                   | 1                   |

All (18) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | C     | 265 | VAL  | CA-CB | 8.51  | 1.60        | 1.54     |
| 1   | L     | 265 | VAL  | CA-CB | 7.45  | 1.60        | 1.54     |
| 1   | G     | 265 | VAL  | CA-CB | 7.27  | 1.59        | 1.54     |
| 1   | H     | 276 | ILE  | CA-CB | 6.13  | 1.61        | 1.54     |
| 1   | B     | 276 | ILE  | CA-CB | 5.91  | 1.61        | 1.54     |
| 1   | K     | 221 | ALA  | CA-CB | -5.77 | 1.43        | 1.53     |
| 1   | E     | 198 | ILE  | CA-CB | 5.65  | 1.62        | 1.54     |
| 1   | E     | 279 | VAL  | CA-CB | -5.63 | 1.47        | 1.54     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 263 | ILE  | CA-CB | -5.62 | 1.47        | 1.55     |
| 1   | B     | 287 | LYS  | C-O   | -5.57 | 1.17        | 1.24     |
| 1   | F     | 277 | ILE  | CA-CB | -5.54 | 1.47        | 1.54     |
| 1   | F     | 146 | ILE  | CA-CB | -5.32 | 1.47        | 1.53     |
| 1   | J     | 146 | ILE  | CA-CB | -5.30 | 1.47        | 1.54     |
| 1   | E     | 276 | ILE  | CA-CB | 5.11  | 1.60        | 1.54     |
| 1   | B     | 177 | ALA  | CA-CB | -5.08 | 1.45        | 1.53     |
| 1   | F     | 211 | ILE  | CA-CB | 5.07  | 1.62        | 1.55     |
| 1   | B     | 169 | VAL  | C-O   | -5.02 | 1.17        | 1.24     |
| 1   | K     | 265 | VAL  | CA-CB | 5.01  | 1.59        | 1.53     |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 198 | ILE  | N-CA-C   | 10.39 | 120.85      | 112.12   |
| 1   | B     | 220 | GLY  | N-CA-C   | -9.02 | 103.51      | 115.32   |
| 1   | G     | 225 | ASP  | N-CA-C   | 7.82  | 118.59      | 108.34   |
| 1   | A     | 223 | ARG  | N-CA-C   | 7.80  | 123.51      | 114.62   |
| 1   | F     | 287 | LYS  | N-CA-C   | -7.64 | 102.95      | 111.28   |
| 1   | I     | 195 | ALA  | CA-C-N   | 7.47  | 128.08      | 120.38   |
| 1   | I     | 195 | ALA  | C-N-CA   | 7.47  | 128.08      | 120.38   |
| 1   | J     | 246 | LEU  | N-CA-C   | -7.16 | 100.20      | 110.59   |
| 1   | H     | 309 | GLU  | N-CA-C   | -7.09 | 104.11      | 114.39   |
| 1   | H     | 220 | GLY  | N-CA-C   | -7.07 | 104.14      | 115.66   |
| 1   | G     | 167 | GLU  | N-CA-C   | -6.96 | 103.62      | 111.07   |
| 1   | H     | 227 | THR  | N-CA-C   | -6.75 | 101.82      | 110.53   |
| 1   | J     | 238 | THR  | CA-C-N   | 6.66  | 128.16      | 119.84   |
| 1   | J     | 238 | THR  | C-N-CA   | 6.66  | 128.16      | 119.84   |
| 1   | L     | 158 | GLY  | N-CA-C   | -6.63 | 104.86      | 112.29   |
| 1   | E     | 227 | THR  | N-CA-C   | -6.60 | 101.20      | 110.50   |
| 1   | A     | 269 | VAL  | N-CA-C   | 6.50  | 122.87      | 109.34   |
| 1   | L     | 195 | ALA  | CA-C-N   | 6.48  | 127.05      | 120.38   |
| 1   | L     | 195 | ALA  | C-N-CA   | 6.48  | 127.05      | 120.38   |
| 1   | B     | 149 | LEU  | CA-CB-CG | 6.45  | 138.87      | 116.30   |
| 1   | F     | 225 | ASP  | N-CA-C   | 6.34  | 117.86      | 108.60   |
| 1   | B     | 302 | ASN  | N-CA-C   | 6.24  | 117.75      | 111.07   |
| 1   | D     | 246 | LEU  | N-CA-C   | -6.23 | 102.14      | 110.55   |
| 1   | L     | 235 | GLU  | N-CA-C   | 6.23  | 119.40      | 108.75   |
| 1   | A     | 219 | ALA  | N-CA-C   | 6.18  | 120.38      | 112.34   |
| 1   | D     | 219 | ALA  | N-CA-C   | 6.04  | 118.66      | 111.71   |
| 1   | D     | 271 | ARG  | N-CA-C   | -6.02 | 101.61      | 110.52   |
| 1   | A     | 226 | THR  | CB-CA-C  | -6.02 | 98.44       | 110.42   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 176 | ILE  | N-CA-C  | -5.98 | 105.89      | 111.45   |
| 1   | D     | 220 | GLY  | N-CA-C  | -5.96 | 105.95      | 115.66   |
| 1   | I     | 139 | MET  | N-CA-C  | 5.93  | 118.43      | 109.41   |
| 1   | F     | 139 | MET  | N-CA-C  | 5.91  | 119.17      | 109.72   |
| 1   | G     | 220 | GLY  | N-CA-C  | -5.91 | 105.00      | 113.86   |
| 1   | F     | 169 | VAL  | N-CA-C  | -5.90 | 104.76      | 110.72   |
| 1   | L     | 196 | PRO  | CA-C-N  | -5.88 | 113.69      | 120.04   |
| 1   | L     | 196 | PRO  | C-N-CA  | -5.88 | 113.69      | 120.04   |
| 1   | J     | 263 | ILE  | N-CA-C  | -5.77 | 99.47       | 108.81   |
| 1   | I     | 156 | ASP  | N-CA-C  | -5.73 | 100.95      | 109.83   |
| 1   | J     | 256 | PHE  | CB-CA-C | -5.72 | 103.45      | 111.80   |
| 1   | J     | 158 | GLY  | N-CA-C  | -5.70 | 106.70      | 113.99   |
| 1   | E     | 219 | ALA  | N-CA-C  | 5.67  | 119.71      | 112.34   |
| 1   | L     | 289 | MET  | N-CA-C  | -5.65 | 104.96      | 113.89   |
| 1   | J     | 136 | ARG  | N-CA-C  | 5.60  | 117.78      | 108.99   |
| 1   | J     | 220 | GLY  | N-CA-C  | -5.58 | 106.02      | 115.34   |
| 1   | F     | 219 | ALA  | N-CA-C  | 5.58  | 119.80      | 112.89   |
| 1   | K     | 301 | LEU  | N-CA-CB | 5.56  | 119.89      | 110.49   |
| 1   | F     | 251 | GLN  | N-CA-C  | 5.53  | 117.20      | 108.96   |
| 1   | C     | 197 | PRO  | CA-C-N  | -5.52 | 116.98      | 122.77   |
| 1   | C     | 197 | PRO  | C-N-CA  | -5.52 | 116.98      | 122.77   |
| 1   | E     | 146 | ILE  | CB-CA-C | -5.52 | 102.91      | 110.96   |
| 1   | H     | 255 | ILE  | N-CA-C  | -5.51 | 99.61       | 107.77   |
| 1   | J     | 275 | ILE  | CB-CA-C | -5.47 | 104.75      | 112.14   |
| 1   | A     | 225 | ASP  | N-CA-C  | 5.46  | 122.42      | 110.80   |
| 1   | K     | 187 | ASP  | N-CA-C  | -5.45 | 100.65      | 108.60   |
| 1   | C     | 158 | GLY  | N-CA-C  | -5.43 | 108.02      | 114.48   |
| 1   | H     | 246 | LEU  | N-CA-C  | -5.41 | 102.75      | 110.59   |
| 1   | C     | 139 | MET  | N-CA-C  | 5.39  | 117.38      | 109.24   |
| 1   | K     | 235 | GLU  | N-CA-C  | 5.38  | 117.02      | 108.79   |
| 1   | D     | 133 | LEU  | N-CA-C  | 5.35  | 117.40      | 107.99   |
| 1   | E     | 269 | VAL  | N-CA-C  | 5.28  | 120.33      | 109.34   |
| 1   | B     | 149 | LEU  | CB-CA-C | -5.28 | 101.05      | 109.75   |
| 1   | I     | 210 | ILE  | CB-CA-C | -5.26 | 104.92      | 111.08   |
| 1   | E     | 196 | PRO  | O-C-N   | 5.26  | 123.62      | 121.15   |
| 1   | E     | 235 | GLU  | N-CA-C  | 5.25  | 117.30      | 108.73   |
| 1   | K     | 227 | THR  | N-CA-C  | -5.24 | 103.62      | 110.53   |
| 1   | H     | 215 | ASN  | N-CA-CB | 5.22  | 117.79      | 110.12   |
| 1   | E     | 157 | SER  | N-CA-C  | -5.18 | 102.53      | 110.30   |
| 1   | A     | 306 | GLU  | N-CA-C  | 5.17  | 119.22      | 112.13   |
| 1   | J     | 269 | VAL  | N-CA-C  | 5.17  | 120.10      | 109.34   |
| 1   | D     | 190 | THR  | N-CA-C  | 5.16  | 116.82      | 108.26   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 251 | GLN  | N-CA-C  | 5.13  | 121.73      | 110.80   |
| 1   | A     | 271 | ARG  | N-CA-C  | 5.12  | 121.70      | 110.80   |
| 1   | H     | 219 | ALA  | N-CA-C  | 5.09  | 118.59      | 112.38   |
| 1   | E     | 294 | THR  | N-CA-CB | 5.04  | 117.63      | 110.16   |
| 1   | L     | 287 | LYS  | N-CA-C  | -5.04 | 105.07      | 111.11   |
| 1   | E     | 255 | ILE  | N-CA-C  | -5.04 | 98.47       | 107.18   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | K     | 300 | ASN  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1242  | 0        | 1268     | 65      | 0            |
| 1   | B     | 1405  | 0        | 1415     | 57      | 0            |
| 1   | C     | 1269  | 0        | 1292     | 51      | 0            |
| 1   | D     | 1405  | 0        | 1415     | 61      | 0            |
| 1   | E     | 1265  | 0        | 1285     | 66      | 0            |
| 1   | F     | 1235  | 0        | 1258     | 72      | 0            |
| 1   | G     | 1238  | 0        | 1265     | 58      | 0            |
| 1   | H     | 1380  | 0        | 1392     | 55      | 0            |
| 1   | I     | 1238  | 0        | 1265     | 55      | 0            |
| 1   | J     | 1383  | 0        | 1391     | 50      | 0            |
| 1   | K     | 1250  | 0        | 1274     | 73      | 0            |
| 1   | L     | 1246  | 0        | 1271     | 62      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 2   | C     | 3     | 0        | 0        | 0       | 0            |
| 2   | D     | 2     | 0        | 0        | 0       | 0            |
| 2   | F     | 3     | 0        | 0        | 0       | 0            |
| 2   | G     | 10    | 0        | 0        | 1       | 0            |
| 2   | H     | 6     | 0        | 0        | 3       | 0            |
| 2   | I     | 4     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 15591 | 0        | 15791    | 674     | 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 22.

All (674) 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:E:137:ARG:HG2  | 1:E:138:SER:H    | 1.10                     | 1.13              |
| 1:L:206:ARG:H    | 1:L:206:ARG:HD2  | 0.97                     | 1.11              |
| 1:D:253:GLN:HB2  | 1:D:262:LYS:NZ   | 1.69                     | 1.06              |
| 1:H:302:ASN:HA   | 1:H:305:ILE:HG22 | 1.41                     | 1.02              |
| 1:G:198:ILE:HG13 | 1:G:199:LEU:H    | 1.25                     | 0.99              |
| 1:C:206:ARG:HD3  | 1:C:206:ARG:H    | 1.24                     | 0.99              |
| 1:G:267:PHE:CE2  | 1:G:271:ARG:HB3  | 2.00                     | 0.96              |
| 1:I:137:ARG:HG2  | 1:I:138:SER:H    | 1.30                     | 0.96              |
| 1:L:206:ARG:HD2  | 1:L:206:ARG:N    | 1.83                     | 0.93              |
| 1:B:156:ASP:O    | 1:B:159:VAL:HG22 | 1.70                     | 0.92              |
| 1:H:263:ILE:HD11 | 1:I:207:GLY:O    | 1.72                     | 0.90              |
| 1:H:137:ARG:HG3  | 1:H:256:PHE:CZ   | 2.06                     | 0.90              |
| 1:J:256:PHE:O    | 1:J:257:ASP:HB2  | 1.72                     | 0.90              |
| 1:G:267:PHE:HE2  | 1:G:271:ARG:HB3  | 1.35                     | 0.89              |
| 1:G:198:ILE:HG13 | 1:G:199:LEU:N    | 1.83                     | 0.89              |
| 1:D:292:ASP:O    | 1:D:294:THR:N    | 2.06                     | 0.88              |
| 1:K:303:HIS:HD2  | 1:K:308:ASN:HA   | 1.37                     | 0.87              |
| 1:A:223:ARG:O    | 1:A:224:GLU:CB   | 2.23                     | 0.87              |
| 1:L:235:GLU:O    | 1:L:267:PHE:HB3  | 1.74                     | 0.87              |
| 1:L:206:ARG:H    | 1:L:206:ARG:CD   | 1.85                     | 0.86              |
| 1:E:137:ARG:HG2  | 1:E:138:SER:N    | 1.90                     | 0.86              |
| 1:H:271:ARG:NH1  | 2:H:324:HOH:O    | 2.08                     | 0.85              |
| 1:H:271:ARG:CZ   | 2:H:324:HOH:O    | 2.24                     | 0.85              |
| 1:J:268:LYS:HZ1  | 1:L:159:VAL:HB   | 1.40                     | 0.83              |
| 1:A:223:ARG:O    | 1:A:224:GLU:HB2  | 1.79                     | 0.83              |
| 1:I:203:LEU:HD22 | 1:I:211:ILE:HD11 | 1.60                     | 0.83              |
| 1:J:309:GLU:O    | 1:J:310:GLU:HB2  | 1.77                     | 0.82              |
| 1:F:272:ASN:HD21 | 1:F:274:ALA:HB3  | 1.43                     | 0.82              |
| 1:F:272:ASN:HD22 | 1:F:272:ASN:C    | 1.88                     | 0.82              |
| 1:D:253:GLN:HB2  | 1:D:262:LYS:HZ3  | 1.46                     | 0.81              |
| 1:F:272:ASN:ND2  | 1:F:275:ILE:H    | 1.78                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:140:HIS:CE1  | 1:B:180:ARG:NH1  | 2.48                     | 0.81              |
| 1:A:205:ILE:HB   | 1:A:208:LEU:HD11 | 1.60                     | 0.81              |
| 1:L:272:ASN:OD1  | 1:L:275:ILE:HG12 | 1.81                     | 0.81              |
| 1:I:303:HIS:C    | 1:I:305:ILE:H    | 1.90                     | 0.79              |
| 1:K:211:ILE:HD12 | 1:K:216:LEU:HD12 | 1.63                     | 0.79              |
| 1:H:291:TYR:HB3  | 1:I:215:ASN:HD21 | 1.47                     | 0.79              |
| 1:E:198:ILE:HG13 | 1:E:199:LEU:N    | 1.97                     | 0.79              |
| 1:H:292:ASP:O    | 1:H:294:THR:N    | 2.15                     | 0.79              |
| 1:H:256:PHE:O    | 1:H:257:ASP:HB2  | 1.80                     | 0.78              |
| 1:A:198:ILE:HG13 | 1:C:304:LEU:HD12 | 1.65                     | 0.78              |
| 1:L:156:ASP:HA   | 1:L:161:LYS:NZ   | 1.97                     | 0.78              |
| 1:I:142:VAL:HG21 | 1:I:161:LYS:HB3  | 1.65                     | 0.78              |
| 1:K:206:ARG:HG2  | 1:K:206:ARG:HH21 | 1.49                     | 0.78              |
| 1:L:211:ILE:HD13 | 1:L:216:LEU:HD12 | 1.66                     | 0.77              |
| 1:C:206:ARG:H    | 1:C:206:ARG:CD   | 1.92                     | 0.77              |
| 1:K:211:ILE:HG22 | 1:L:283:ASN:ND2  | 2.00                     | 0.77              |
| 1:E:137:ARG:CG   | 1:E:138:SER:H    | 1.96                     | 0.76              |
| 1:G:136:ARG:O    | 1:G:137:ARG:HB2  | 1.86                     | 0.76              |
| 1:B:254:LEU:HD21 | 1:B:257:ASP:H    | 1.51                     | 0.75              |
| 1:G:279:VAL:HA   | 1:G:282:MET:HE3  | 1.67                     | 0.75              |
| 1:K:191:ILE:CD1  | 1:K:255:ILE:HB   | 2.16                     | 0.75              |
| 1:K:136:ARG:HH11 | 1:K:136:ARG:CG   | 1.99                     | 0.75              |
| 1:A:223:ARG:NH1  | 1:A:226:THR:HG23 | 2.01                     | 0.75              |
| 1:C:191:ILE:HD11 | 1:C:258:VAL:HB   | 1.68                     | 0.75              |
| 1:G:198:ILE:CG1  | 1:G:199:LEU:N    | 2.49                     | 0.74              |
| 1:A:198:ILE:HG23 | 1:A:199:LEU:H    | 1.51                     | 0.74              |
| 1:E:292:ASP:O    | 1:E:293:ALA:CB   | 2.33                     | 0.74              |
| 1:E:305:ILE:CG2  | 1:J:180:ARG:HG2  | 2.16                     | 0.74              |
| 1:A:176:ILE:CD1  | 1:A:226:THR:OG1  | 2.35                     | 0.74              |
| 1:B:137:ARG:HH12 | 1:B:255:ILE:HA   | 1.52                     | 0.74              |
| 1:L:156:ASP:HA   | 1:L:161:LYS:HZ1  | 1.52                     | 0.74              |
| 1:K:189:GLN:O    | 1:K:189:GLN:HG2  | 1.87                     | 0.74              |
| 1:A:136:ARG:O    | 1:A:137:ARG:HB2  | 1.87                     | 0.74              |
| 1:I:292:ASP:O    | 1:I:293:ALA:HB3  | 1.87                     | 0.73              |
| 1:F:292:ASP:O    | 1:F:293:ALA:HB3  | 1.86                     | 0.73              |
| 1:G:176:ILE:HG12 | 1:G:226:THR:HG22 | 1.69                     | 0.73              |
| 1:I:191:ILE:HD11 | 1:I:258:VAL:HB   | 1.70                     | 0.73              |
| 1:G:170:GLN:OE1  | 2:G:325:HOH:O    | 2.05                     | 0.72              |
| 1:G:180:ARG:HH21 | 1:G:199:LEU:CD1  | 2.01                     | 0.72              |
| 1:A:235:GLU:HB3  | 1:A:267:PHE:HB3  | 1.69                     | 0.72              |
| 1:J:216:LEU:HD21 | 1:K:283:ASN:HD22 | 1.53                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:254:LEU:CD2  | 1:K:257:ASP:HA   | 2.20                     | 0.72              |
| 1:B:211:ILE:HD12 | 1:B:216:LEU:HD12 | 1.69                     | 0.72              |
| 1:D:255:ILE:HD12 | 1:D:260:VAL:HG21 | 1.72                     | 0.72              |
| 1:J:301:LEU:O    | 1:J:305:ILE:HG12 | 1.91                     | 0.71              |
| 1:D:137:ARG:HB3  | 1:D:256:PHE:CE1  | 2.26                     | 0.71              |
| 1:B:271:ARG:HD2  | 1:C:163:GLU:OE1  | 1.90                     | 0.71              |
| 1:D:253:GLN:HB2  | 1:D:262:LYS:HZ1  | 1.54                     | 0.71              |
| 1:A:272:ASN:C    | 1:A:272:ASN:HD22 | 1.97                     | 0.70              |
| 1:B:140:HIS:CE1  | 1:B:180:ARG:HH12 | 2.07                     | 0.70              |
| 1:C:162:SER:O    | 1:C:165:ALA:HB3  | 1.90                     | 0.70              |
| 1:I:299:LYS:NZ   | 2:I:323:HOH:O    | 2.24                     | 0.70              |
| 1:E:292:ASP:O    | 1:E:293:ALA:HB3  | 1.89                     | 0.70              |
| 1:K:254:LEU:HD23 | 1:K:257:ASP:HA   | 1.74                     | 0.70              |
| 1:B:147:TYR:O    | 1:B:285:ARG:NH2  | 2.24                     | 0.69              |
| 1:C:266:PRO:O    | 1:C:271:ARG:NH1  | 2.26                     | 0.69              |
| 1:E:185:GLN:OE1  | 1:E:256:PHE:HB3  | 1.93                     | 0.69              |
| 1:H:291:TYR:HB3  | 1:I:215:ASN:ND2  | 2.08                     | 0.69              |
| 1:K:211:ILE:HG22 | 1:L:283:ASN:HD21 | 1.57                     | 0.69              |
| 1:J:142:VAL:HG11 | 1:J:165:ALA:HB2  | 1.75                     | 0.68              |
| 1:A:180:ARG:HH21 | 1:A:199:LEU:CD2  | 2.07                     | 0.68              |
| 1:A:171:ARG:NH2  | 1:A:278:GLU:OE1  | 2.26                     | 0.67              |
| 1:E:205:ILE:HB   | 1:E:208:LEU:HD11 | 1.77                     | 0.67              |
| 1:F:137:ARG:HB2  | 1:F:256:PHE:HE1  | 1.57                     | 0.67              |
| 1:B:271:ARG:HG3  | 1:B:272:ASN:H    | 1.60                     | 0.67              |
| 1:E:156:ASP:HB3  | 1:E:161:LYS:HZ3  | 1.61                     | 0.66              |
| 1:H:256:PHE:O    | 1:H:257:ASP:CB   | 2.42                     | 0.66              |
| 1:K:303:HIS:CD2  | 1:K:308:ASN:HA   | 2.25                     | 0.66              |
| 1:L:275:ILE:O    | 1:L:279:VAL:HG23 | 1.95                     | 0.66              |
| 1:B:246:LEU:HD12 | 1:B:248:SER:OG   | 1.95                     | 0.66              |
| 1:L:256:PHE:O    | 1:L:257:ASP:HB2  | 1.94                     | 0.66              |
| 1:E:171:ARG:NH2  | 1:E:278:GLU:OE2  | 2.28                     | 0.66              |
| 1:E:198:ILE:CG1  | 1:E:199:LEU:N    | 2.59                     | 0.66              |
| 1:I:203:LEU:HD22 | 1:I:211:ILE:CD1  | 2.26                     | 0.66              |
| 1:K:180:ARG:NH2  | 1:K:199:LEU:CD1  | 2.59                     | 0.66              |
| 1:H:272:ASN:C    | 1:H:272:ASN:HD22 | 2.02                     | 0.66              |
| 1:C:292:ASP:O    | 1:C:293:ALA:HB3  | 1.96                     | 0.66              |
| 1:H:302:ASN:CA   | 1:H:305:ILE:HG22 | 2.24                     | 0.66              |
| 1:J:300:ASN:HD22 | 1:J:303:HIS:HD2  | 1.42                     | 0.65              |
| 1:F:235:GLU:O    | 1:F:267:PHE:HB3  | 1.96                     | 0.65              |
| 1:B:246:LEU:CD1  | 1:B:248:SER:OG   | 2.45                     | 0.65              |
| 1:G:292:ASP:O    | 1:G:293:ALA:CB   | 2.43                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:183:VAL:O    | 1:K:184:TYR:HB3  | 1.95                     | 0.65              |
| 1:D:309:GLU:C    | 1:D:311:THR:H    | 2.04                     | 0.65              |
| 1:K:191:ILE:HD11 | 1:K:255:ILE:HB   | 1.76                     | 0.65              |
| 1:D:304:LEU:HD13 | 1:F:199:LEU:HD23 | 1.79                     | 0.65              |
| 1:C:154:THR:O    | 1:C:233:HIS:HA   | 1.97                     | 0.65              |
| 1:I:137:ARG:HG2  | 1:I:138:SER:N    | 2.09                     | 0.65              |
| 1:I:292:ASP:O    | 1:I:293:ALA:CB   | 2.45                     | 0.65              |
| 1:D:263:ILE:HG22 | 1:D:264:THR:N    | 2.12                     | 0.65              |
| 1:E:156:ASP:HB3  | 1:E:161:LYS:NZ   | 2.11                     | 0.65              |
| 1:B:266:PRO:HG2  | 1:B:271:ARG:NH2  | 2.12                     | 0.64              |
| 1:K:268:LYS:O    | 1:K:269:VAL:HG13 | 1.97                     | 0.64              |
| 1:E:185:GLN:HA   | 1:E:191:ILE:HD13 | 1.79                     | 0.64              |
| 1:A:176:ILE:HD13 | 1:A:226:THR:OG1  | 1.96                     | 0.64              |
| 1:K:142:VAL:HG12 | 1:K:144:VAL:HG13 | 1.80                     | 0.64              |
| 1:B:196:PRO:HG2  | 1:B:199:LEU:HD12 | 1.79                     | 0.64              |
| 1:B:271:ARG:HG3  | 1:B:272:ASN:N    | 2.12                     | 0.64              |
| 1:H:302:ASN:HA   | 1:H:305:ILE:CG2  | 2.24                     | 0.64              |
| 1:K:154:THR:O    | 1:K:233:HIS:HA   | 1.97                     | 0.63              |
| 1:D:149:LEU:HD22 | 1:D:229:SER:HB2  | 1.79                     | 0.63              |
| 1:I:142:VAL:CG2  | 1:I:161:LYS:HB3  | 2.28                     | 0.63              |
| 1:F:156:ASP:CG   | 1:F:157:SER:H    | 2.05                     | 0.63              |
| 1:K:180:ARG:HH21 | 1:K:199:LEU:CD1  | 2.12                     | 0.63              |
| 1:C:136:ARG:HA   | 1:C:256:PHE:HZ   | 1.64                     | 0.63              |
| 1:C:153:ILE:HD12 | 1:C:277:ILE:HD13 | 1.80                     | 0.63              |
| 1:B:254:LEU:CD2  | 1:B:257:ASP:H    | 2.12                     | 0.63              |
| 1:D:266:PRO:HG2  | 1:D:271:ARG:NH2  | 2.14                     | 0.62              |
| 1:F:272:ASN:C    | 1:F:272:ASN:ND2  | 2.57                     | 0.62              |
| 1:A:305:ILE:HG22 | 1:A:306:GLU:HG3  | 1.80                     | 0.62              |
| 1:B:256:PHE:O    | 1:B:257:ASP:HB2  | 1.98                     | 0.62              |
| 1:E:170:GLN:HG2  | 1:E:217:PHE:CE2  | 2.34                     | 0.62              |
| 1:E:272:ASN:C    | 1:E:272:ASN:HD22 | 2.08                     | 0.62              |
| 1:A:198:ILE:HG13 | 1:C:304:LEU:CD1  | 2.30                     | 0.62              |
| 1:K:180:ARG:HH21 | 1:K:199:LEU:HD11 | 1.63                     | 0.62              |
| 1:L:191:ILE:HD11 | 1:L:258:VAL:HB   | 1.82                     | 0.62              |
| 1:L:292:ASP:O    | 1:L:293:ALA:HB3  | 2.00                     | 0.62              |
| 1:A:180:ARG:HH21 | 1:A:199:LEU:HD21 | 1.64                     | 0.61              |
| 1:I:294:THR:O    | 1:I:298:GLU:HG3  | 2.00                     | 0.61              |
| 1:I:211:ILE:C    | 1:I:211:ILE:HD12 | 2.25                     | 0.61              |
| 1:K:185:GLN:HE21 | 1:K:188:GLU:HA   | 1.65                     | 0.61              |
| 1:E:188:GLU:O    | 1:E:189:GLN:HG2  | 2.01                     | 0.61              |
| 1:H:191:ILE:CD1  | 1:H:255:ILE:HB   | 2.31                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:137:ARG:HB2  | 1:F:256:PHE:CE1  | 2.36                     | 0.61              |
| 1:K:166:LEU:HD21 | 1:L:279:VAL:HG21 | 1.83                     | 0.61              |
| 1:K:180:ARG:NH2  | 1:K:199:LEU:HD13 | 2.15                     | 0.61              |
| 1:B:145:ASP:CG   | 1:B:174:ARG:HH21 | 2.08                     | 0.61              |
| 1:C:136:ARG:HA   | 1:C:256:PHE:CZ   | 2.35                     | 0.61              |
| 1:A:141:GLY:HA2  | 1:A:161:LYS:HE3  | 1.82                     | 0.61              |
| 1:G:170:GLN:HG3  | 1:I:275:ILE:HD12 | 1.83                     | 0.61              |
| 1:L:267:PHE:HD1  | 1:L:267:PHE:C    | 2.09                     | 0.61              |
| 1:B:234:LEU:HD23 | 1:B:265:VAL:HG23 | 1.83                     | 0.60              |
| 1:H:144:VAL:HG22 | 1:H:145:ASP:N    | 2.15                     | 0.60              |
| 1:D:237:TRP:HZ3  | 1:D:239:PRO:HB3  | 1.66                     | 0.60              |
| 1:G:180:ARG:HH21 | 1:G:199:LEU:HD13 | 1.66                     | 0.60              |
| 1:L:272:ASN:CG   | 1:L:275:ILE:HG12 | 2.26                     | 0.60              |
| 1:F:214:MET:HG3  | 1:F:222:VAL:HG21 | 1.82                     | 0.60              |
| 1:D:301:LEU:O    | 1:D:305:ILE:HG13 | 2.02                     | 0.60              |
| 1:G:292:ASP:O    | 1:G:293:ALA:HB3  | 2.01                     | 0.60              |
| 1:G:286:ALA:HA   | 1:G:289:MET:HE2  | 1.84                     | 0.60              |
| 1:B:309:GLU:C    | 1:B:311:THR:H    | 2.08                     | 0.60              |
| 1:G:157:SER:O    | 1:G:160:GLY:HA3  | 2.01                     | 0.60              |
| 1:J:246:LEU:HD13 | 1:J:248:SER:OG   | 2.02                     | 0.60              |
| 1:K:161:LYS:O    | 1:K:164:THR:HG22 | 2.02                     | 0.60              |
| 1:E:176:ILE:HG12 | 1:E:226:THR:HG22 | 1.84                     | 0.60              |
| 1:K:189:GLN:O    | 1:K:189:GLN:CG   | 2.48                     | 0.60              |
| 1:B:187:ASP:C    | 1:B:187:ASP:OD2  | 2.45                     | 0.59              |
| 1:H:159:VAL:HG12 | 1:H:267:PHE:CD2  | 2.37                     | 0.59              |
| 1:I:266:PRO:O    | 1:I:271:ARG:NH2  | 2.35                     | 0.59              |
| 1:D:237:TRP:HZ2  | 1:F:206:ARG:NH1  | 2.01                     | 0.59              |
| 1:J:272:ASN:OD1  | 1:J:275:ILE:HG12 | 2.02                     | 0.58              |
| 1:K:185:GLN:NE2  | 1:K:188:GLU:HA   | 2.18                     | 0.58              |
| 1:A:283:ASN:HD22 | 1:B:216:LEU:HD21 | 1.68                     | 0.58              |
| 1:E:142:VAL:HG11 | 1:E:165:ALA:HB2  | 1.85                     | 0.58              |
| 1:I:165:ALA:O    | 1:I:169:VAL:HG13 | 2.03                     | 0.58              |
| 1:B:141:GLY:HA2  | 1:B:161:LYS:HE3  | 1.86                     | 0.58              |
| 1:K:136:ARG:HH11 | 1:K:136:ARG:HG3  | 1.68                     | 0.58              |
| 1:G:145:ASP:C    | 1:G:145:ASP:OD2  | 2.46                     | 0.58              |
| 1:A:136:ARG:HG2  | 1:A:137:ARG:H    | 1.68                     | 0.58              |
| 1:D:244:ASP:OD2  | 1:D:246:LEU:O    | 2.21                     | 0.58              |
| 1:G:272:ASN:O    | 1:G:276:ILE:HG12 | 2.03                     | 0.58              |
| 1:K:206:ARG:HG2  | 1:K:206:ARG:NH2  | 2.15                     | 0.58              |
| 1:E:272:ASN:O    | 1:E:276:ILE:HG12 | 2.03                     | 0.58              |
| 1:H:263:ILE:CD1  | 1:I:207:GLY:O    | 2.51                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:256:PHE:O    | 1:J:257:ASP:CB   | 2.46                     | 0.58              |
| 1:L:267:PHE:C    | 1:L:267:PHE:CD1  | 2.82                     | 0.58              |
| 1:L:269:VAL:O    | 1:L:271:ARG:N    | 2.37                     | 0.58              |
| 1:F:266:PRO:O    | 1:F:267:PHE:O    | 2.22                     | 0.58              |
| 1:H:300:ASN:HB2  | 1:I:199:LEU:HD21 | 1.86                     | 0.57              |
| 1:I:171:ARG:HE   | 1:I:278:GLU:CD   | 2.12                     | 0.57              |
| 1:A:216:LEU:HD21 | 1:C:283:ASN:HD22 | 1.69                     | 0.57              |
| 1:D:242:THR:HG23 | 1:D:243:PHE:N    | 2.18                     | 0.57              |
| 1:A:205:ILE:HB   | 1:A:208:LEU:CD1  | 2.34                     | 0.57              |
| 1:B:244:ASP:OD1  | 1:B:246:LEU:O    | 2.23                     | 0.57              |
| 1:H:144:VAL:CG2  | 1:H:145:ASP:N    | 2.67                     | 0.57              |
| 1:F:140:HIS:HD2  | 1:F:141:GLY:H    | 1.51                     | 0.57              |
| 1:K:198:ILE:HG22 | 1:K:199:LEU:N    | 2.19                     | 0.57              |
| 1:C:256:PHE:O    | 1:C:257:ASP:HB2  | 2.05                     | 0.57              |
| 1:J:204:GLU:OE1  | 1:J:206:ARG:HG3  | 2.04                     | 0.57              |
| 1:A:214:MET:HE2  | 1:F:215:ASN:ND2  | 2.19                     | 0.57              |
| 1:B:271:ARG:CD   | 1:C:163:GLU:OE1  | 2.52                     | 0.57              |
| 1:E:145:ASP:OD2  | 1:E:145:ASP:C    | 2.47                     | 0.57              |
| 1:K:145:ASP:OD2  | 1:K:145:ASP:C    | 2.48                     | 0.57              |
| 1:K:292:ASP:O    | 1:K:293:ALA:CB   | 2.52                     | 0.57              |
| 1:D:262:LYS:HG2  | 1:D:263:ILE:N    | 2.20                     | 0.56              |
| 1:K:136:ARG:CG   | 1:K:136:ARG:NH1  | 2.66                     | 0.56              |
| 1:G:272:ASN:C    | 1:G:272:ASN:HD22 | 2.13                     | 0.56              |
| 1:K:184:TYR:HA   | 1:K:256:PHE:CE1  | 2.41                     | 0.56              |
| 1:D:280:ALA:HB2  | 1:F:208:LEU:HD11 | 1.88                     | 0.56              |
| 1:A:178:ASP:OD2  | 1:A:179:ASP:N    | 2.39                     | 0.56              |
| 1:E:143:LEU:HD13 | 1:E:176:ILE:HB   | 1.87                     | 0.56              |
| 1:C:206:ARG:HD3  | 1:C:206:ARG:N    | 2.08                     | 0.56              |
| 1:G:185:GLN:OE1  | 1:G:256:PHE:HB3  | 2.06                     | 0.56              |
| 1:I:214:MET:HE3  | 1:I:219:ALA:HB2  | 1.88                     | 0.56              |
| 1:I:303:HIS:C    | 1:I:305:ILE:N    | 2.54                     | 0.56              |
| 1:A:215:ASN:ND2  | 1:F:214:MET:HE1  | 2.21                     | 0.55              |
| 1:D:149:LEU:HD22 | 1:D:229:SER:CB   | 2.36                     | 0.55              |
| 1:K:307:HIS:O    | 1:K:307:HIS:ND1  | 2.38                     | 0.55              |
| 1:F:159:VAL:O    | 1:F:159:VAL:HG13 | 2.06                     | 0.55              |
| 1:A:145:ASP:OD1  | 1:A:145:ASP:C    | 2.46                     | 0.55              |
| 1:B:279:VAL:HG21 | 1:C:166:LEU:HD21 | 1.88                     | 0.55              |
| 1:B:204:GLU:OE1  | 1:B:206:ARG:HG3  | 2.06                     | 0.55              |
| 1:D:237:TRP:HZ3  | 1:D:239:PRO:CB   | 2.20                     | 0.55              |
| 1:G:166:LEU:HD21 | 1:I:279:VAL:HG21 | 1.89                     | 0.55              |
| 1:A:176:ILE:HD11 | 1:A:226:THR:OG1  | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:137:ARG:NH1  | 1:B:255:ILE:HA   | 2.19                     | 0.55              |
| 1:L:160:GLY:HA3  | 1:L:206:ARG:HH22 | 1.70                     | 0.55              |
| 1:L:273:LEU:O    | 1:L:277:ILE:HG13 | 2.07                     | 0.55              |
| 1:A:163:GLU:O    | 1:A:166:LEU:HB3  | 2.06                     | 0.55              |
| 1:E:139:MET:CE   | 1:E:183:VAL:HG21 | 2.36                     | 0.55              |
| 1:I:186:GLN:HG2  | 1:I:187:ASP:H    | 1.70                     | 0.55              |
| 1:J:276:ILE:HD11 | 1:L:163:GLU:HG3  | 1.88                     | 0.55              |
| 1:C:211:ILE:HD13 | 1:C:216:LEU:HD12 | 1.89                     | 0.55              |
| 1:I:302:ASN:C    | 1:I:304:LEU:H    | 2.15                     | 0.55              |
| 1:H:157:SER:C    | 1:H:159:VAL:H    | 2.15                     | 0.54              |
| 1:C:256:PHE:O    | 1:C:257:ASP:CB   | 2.55                     | 0.54              |
| 1:D:185:GLN:OE1  | 1:D:256:PHE:O    | 2.24                     | 0.54              |
| 1:K:199:LEU:HD12 | 1:K:199:LEU:H    | 1.73                     | 0.54              |
| 1:A:211:ILE:HD12 | 1:A:216:LEU:HD12 | 1.89                     | 0.54              |
| 1:D:237:TRP:CZ3  | 1:D:239:PRO:HB3  | 2.42                     | 0.54              |
| 1:I:163:GLU:OE2  | 1:I:163:GLU:N    | 2.38                     | 0.54              |
| 1:L:174:ARG:HG2  | 1:L:223:ARG:HB2  | 1.90                     | 0.54              |
| 1:A:215:ASN:HD21 | 1:F:214:MET:HE1  | 1.72                     | 0.54              |
| 1:D:145:ASP:CG   | 1:D:174:ARG:HH21 | 2.16                     | 0.54              |
| 1:J:268:LYS:NZ   | 1:L:159:VAL:HB   | 2.19                     | 0.54              |
| 1:J:304:LEU:HD12 | 1:L:199:LEU:HD12 | 1.90                     | 0.54              |
| 1:E:198:ILE:C    | 1:E:198:ILE:HD12 | 2.32                     | 0.54              |
| 1:J:147:TYR:O    | 1:J:285:ARG:NH2  | 2.31                     | 0.54              |
| 1:J:253:GLN:HB2  | 1:J:262:LYS:NZ   | 2.22                     | 0.54              |
| 1:A:289:MET:HE1  | 1:D:222:VAL:HG23 | 1.90                     | 0.54              |
| 1:D:196:PRO:HG2  | 1:D:199:LEU:HD12 | 1.89                     | 0.54              |
| 1:I:302:ASN:C    | 1:I:304:LEU:N    | 2.65                     | 0.54              |
| 1:E:136:ARG:HG3  | 1:E:136:ARG:HH11 | 1.71                     | 0.54              |
| 1:G:180:ARG:HH21 | 1:G:199:LEU:HD11 | 1.73                     | 0.54              |
| 1:H:207:GLY:O    | 1:H:208:LEU:HB2  | 2.07                     | 0.54              |
| 1:H:155:GLY:O    | 1:H:159:VAL:HG21 | 2.08                     | 0.54              |
| 1:H:272:ASN:C    | 1:H:272:ASN:ND2  | 2.63                     | 0.54              |
| 1:D:263:ILE:CG2  | 1:D:264:THR:N    | 2.70                     | 0.54              |
| 1:F:235:GLU:O    | 1:F:236:ASN:HB3  | 2.08                     | 0.54              |
| 1:F:235:GLU:HB3  | 1:F:266:PRO:HA   | 1.89                     | 0.54              |
| 1:L:256:PHE:O    | 1:L:257:ASP:CB   | 2.54                     | 0.54              |
| 1:G:191:ILE:HG22 | 1:G:228:ILE:HB   | 1.90                     | 0.53              |
| 1:J:255:ILE:HD12 | 1:J:260:VAL:HG21 | 1.90                     | 0.53              |
| 1:K:303:HIS:HD2  | 1:K:308:ASN:CA   | 2.15                     | 0.53              |
| 1:B:185:GLN:OE1  | 1:B:256:PHE:O    | 2.26                     | 0.53              |
| 1:K:268:LYS:HG3  | 1:K:269:VAL:H    | 1.72                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:267:PHE:CD2  | 1:G:271:ARG:HB3  | 2.41                     | 0.53              |
| 1:L:158:GLY:O    | 1:L:159:VAL:C    | 2.52                     | 0.53              |
| 1:L:254:LEU:HD21 | 1:L:257:ASP:HA   | 1.90                     | 0.53              |
| 1:D:308:ASN:HA   | 1:F:180:ARG:HH21 | 1.73                     | 0.53              |
| 1:F:292:ASP:O    | 1:F:293:ALA:CB   | 2.50                     | 0.53              |
| 1:G:180:ARG:NH2  | 1:G:199:LEU:HD13 | 2.24                     | 0.53              |
| 1:K:136:ARG:HH11 | 1:K:136:ARG:HG2  | 1.71                     | 0.53              |
| 1:L:272:ASN:OD1  | 1:L:275:ILE:CG1  | 2.52                     | 0.53              |
| 1:C:189:GLN:HG3  | 1:C:190:THR:OG1  | 2.09                     | 0.53              |
| 1:F:266:PRO:HG2  | 1:F:271:ARG:HH12 | 1.72                     | 0.53              |
| 1:D:300:ASN:HD22 | 1:D:303:HIS:HD2  | 1.56                     | 0.53              |
| 1:H:191:ILE:HD11 | 1:H:255:ILE:HB   | 1.90                     | 0.53              |
| 1:L:187:ASP:OD2  | 1:L:189:GLN:HG3  | 2.08                     | 0.53              |
| 1:C:273:LEU:O    | 1:C:277:ILE:HG13 | 2.08                     | 0.53              |
| 1:G:211:ILE:C    | 1:G:211:ILE:HD12 | 2.33                     | 0.53              |
| 1:K:272:ASN:HD22 | 1:K:272:ASN:C    | 2.17                     | 0.53              |
| 1:K:184:TYR:HD1  | 1:K:185:GLN:O    | 1.92                     | 0.52              |
| 1:D:166:LEU:HD13 | 1:D:203:LEU:HD13 | 1.91                     | 0.52              |
| 1:F:171:ARG:HE   | 1:F:278:GLU:CD   | 2.17                     | 0.52              |
| 1:G:141:GLY:HA2  | 1:G:161:LYS:HE3  | 1.90                     | 0.52              |
| 1:A:254:LEU:HD12 | 1:A:257:ASP:HA   | 1.91                     | 0.52              |
| 1:D:156:ASP:OD2  | 1:D:156:ASP:N    | 2.38                     | 0.52              |
| 1:B:254:LEU:HD21 | 1:B:257:ASP:N    | 2.21                     | 0.52              |
| 1:C:292:ASP:O    | 1:C:293:ALA:CB   | 2.57                     | 0.52              |
| 1:A:254:LEU:HA   | 1:A:258:VAL:O    | 2.09                     | 0.52              |
| 1:E:198:ILE:HG13 | 1:E:199:LEU:H    | 1.74                     | 0.52              |
| 1:J:244:ASP:OD1  | 1:J:246:LEU:O    | 2.26                     | 0.52              |
| 1:A:143:LEU:HG   | 1:A:176:ILE:HD12 | 1.91                     | 0.52              |
| 1:G:188:GLU:O    | 1:G:189:GLN:HB3  | 2.09                     | 0.52              |
| 1:L:268:LYS:O    | 1:L:269:VAL:O    | 2.28                     | 0.52              |
| 1:A:272:ASN:C    | 1:A:272:ASN:ND2  | 2.64                     | 0.52              |
| 1:D:161:LYS:O    | 1:D:164:THR:HB   | 2.09                     | 0.52              |
| 1:F:273:LEU:O    | 1:F:277:ILE:HG13 | 2.10                     | 0.52              |
| 1:C:285:ARG:HG2  | 1:C:289:MET:HE2  | 1.92                     | 0.52              |
| 1:E:211:ILE:C    | 1:E:211:ILE:HD12 | 2.35                     | 0.52              |
| 1:H:275:ILE:CG2  | 1:H:276:ILE:HD13 | 2.39                     | 0.52              |
| 1:J:171:ARG:HH22 | 1:J:275:ILE:CD1  | 2.23                     | 0.52              |
| 1:J:301:LEU:CD2  | 1:J:305:ILE:HD11 | 2.40                     | 0.52              |
| 1:K:180:ARG:NH2  | 1:K:199:LEU:HD11 | 2.23                     | 0.52              |
| 1:A:183:VAL:HG23 | 1:A:191:ILE:HG23 | 1.91                     | 0.51              |
| 1:F:149:LEU:HD22 | 1:F:229:SER:HB2  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:279:VAL:HG21 | 1:L:166:LEU:HD21 | 1.92                     | 0.51              |
| 1:G:163:GLU:O    | 1:G:166:LEU:HB3  | 2.10                     | 0.51              |
| 1:K:187:ASP:OD2  | 1:K:188:GLU:N    | 2.43                     | 0.51              |
| 1:E:149:LEU:HD21 | 1:E:229:SER:HB2  | 1.91                     | 0.51              |
| 1:J:275:ILE:HD11 | 1:L:167:GLU:OE2  | 2.11                     | 0.51              |
| 1:H:269:VAL:C    | 1:H:271:ARG:H    | 2.19                     | 0.51              |
| 1:F:272:ASN:ND2  | 1:F:275:ILE:HG12 | 2.26                     | 0.51              |
| 1:K:176:ILE:HG12 | 1:K:226:THR:HG22 | 1.91                     | 0.51              |
| 1:E:305:ILE:HG22 | 1:J:180:ARG:HG2  | 1.93                     | 0.51              |
| 1:I:153:ILE:HD13 | 1:I:277:ILE:HD13 | 1.93                     | 0.51              |
| 1:B:145:ASP:OD2  | 1:B:174:ARG:NH2  | 2.44                     | 0.51              |
| 1:G:170:GLN:OE1  | 1:G:170:GLN:HA   | 2.11                     | 0.51              |
| 1:K:178:ASP:CG   | 1:K:203:LEU:HD23 | 2.36                     | 0.51              |
| 1:E:268:LYS:O    | 1:E:270:GLY:N    | 2.43                     | 0.51              |
| 1:D:234:LEU:HD21 | 1:D:273:LEU:HD21 | 1.93                     | 0.50              |
| 1:F:157:SER:O    | 1:F:158:GLY:C    | 2.54                     | 0.50              |
| 1:A:142:VAL:HG12 | 1:A:144:VAL:HG13 | 1.93                     | 0.50              |
| 1:F:145:ASP:CG   | 1:F:174:ARG:HH21 | 2.20                     | 0.50              |
| 1:H:155:GLY:O    | 1:H:159:VAL:CG2  | 2.59                     | 0.50              |
| 1:H:205:ILE:O    | 1:H:206:ARG:C    | 2.55                     | 0.50              |
| 1:A:159:VAL:O    | 1:A:159:VAL:HG13 | 2.11                     | 0.50              |
| 1:B:189:GLN:HE21 | 1:B:189:GLN:N    | 2.09                     | 0.50              |
| 1:E:216:LEU:HD21 | 1:F:283:ASN:HD22 | 1.77                     | 0.50              |
| 1:B:212:ASP:OD2  | 1:B:212:ASP:C    | 2.55                     | 0.50              |
| 1:C:188:GLU:OE1  | 1:C:188:GLU:N    | 2.44                     | 0.50              |
| 1:J:246:LEU:CD1  | 1:J:248:SER:OG   | 2.60                     | 0.50              |
| 1:K:292:ASP:O    | 1:K:293:ALA:HB3  | 2.11                     | 0.50              |
| 1:L:156:ASP:HA   | 1:L:161:LYS:HZ2  | 1.74                     | 0.50              |
| 1:A:198:ILE:HD13 | 1:A:198:ILE:C    | 2.37                     | 0.50              |
| 1:F:254:LEU:HD22 | 1:F:257:ASP:O    | 2.11                     | 0.50              |
| 1:G:155:GLY:O    | 1:G:156:ASP:HB3  | 2.12                     | 0.50              |
| 1:J:246:LEU:HD22 | 1:J:294:THR:HG23 | 1.94                     | 0.50              |
| 1:D:279:VAL:O    | 1:D:280:ALA:C    | 2.50                     | 0.50              |
| 1:H:187:ASP:OD2  | 1:H:187:ASP:C    | 2.55                     | 0.50              |
| 1:K:204:GLU:O    | 1:K:206:ARG:NH2  | 2.45                     | 0.50              |
| 1:L:159:VAL:HG12 | 1:L:267:PHE:CZ   | 2.47                     | 0.50              |
| 1:H:269:VAL:HG23 | 1:H:270:GLY:N    | 2.26                     | 0.49              |
| 1:H:292:ASP:O    | 1:H:293:ALA:C    | 2.55                     | 0.49              |
| 1:L:142:VAL:HG21 | 1:L:161:LYS:HB3  | 1.94                     | 0.49              |
| 1:A:198:ILE:HD13 | 1:A:199:LEU:N    | 2.25                     | 0.49              |
| 1:G:159:VAL:O    | 1:G:160:GLY:O    | 2.29                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:191:ILE:HD13 | 1:H:255:ILE:HB   | 1.94                     | 0.49              |
| 1:I:212:ASP:OD1  | 1:I:215:ASN:HB2  | 2.12                     | 0.49              |
| 1:A:223:ARG:NH1  | 1:A:226:THR:CG2  | 2.74                     | 0.49              |
| 1:H:225:ASP:OD2  | 1:H:225:ASP:C    | 2.55                     | 0.49              |
| 1:J:145:ASP:CG   | 1:J:174:ARG:HH21 | 2.20                     | 0.49              |
| 1:I:151:VAL:HG22 | 1:I:230:LEU:HD23 | 1.93                     | 0.49              |
| 1:J:145:ASP:OD2  | 1:J:145:ASP:C    | 2.55                     | 0.49              |
| 1:B:282:MET:HB3  | 1:C:216:LEU:HD22 | 1.95                     | 0.49              |
| 1:A:153:ILE:HA   | 1:A:232:VAL:O    | 2.10                     | 0.49              |
| 1:C:174:ARG:HG2  | 1:C:223:ARG:HB2  | 1.95                     | 0.49              |
| 1:D:242:THR:CG2  | 1:D:243:PHE:N    | 2.75                     | 0.49              |
| 1:J:196:PRO:O    | 1:J:197:PRO:C    | 2.55                     | 0.49              |
| 1:F:272:ASN:CG   | 1:F:275:ILE:HG12 | 2.38                     | 0.49              |
| 1:H:145:ASP:OD2  | 1:H:145:ASP:C    | 2.55                     | 0.49              |
| 1:J:205:ILE:O    | 1:J:205:ILE:HG22 | 2.13                     | 0.49              |
| 1:D:237:TRP:HZ2  | 1:F:206:ARG:HH12 | 1.60                     | 0.49              |
| 1:G:286:ALA:HA   | 1:G:289:MET:CE   | 2.41                     | 0.49              |
| 1:I:180:ARG:HD2  | 1:I:196:PRO:HG3  | 1.94                     | 0.49              |
| 1:J:167:GLU:O    | 1:J:171:ARG:HG3  | 2.12                     | 0.49              |
| 1:K:145:ASP:O    | 1:K:173:HIS:HB3  | 2.13                     | 0.49              |
| 1:E:170:GLN:HG2  | 1:E:217:PHE:HE2  | 1.77                     | 0.49              |
| 1:D:156:ASP:O    | 1:D:159:VAL:HG22 | 2.13                     | 0.49              |
| 1:F:290:GLY:O    | 1:F:291:TYR:C    | 2.56                     | 0.49              |
| 1:D:292:ASP:O    | 1:D:292:ASP:OD2  | 2.31                     | 0.48              |
| 1:H:242:THR:O    | 1:H:243:PHE:O    | 2.31                     | 0.48              |
| 1:H:275:ILE:HG22 | 1:H:276:ILE:HD13 | 1.94                     | 0.48              |
| 1:J:185:GLN:OE1  | 1:J:256:PHE:O    | 2.30                     | 0.48              |
| 1:I:167:GLU:O    | 1:I:171:ARG:HG3  | 2.13                     | 0.48              |
| 1:G:176:ILE:HG12 | 1:G:226:THR:CG2  | 2.42                     | 0.48              |
| 1:A:211:ILE:CD1  | 1:A:216:LEU:HD12 | 2.43                     | 0.48              |
| 1:F:174:ARG:HD3  | 1:F:220:GLY:O    | 2.14                     | 0.48              |
| 1:L:137:ARG:NH2  | 1:L:256:PHE:H    | 2.11                     | 0.48              |
| 1:B:275:ILE:HG23 | 1:B:276:ILE:N    | 2.28                     | 0.48              |
| 1:B:275:ILE:O    | 1:B:279:VAL:HG23 | 2.14                     | 0.48              |
| 1:E:163:GLU:O    | 1:E:166:LEU:HB3  | 2.13                     | 0.48              |
| 1:F:179:ASP:O    | 1:F:180:ARG:C    | 2.56                     | 0.48              |
| 1:K:136:ARG:NH1  | 1:K:136:ARG:HG2  | 2.28                     | 0.48              |
| 1:J:268:LYS:O    | 1:J:268:LYS:HG2  | 2.14                     | 0.48              |
| 1:D:263:ILE:CG2  | 1:D:264:THR:H    | 2.27                     | 0.48              |
| 1:E:147:TYR:HE1  | 1:E:282:MET:HE2  | 1.79                     | 0.48              |
| 1:F:140:HIS:HD2  | 1:F:141:GLY:N    | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:203:LEU:C    | 1:I:203:LEU:HD23 | 2.39                     | 0.48              |
| 1:I:214:MET:O    | 1:I:214:MET:HG2  | 2.12                     | 0.48              |
| 1:J:187:ASP:OD2  | 1:J:187:ASP:C    | 2.57                     | 0.48              |
| 1:J:279:VAL:O    | 1:J:280:ALA:C    | 2.54                     | 0.48              |
| 1:A:198:ILE:HG23 | 1:A:199:LEU:N    | 2.26                     | 0.48              |
| 1:F:211:ILE:HD13 | 1:F:216:LEU:HD12 | 1.96                     | 0.48              |
| 1:C:170:GLN:HG2  | 1:C:217:PHE:CE2  | 2.49                     | 0.47              |
| 1:C:203:LEU:C    | 1:C:203:LEU:HD23 | 2.39                     | 0.47              |
| 1:L:195:ALA:HA   | 1:L:196:PRO:HD2  | 1.65                     | 0.47              |
| 1:G:304:LEU:HA   | 1:G:304:LEU:HD22 | 1.67                     | 0.47              |
| 1:K:272:ASN:O    | 1:K:276:ILE:HG12 | 2.15                     | 0.47              |
| 1:C:203:LEU:HD23 | 1:C:211:ILE:HG13 | 1.95                     | 0.47              |
| 1:H:150:GLY:HA3  | 1:H:227:THR:O    | 2.15                     | 0.47              |
| 1:I:195:ALA:HA   | 1:I:196:PRO:HD2  | 1.63                     | 0.47              |
| 1:E:166:LEU:HD21 | 1:F:279:VAL:HG21 | 1.95                     | 0.47              |
| 1:E:174:ARG:HD3  | 1:E:220:GLY:O    | 2.15                     | 0.47              |
| 1:F:272:ASN:HD21 | 1:F:275:ILE:H    | 1.57                     | 0.47              |
| 1:G:178:ASP:CG   | 1:G:203:LEU:HD12 | 2.39                     | 0.47              |
| 1:H:244:ASP:OD1  | 1:H:246:LEU:O    | 2.32                     | 0.47              |
| 1:I:203:LEU:CD2  | 1:I:211:ILE:HD11 | 2.39                     | 0.47              |
| 1:L:292:ASP:O    | 1:L:293:ALA:CB   | 2.63                     | 0.47              |
| 1:A:170:GLN:HB2  | 1:C:275:ILE:HD11 | 1.96                     | 0.47              |
| 1:C:185:GLN:HG3  | 1:C:186:GLN:H    | 1.80                     | 0.47              |
| 1:E:254:LEU:HD23 | 1:E:257:ASP:HA   | 1.97                     | 0.47              |
| 1:H:196:PRO:O    | 1:H:197:PRO:C    | 2.58                     | 0.47              |
| 1:F:166:LEU:O    | 1:F:169:VAL:HG22 | 2.15                     | 0.47              |
| 1:A:160:GLY:O    | 1:A:162:SER:N    | 2.48                     | 0.46              |
| 1:L:166:LEU:HD13 | 1:L:203:LEU:HD21 | 1.97                     | 0.46              |
| 1:L:235:GLU:O    | 1:L:267:PHE:CB   | 2.54                     | 0.46              |
| 1:A:214:MET:CE   | 1:F:215:ASN:HD22 | 2.28                     | 0.46              |
| 1:A:214:MET:CE   | 1:F:215:ASN:ND2  | 2.79                     | 0.46              |
| 1:B:176:ILE:O    | 1:B:195:ALA:HB2  | 2.16                     | 0.46              |
| 1:B:262:LYS:HG2  | 1:B:263:ILE:N    | 2.29                     | 0.46              |
| 1:C:184:TYR:HD1  | 1:C:185:GLN:O    | 1.98                     | 0.46              |
| 1:D:205:ILE:O    | 1:D:206:ARG:C    | 2.58                     | 0.46              |
| 1:G:192:VAL:HA   | 1:G:227:THR:HA   | 1.98                     | 0.46              |
| 1:A:255:ILE:O    | 1:A:256:PHE:HB2  | 2.16                     | 0.46              |
| 1:B:142:VAL:HG11 | 1:B:165:ALA:HB2  | 1.98                     | 0.46              |
| 1:G:146:ILE:HG22 | 1:G:147:TYR:CD1  | 2.51                     | 0.46              |
| 1:D:237:TRP:HZ3  | 1:D:239:PRO:CA   | 2.29                     | 0.46              |
| 1:F:307:HIS:ND1  | 1:F:308:ASN:N    | 2.64                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:283:ASN:HD22 | 1:H:216:LEU:HD21 | 1.80                     | 0.46              |
| 1:H:255:ILE:HD12 | 1:H:260:VAL:HG21 | 1.97                     | 0.46              |
| 1:I:253:GLN:CB   | 1:I:262:LYS:HD2  | 2.46                     | 0.46              |
| 1:L:234:LEU:HD22 | 1:L:273:LEU:HD13 | 1.97                     | 0.46              |
| 1:D:212:ASP:C    | 1:D:212:ASP:OD2  | 2.59                     | 0.46              |
| 1:F:156:ASP:CG   | 1:F:157:SER:N    | 2.73                     | 0.46              |
| 1:K:286:ALA:HA   | 1:K:289:MET:HE2  | 1.98                     | 0.46              |
| 1:A:163:GLU:OE1  | 1:C:271:ARG:HB2  | 2.16                     | 0.46              |
| 1:B:309:GLU:C    | 1:B:311:THR:N    | 2.70                     | 0.46              |
| 1:D:145:ASP:O    | 1:D:173:HIS:HB3  | 2.16                     | 0.46              |
| 1:D:191:ILE:CD1  | 1:D:260:VAL:CG2  | 2.93                     | 0.46              |
| 1:F:275:ILE:O    | 1:F:279:VAL:HG23 | 2.15                     | 0.46              |
| 1:H:285:ARG:NH1  | 2:H:325:HOH:O    | 2.47                     | 0.46              |
| 1:D:292:ASP:CG   | 1:D:295:LYS:HG3  | 2.40                     | 0.46              |
| 1:E:248:SER:HB2  | 1:E:249:GLY:H    | 1.60                     | 0.46              |
| 1:I:269:VAL:O    | 1:I:271:ARG:N    | 2.48                     | 0.46              |
| 1:K:187:ASP:CG   | 1:K:189:GLN:H    | 2.24                     | 0.46              |
| 1:F:179:ASP:CG   | 1:F:180:ARG:HG2  | 2.41                     | 0.46              |
| 1:K:198:ILE:HG22 | 1:K:199:LEU:H    | 1.80                     | 0.46              |
| 1:D:137:ARG:NH2  | 1:D:256:PHE:H    | 2.14                     | 0.46              |
| 1:D:203:LEU:C    | 1:D:203:LEU:HD23 | 2.41                     | 0.46              |
| 1:G:158:GLY:C    | 1:G:160:GLY:H    | 2.24                     | 0.46              |
| 1:C:162:SER:HB3  | 1:C:178:ASP:OD1  | 2.16                     | 0.46              |
| 1:D:196:PRO:O    | 1:D:197:PRO:C    | 2.57                     | 0.46              |
| 1:L:184:TYR:CD1  | 1:L:184:TYR:C    | 2.94                     | 0.46              |
| 1:G:196:PRO:O    | 1:G:200:SER:HB2  | 2.16                     | 0.45              |
| 1:I:186:GLN:O    | 1:I:187:ASP:C    | 2.59                     | 0.45              |
| 1:J:149:LEU:C    | 1:J:149:LEU:HD23 | 2.41                     | 0.45              |
| 1:K:301:LEU:HD23 | 1:K:301:LEU:HA   | 1.69                     | 0.45              |
| 1:L:178:ASP:O    | 1:L:179:ASP:C    | 2.58                     | 0.45              |
| 1:B:308:ASN:O    | 1:B:311:THR:OG1  | 2.20                     | 0.45              |
| 1:A:183:VAL:HG23 | 1:A:191:ILE:CG2  | 2.46                     | 0.45              |
| 1:D:268:LYS:O    | 1:D:269:VAL:C    | 2.59                     | 0.45              |
| 1:G:170:GLN:OE1  | 1:G:217:PHE:HE2  | 1.98                     | 0.45              |
| 1:K:183:VAL:HG23 | 1:K:256:PHE:HE1  | 1.82                     | 0.45              |
| 1:G:212:ASP:HB3  | 1:G:215:ASN:HB3  | 1.99                     | 0.45              |
| 1:H:137:ARG:HG3  | 1:H:256:PHE:HZ   | 1.75                     | 0.45              |
| 1:H:142:VAL:HG11 | 1:H:165:ALA:HB2  | 1.98                     | 0.45              |
| 1:L:142:VAL:CG2  | 1:L:161:LYS:HB3  | 2.46                     | 0.45              |
| 1:E:184:TYR:HA   | 1:E:256:PHE:HE1  | 1.80                     | 0.45              |
| 1:L:203:LEU:HD22 | 1:L:211:ILE:HG13 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:251:GLN:HB3  | 1:L:252:THR:H    | 1.54                     | 0.45              |
| 1:B:279:VAL:HG13 | 1:C:216:LEU:HD13 | 1.99                     | 0.45              |
| 1:B:292:ASP:CG   | 1:B:295:LYS:HD3  | 2.41                     | 0.45              |
| 1:E:251:GLN:HE21 | 1:E:262:LYS:HD3  | 1.82                     | 0.45              |
| 1:G:159:VAL:HG11 | 1:G:206:ARG:HG3  | 1.98                     | 0.45              |
| 1:H:185:GLN:OE1  | 1:H:256:PHE:O    | 2.35                     | 0.45              |
| 1:C:144:VAL:HG23 | 1:C:146:ILE:HG13 | 1.99                     | 0.45              |
| 1:E:174:ARG:CD   | 1:E:220:GLY:O    | 2.64                     | 0.45              |
| 1:E:211:ILE:HD13 | 1:E:216:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:149:LEU:HD11 | 1:A:229:SER:CB   | 2.47                     | 0.45              |
| 1:A:160:GLY:O    | 1:A:161:LYS:C    | 2.60                     | 0.45              |
| 1:E:149:LEU:CD2  | 1:E:229:SER:HB2  | 2.47                     | 0.45              |
| 1:G:145:ASP:O    | 1:G:173:HIS:HB3  | 2.16                     | 0.45              |
| 1:L:272:ASN:C    | 1:L:272:ASN:HD22 | 2.25                     | 0.45              |
| 1:C:171:ARG:HG2  | 1:C:171:ARG:HH11 | 1.82                     | 0.44              |
| 1:K:180:ARG:HH22 | 1:K:199:LEU:HD13 | 1.82                     | 0.44              |
| 1:L:191:ILE:HD12 | 1:L:260:VAL:CG2  | 2.47                     | 0.44              |
| 1:B:279:VAL:O    | 1:B:280:ALA:C    | 2.58                     | 0.44              |
| 1:E:136:ARG:HG3  | 1:E:136:ARG:NH1  | 2.32                     | 0.44              |
| 1:F:154:THR:O    | 1:F:233:HIS:HA   | 2.17                     | 0.44              |
| 1:I:216:LEU:HD23 | 1:I:216:LEU:HA   | 1.74                     | 0.44              |
| 1:J:234:LEU:HD23 | 1:J:265:VAL:HG22 | 2.00                     | 0.44              |
| 1:L:170:GLN:OE1  | 1:L:170:GLN:HA   | 2.17                     | 0.44              |
| 1:A:267:PHE:HE1  | 1:A:271:ARG:HB3  | 1.82                     | 0.44              |
| 1:F:235:GLU:O    | 1:F:236:ASN:CB   | 2.65                     | 0.44              |
| 1:G:287:LYS:HB2  | 1:G:287:LYS:HE3  | 1.89                     | 0.44              |
| 1:G:157:SER:O    | 1:G:160:GLY:N    | 2.50                     | 0.44              |
| 1:G:157:SER:O    | 1:G:160:GLY:CA   | 2.64                     | 0.44              |
| 1:G:204:GLU:O    | 1:G:206:ARG:NH1  | 2.51                     | 0.44              |
| 1:J:140:HIS:CD2  | 1:J:180:ARG:HH11 | 2.36                     | 0.44              |
| 1:J:196:PRO:HG2  | 1:J:199:LEU:HD12 | 1.99                     | 0.44              |
| 1:K:274:ALA:O    | 1:K:278:GLU:HG3  | 2.17                     | 0.44              |
| 1:D:160:GLY:O    | 1:D:161:LYS:C    | 2.61                     | 0.44              |
| 1:I:180:ARG:HD2  | 1:I:196:PRO:HB3  | 1.98                     | 0.44              |
| 1:J:162:SER:O    | 1:J:165:ALA:HB3  | 2.17                     | 0.44              |
| 1:F:254:LEU:HA   | 1:F:258:VAL:O    | 2.18                     | 0.44              |
| 1:I:211:ILE:HD12 | 1:I:211:ILE:O    | 2.16                     | 0.44              |
| 1:A:226:THR:HB   | 1:A:227:THR:O    | 2.17                     | 0.44              |
| 1:I:137:ARG:H    | 1:I:256:PHE:HZ   | 1.65                     | 0.44              |
| 1:K:235:GLU:O    | 1:K:267:PHE:HB3  | 2.18                     | 0.44              |
| 1:A:225:ASP:O    | 1:A:226:THR:O    | 2.36                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:137:ARG:HB2  | 1:B:256:PHE:CZ   | 2.53                     | 0.44              |
| 1:D:309:GLU:C    | 1:D:311:THR:N    | 2.72                     | 0.44              |
| 1:F:185:GLN:HG2  | 1:F:186:GLN:H    | 1.83                     | 0.44              |
| 1:A:175:LEU:HD23 | 1:A:213:VAL:HG21 | 2.00                     | 0.43              |
| 1:B:160:GLY:O    | 1:B:163:GLU:HG2  | 2.18                     | 0.43              |
| 1:C:285:ARG:O    | 1:C:289:MET:HG3  | 2.18                     | 0.43              |
| 1:E:184:TYR:HD1  | 1:E:185:GLN:O    | 2.01                     | 0.43              |
| 1:G:184:TYR:HA   | 1:G:256:PHE:HE1  | 1.83                     | 0.43              |
| 1:H:219:ALA:C    | 1:H:221:ALA:H    | 2.25                     | 0.43              |
| 1:H:270:GLY:O    | 1:I:159:VAL:HG11 | 2.18                     | 0.43              |
| 1:F:253:GLN:HB2  | 1:F:262:LYS:HD2  | 1.99                     | 0.43              |
| 1:J:272:ASN:HD21 | 1:J:274:ALA:HB3  | 1.83                     | 0.43              |
| 1:A:175:LEU:CD2  | 1:A:213:VAL:HG21 | 2.48                     | 0.43              |
| 1:A:223:ARG:O    | 1:A:224:GLU:HB3  | 2.14                     | 0.43              |
| 1:E:138:SER:HB2  | 1:E:182:ASP:OD1  | 2.19                     | 0.43              |
| 1:J:301:LEU:HD23 | 1:J:305:ILE:HD11 | 2.00                     | 0.43              |
| 1:K:304:LEU:HD22 | 1:K:304:LEU:O    | 2.18                     | 0.43              |
| 1:F:156:ASP:O    | 1:F:161:LYS:NZ   | 2.51                     | 0.43              |
| 1:H:145:ASP:O    | 1:H:173:HIS:HB3  | 2.17                     | 0.43              |
| 1:H:280:ALA:HB2  | 1:I:208:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:234:LEU:CD2  | 1:D:273:LEU:HD21 | 2.48                     | 0.43              |
| 1:E:201:HIS:HE1  | 1:E:223:ARG:O    | 2.02                     | 0.43              |
| 1:K:146:ILE:CD1  | 1:K:277:ILE:HG22 | 2.49                     | 0.43              |
| 1:D:237:TRP:CZ2  | 1:F:206:ARG:NH1  | 2.85                     | 0.43              |
| 1:F:184:TYR:HD1  | 1:F:184:TYR:O    | 2.02                     | 0.43              |
| 1:K:295:LYS:O    | 1:K:299:LYS:HB2  | 2.18                     | 0.43              |
| 1:C:170:GLN:HG2  | 1:C:217:PHE:HE2  | 1.84                     | 0.43              |
| 1:H:165:ALA:O    | 1:H:169:VAL:HG13 | 2.19                     | 0.43              |
| 1:B:145:ASP:OD2  | 1:B:145:ASP:C    | 2.62                     | 0.43              |
| 1:B:279:VAL:HG21 | 1:C:166:LEU:CD2  | 2.49                     | 0.43              |
| 1:D:269:VAL:HG23 | 1:D:269:VAL:O    | 2.19                     | 0.43              |
| 1:F:143:LEU:HD13 | 1:F:176:ILE:HB   | 2.01                     | 0.43              |
| 1:D:275:ILE:O    | 1:D:279:VAL:HG23 | 2.18                     | 0.43              |
| 1:E:158:GLY:O    | 1:E:159:VAL:C    | 2.62                     | 0.43              |
| 1:F:292:ASP:HB3  | 1:F:295:LYS:HB2  | 2.01                     | 0.43              |
| 1:G:272:ASN:C    | 1:G:272:ASN:ND2  | 2.76                     | 0.43              |
| 1:H:279:VAL:O    | 1:H:280:ALA:C    | 2.58                     | 0.43              |
| 1:D:242:THR:HG23 | 1:D:243:PHE:H    | 1.81                     | 0.42              |
| 1:J:171:ARG:HH22 | 1:J:275:ILE:HD11 | 1.83                     | 0.42              |
| 1:B:246:LEU:HD13 | 1:B:248:SER:OG   | 2.19                     | 0.42              |
| 1:H:263:ILE:HG13 | 1:H:264:THR:N    | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:136:ARG:HG3  | 1:I:184:TYR:HB3  | 2.02                     | 0.42              |
| 1:J:145:ASP:OD1  | 1:J:223:ARG:NH1  | 2.50                     | 0.42              |
| 1:L:136:ARG:HG3  | 1:L:184:TYR:HB3  | 2.01                     | 0.42              |
| 1:B:145:ASP:CG   | 1:B:174:ARG:NH2  | 2.74                     | 0.42              |
| 1:E:145:ASP:O    | 1:E:173:HIS:HB3  | 2.20                     | 0.42              |
| 1:F:161:LYS:O    | 1:F:164:THR:HB   | 2.19                     | 0.42              |
| 1:K:196:PRO:HG3  | 1:K:199:LEU:HB2  | 2.00                     | 0.42              |
| 1:K:296:THR:O    | 1:K:299:LYS:HB3  | 2.19                     | 0.42              |
| 1:E:149:LEU:HD23 | 1:E:149:LEU:HA   | 1.85                     | 0.42              |
| 1:E:156:ASP:N    | 1:E:161:LYS:HZ2  | 2.17                     | 0.42              |
| 1:E:196:PRO:CG   | 1:E:199:LEU:HB2  | 2.49                     | 0.42              |
| 1:E:198:ILE:C    | 1:E:198:ILE:CD1  | 2.92                     | 0.42              |
| 1:C:153:ILE:CD1  | 1:C:277:ILE:HD13 | 2.48                     | 0.42              |
| 1:F:265:VAL:HA   | 1:F:266:PRO:HD2  | 1.86                     | 0.42              |
| 1:K:141:GLY:HA2  | 1:K:161:LYS:HE3  | 2.02                     | 0.42              |
| 1:K:283:ASN:O    | 1:K:287:LYS:HB2  | 2.19                     | 0.42              |
| 1:K:268:LYS:HG3  | 1:K:269:VAL:N    | 2.34                     | 0.42              |
| 1:B:275:ILE:HD12 | 1:C:167:GLU:HA   | 2.02                     | 0.42              |
| 1:F:273:LEU:O    | 1:F:274:ALA:C    | 2.63                     | 0.42              |
| 1:G:183:VAL:HG12 | 1:G:184:TYR:N    | 2.34                     | 0.42              |
| 1:D:262:LYS:HG2  | 1:D:263:ILE:H    | 1.85                     | 0.42              |
| 1:E:160:GLY:O    | 1:E:163:GLU:N    | 2.46                     | 0.42              |
| 1:F:140:HIS:CD2  | 1:F:141:GLY:N    | 2.88                     | 0.42              |
| 1:K:139:MET:HE2  | 1:K:139:MET:HB3  | 1.92                     | 0.42              |
| 1:L:137:ARG:HB2  | 1:L:256:PHE:CE1  | 2.55                     | 0.42              |
| 1:A:183:VAL:CG2  | 1:A:191:ILE:HG23 | 2.49                     | 0.41              |
| 1:J:238:THR:C    | 1:J:240:ASP:H    | 2.28                     | 0.41              |
| 1:A:213:VAL:O    | 1:A:214:MET:C    | 2.63                     | 0.41              |
| 1:B:310:GLU:O    | 1:B:310:GLU:HG3  | 2.20                     | 0.41              |
| 1:F:185:GLN:OE1  | 1:F:256:PHE:HB3  | 2.20                     | 0.41              |
| 1:F:272:ASN:HD21 | 1:F:274:ALA:CB   | 2.23                     | 0.41              |
| 1:H:300:ASN:O    | 1:H:301:LEU:C    | 2.63                     | 0.41              |
| 1:I:156:ASP:HA   | 1:I:161:LYS:NZ   | 2.36                     | 0.41              |
| 1:L:178:ASP:O    | 1:L:180:ARG:N    | 2.53                     | 0.41              |
| 1:G:174:ARG:CD   | 1:G:220:GLY:O    | 2.68                     | 0.41              |
| 1:G:187:ASP:C    | 1:G:189:GLN:H    | 2.28                     | 0.41              |
| 1:I:157:SER:O    | 1:I:158:GLY:C    | 2.62                     | 0.41              |
| 1:I:184:TYR:CD1  | 1:I:184:TYR:C    | 2.98                     | 0.41              |
| 1:L:272:ASN:C    | 1:L:272:ASN:ND2  | 2.78                     | 0.41              |
| 1:A:205:ILE:CB   | 1:A:208:LEU:HD11 | 2.41                     | 0.41              |
| 1:A:267:PHE:CE1  | 1:A:271:ARG:HB3  | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:237:TRP:H    | 1:C:237:TRP:CD1  | 2.38                     | 0.41              |
| 1:D:309:GLU:O    | 1:D:311:THR:N    | 2.53                     | 0.41              |
| 1:E:272:ASN:HD22 | 1:E:273:LEU:N    | 2.18                     | 0.41              |
| 1:E:286:ALA:HA   | 1:E:289:MET:CE   | 2.50                     | 0.41              |
| 1:K:250:GLU:H    | 1:K:250:GLU:HG2  | 1.56                     | 0.41              |
| 1:E:180:ARG:HH21 | 1:E:199:LEU:HD12 | 1.84                     | 0.41              |
| 1:E:304:LEU:HD12 | 1:E:304:LEU:O    | 2.20                     | 0.41              |
| 1:F:152:LEU:HB3  | 1:F:231:ILE:HG12 | 2.01                     | 0.41              |
| 1:G:198:ILE:HG23 | 1:G:199:LEU:HD12 | 2.02                     | 0.41              |
| 1:B:300:ASN:O    | 1:B:301:LEU:C    | 2.64                     | 0.41              |
| 1:C:253:GLN:HB2  | 1:C:262:LYS:HZ3  | 1.86                     | 0.41              |
| 1:I:233:HIS:CD2  | 1:I:233:HIS:C    | 2.98                     | 0.41              |
| 1:A:145:ASP:O    | 1:A:173:HIS:HB3  | 2.21                     | 0.41              |
| 1:A:153:ILE:H    | 1:A:153:ILE:HG12 | 1.76                     | 0.41              |
| 1:E:174:ARG:HD3  | 1:E:174:ARG:HH11 | 1.69                     | 0.41              |
| 1:E:267:PHE:CE2  | 1:E:271:ARG:HB2  | 2.55                     | 0.41              |
| 1:F:139:MET:CE   | 1:F:183:VAL:HG21 | 2.50                     | 0.41              |
| 1:K:174:ARG:CD   | 1:K:220:GLY:O    | 2.68                     | 0.41              |
| 1:K:176:ILE:N    | 1:K:176:ILE:HD12 | 2.35                     | 0.41              |
| 1:L:191:ILE:HD12 | 1:L:260:VAL:HG21 | 2.03                     | 0.41              |
| 1:G:186:GLN:O    | 1:G:187:ASP:HB3  | 2.21                     | 0.41              |
| 1:H:161:LYS:H    | 1:H:161:LYS:HE3  | 1.85                     | 0.41              |
| 1:I:139:MET:SD   | 1:I:183:VAL:HG21 | 2.61                     | 0.41              |
| 1:B:254:LEU:HD23 | 1:B:255:ILE:N    | 2.35                     | 0.41              |
| 1:B:275:ILE:CG2  | 1:B:276:ILE:N    | 2.83                     | 0.41              |
| 1:C:171:ARG:HG2  | 1:C:171:ARG:NH1  | 2.36                     | 0.41              |
| 1:C:303:HIS:O    | 1:C:303:HIS:ND1  | 2.54                     | 0.41              |
| 1:E:191:ILE:HD13 | 1:E:191:ILE:HA   | 1.94                     | 0.41              |
| 1:F:263:ILE:CG2  | 1:F:264:THR:N    | 2.82                     | 0.41              |
| 1:G:139:MET:HE2  | 1:G:139:MET:HB3  | 1.84                     | 0.41              |
| 1:H:166:LEU:HD12 | 1:H:166:LEU:HA   | 1.71                     | 0.41              |
| 1:J:145:ASP:OD2  | 1:J:174:ARG:NH2  | 2.54                     | 0.41              |
| 1:J:171:ARG:NH2  | 1:J:275:ILE:CD1  | 2.84                     | 0.41              |
| 1:K:224:GLU:OE2  | 1:K:224:GLU:HA   | 2.20                     | 0.41              |
| 1:K:272:ASN:HD22 | 1:K:273:LEU:N    | 2.19                     | 0.41              |
| 1:L:216:LEU:HD23 | 1:L:216:LEU:HA   | 1.84                     | 0.41              |
| 1:L:265:VAL:HA   | 1:L:266:PRO:HD2  | 1.93                     | 0.41              |
| 1:B:273:LEU:HD23 | 1:B:273:LEU:HA   | 1.88                     | 0.41              |
| 1:D:162:SER:OG   | 1:D:178:ASP:OD2  | 2.25                     | 0.41              |
| 1:D:237:TRP:C    | 1:D:237:TRP:HE3  | 2.29                     | 0.41              |
| 1:E:143:LEU:HD13 | 1:E:176:ILE:CB   | 2.51                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:170:GLN:HG2  | 1:F:217:PHE:HE2  | 1.86                     | 0.41              |
| 1:L:187:ASP:C    | 1:L:189:GLN:H    | 2.29                     | 0.41              |
| 1:L:199:LEU:HD23 | 1:L:199:LEU:HA   | 1.87                     | 0.41              |
| 1:A:254:LEU:CD1  | 1:A:257:ASP:HA   | 2.51                     | 0.40              |
| 1:B:256:PHE:O    | 1:B:257:ASP:CB   | 2.64                     | 0.40              |
| 1:D:166:LEU:HD12 | 1:D:166:LEU:HA   | 1.87                     | 0.40              |
| 1:D:206:ARG:O    | 1:E:271:ARG:NH2  | 2.49                     | 0.40              |
| 1:E:157:SER:O    | 1:E:158:GLY:C    | 2.64                     | 0.40              |
| 1:E:178:ASP:CB   | 1:E:203:LEU:HD23 | 2.51                     | 0.40              |
| 1:G:235:GLU:O    | 1:G:267:PHE:HB3  | 2.21                     | 0.40              |
| 1:I:253:GLN:HB3  | 1:I:262:LYS:HD2  | 2.03                     | 0.40              |
| 1:C:136:ARG:CA   | 1:C:256:PHE:HZ   | 2.30                     | 0.40              |
| 1:C:171:ARG:NH2  | 1:C:275:ILE:HG12 | 2.36                     | 0.40              |
| 1:J:186:GLN:HE21 | 1:J:190:THR:HG21 | 1.86                     | 0.40              |
| 1:E:162:SER:HB2  | 1:E:203:LEU:HD22 | 2.03                     | 0.40              |
| 1:F:195:ALA:HA   | 1:F:196:PRO:HD3  | 1.99                     | 0.40              |
| 1:K:272:ASN:C    | 1:K:272:ASN:ND2  | 2.80                     | 0.40              |
| 1:L:156:ASP:O    | 1:L:157:SER:O    | 2.40                     | 0.40              |
| 1:F:166:LEU:HD13 | 1:F:203:LEU:HD23 | 2.04                     | 0.40              |
| 1:F:214:MET:HE2  | 1:F:214:MET:HB3  | 1.94                     | 0.40              |
| 1:F:285:ARG:O    | 1:F:289:MET:HG3  | 2.22                     | 0.40              |
| 1:I:166:LEU:HD13 | 1:I:203:LEU:HD21 | 2.02                     | 0.40              |
| 1:J:268:LYS:O    | 1:J:270:GLY:N    | 2.54                     | 0.40              |
| 1:B:283:ASN:HA   | 1:C:216:LEU:HD21 | 2.04                     | 0.40              |
| 1:C:171:ARG:HH11 | 1:C:171:ARG:CG   | 2.34                     | 0.40              |
| 1:J:170:GLN:HA   | 1:J:170:GLN:HE21 | 1.86                     | 0.40              |
| 1:K:279:VAL:HA   | 1:K:282:MET:HE3  | 2.03                     | 0.40              |
| 1:L:212:ASP:HB3  | 1:L:215:ASN:HB2  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 157/205 (77%)   | 127 (81%)  | 23 (15%)  | 7 (4%)   | 2           | 2  |
| 1   | B     | 179/205 (87%)   | 161 (90%)  | 16 (9%)   | 2 (1%)   | 11          | 25 |
| 1   | C     | 160/205 (78%)   | 140 (88%)  | 12 (8%)   | 8 (5%)   | 1           | 2  |
| 1   | D     | 179/205 (87%)   | 155 (87%)  | 17 (10%)  | 7 (4%)   | 2           | 3  |
| 1   | E     | 160/205 (78%)   | 132 (82%)  | 23 (14%)  | 5 (3%)   | 3           | 5  |
| 1   | F     | 156/205 (76%)   | 142 (91%)  | 10 (6%)   | 4 (3%)   | 4           | 7  |
| 1   | G     | 156/205 (76%)   | 130 (83%)  | 14 (9%)   | 12 (8%)  | 1           | 1  |
| 1   | H     | 176/205 (86%)   | 149 (85%)  | 17 (10%)  | 10 (6%)  | 1           | 1  |
| 1   | I     | 156/205 (76%)   | 134 (86%)  | 11 (7%)   | 11 (7%)  | 1           | 1  |
| 1   | J     | 176/205 (86%)   | 151 (86%)  | 18 (10%)  | 7 (4%)   | 2           | 3  |
| 1   | K     | 158/205 (77%)   | 129 (82%)  | 20 (13%)  | 9 (6%)   | 1           | 1  |
| 1   | L     | 157/205 (77%)   | 130 (83%)  | 19 (12%)  | 8 (5%)   | 1           | 2  |
| All | All   | 1970/2460 (80%) | 1680 (85%) | 200 (10%) | 90 (5%)  | 2           | 2  |

All (90) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 137 | ARG  |
| 1   | A     | 226 | THR  |
| 1   | B     | 133 | LEU  |
| 1   | D     | 269 | VAL  |
| 1   | D     | 293 | ALA  |
| 1   | E     | 156 | ASP  |
| 1   | E     | 159 | VAL  |
| 1   | F     | 159 | VAL  |
| 1   | F     | 267 | PHE  |
| 1   | F     | 269 | VAL  |
| 1   | F     | 291 | TYR  |
| 1   | G     | 137 | ARG  |
| 1   | G     | 189 | GLN  |
| 1   | G     | 251 | GLN  |
| 1   | G     | 293 | ALA  |
| 1   | H     | 157 | SER  |
| 1   | H     | 243 | PHE  |
| 1   | H     | 269 | VAL  |
| 1   | H     | 293 | ALA  |
| 1   | I     | 159 | VAL  |
| 1   | I     | 269 | VAL  |
| 1   | I     | 303 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 269 | VAL  |
| 1   | J     | 293 | ALA  |
| 1   | J     | 310 | GLU  |
| 1   | K     | 199 | LEU  |
| 1   | K     | 269 | VAL  |
| 1   | K     | 293 | ALA  |
| 1   | K     | 301 | LEU  |
| 1   | L     | 156 | ASP  |
| 1   | L     | 157 | SER  |
| 1   | L     | 269 | VAL  |
| 1   | L     | 270 | GLY  |
| 1   | A     | 160 | GLY  |
| 1   | A     | 161 | LYS  |
| 1   | A     | 224 | GLU  |
| 1   | A     | 271 | ARG  |
| 1   | B     | 310 | GLU  |
| 1   | C     | 200 | SER  |
| 1   | C     | 257 | ASP  |
| 1   | D     | 308 | ASN  |
| 1   | D     | 310 | GLU  |
| 1   | E     | 269 | VAL  |
| 1   | E     | 293 | ALA  |
| 1   | G     | 160 | GLY  |
| 1   | G     | 199 | LEU  |
| 1   | G     | 200 | SER  |
| 1   | G     | 269 | VAL  |
| 1   | H     | 156 | ASP  |
| 1   | H     | 208 | LEU  |
| 1   | I     | 270 | GLY  |
| 1   | I     | 293 | ALA  |
| 1   | I     | 304 | LEU  |
| 1   | J     | 206 | ARG  |
| 1   | J     | 237 | TRP  |
| 1   | K     | 137 | ARG  |
| 1   | L     | 257 | ASP  |
| 1   | C     | 156 | ASP  |
| 1   | C     | 293 | ALA  |
| 1   | D     | 237 | TRP  |
| 1   | D     | 256 | PHE  |
| 1   | G     | 306 | GLU  |
| 1   | I     | 187 | ASP  |
| 1   | J     | 239 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 157 | SER  |
| 1   | K     | 184 | TYR  |
| 1   | L     | 268 | LYS  |
| 1   | C     | 179 | ASP  |
| 1   | C     | 302 | ASN  |
| 1   | G     | 156 | ASP  |
| 1   | G     | 161 | LYS  |
| 1   | H     | 257 | ASP  |
| 1   | K     | 200 | SER  |
| 1   | C     | 137 | ARG  |
| 1   | D     | 309 | GLU  |
| 1   | E     | 199 | LEU  |
| 1   | G     | 188 | GLU  |
| 1   | H     | 241 | LYS  |
| 1   | I     | 137 | ARG  |
| 1   | I     | 188 | GLU  |
| 1   | I     | 251 | GLN  |
| 1   | J     | 257 | ASP  |
| 1   | K     | 138 | SER  |
| 1   | L     | 252 | THR  |
| 1   | L     | 306 | GLU  |
| 1   | C     | 197 | PRO  |
| 1   | H     | 207 | GLY  |
| 1   | H     | 270 | GLY  |
| 1   | I     | 158 | GLY  |
| 1   | A     | 269 | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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     | 135/174 (78%) | 115 (85%) | 20 (15%) | 3           | 6 |
| 1   | B     | 153/174 (88%) | 128 (84%) | 25 (16%) | 2           | 4 |
| 1   | C     | 138/174 (79%) | 115 (83%) | 23 (17%) | 2           | 4 |
| 1   | D     | 153/174 (88%) | 126 (82%) | 27 (18%) | 2           | 3 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | E     | 138/174 (79%)   | 117 (85%)  | 21 (15%)  | 3           | 5 |
| 1   | F     | 135/174 (78%)   | 115 (85%)  | 20 (15%)  | 3           | 6 |
| 1   | G     | 135/174 (78%)   | 114 (84%)  | 21 (16%)  | 2           | 4 |
| 1   | H     | 150/174 (86%)   | 129 (86%)  | 21 (14%)  | 3           | 6 |
| 1   | I     | 135/174 (78%)   | 113 (84%)  | 22 (16%)  | 2           | 4 |
| 1   | J     | 151/174 (87%)   | 123 (82%)  | 28 (18%)  | 1           | 3 |
| 1   | K     | 136/174 (78%)   | 111 (82%)  | 25 (18%)  | 1           | 3 |
| 1   | L     | 136/174 (78%)   | 112 (82%)  | 24 (18%)  | 2           | 3 |
| All | All   | 1695/2088 (81%) | 1418 (84%) | 277 (16%) | 2           | 4 |

All (277) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 138 | SER  |
| 1   | A     | 145 | ASP  |
| 1   | A     | 151 | VAL  |
| 1   | A     | 153 | ILE  |
| 1   | A     | 162 | SER  |
| 1   | A     | 164 | THR  |
| 1   | A     | 170 | GLN  |
| 1   | A     | 198 | ILE  |
| 1   | A     | 203 | LEU  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 211 | ILE  |
| 1   | A     | 250 | GLU  |
| 1   | A     | 255 | ILE  |
| 1   | A     | 263 | ILE  |
| 1   | A     | 273 | LEU  |
| 1   | A     | 275 | ILE  |
| 1   | A     | 285 | ARG  |
| 1   | A     | 294 | THR  |
| 1   | A     | 299 | LYS  |
| 1   | A     | 302 | ASN  |
| 1   | B     | 133 | LEU  |
| 1   | B     | 143 | LEU  |
| 1   | B     | 145 | ASP  |
| 1   | B     | 157 | SER  |
| 1   | B     | 169 | VAL  |
| 1   | B     | 174 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 179 | ASP  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 204 | GLU  |
| 1   | B     | 205 | ILE  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 210 | ILE  |
| 1   | B     | 214 | MET  |
| 1   | B     | 224 | GLU  |
| 1   | B     | 237 | TRP  |
| 1   | B     | 238 | THR  |
| 1   | B     | 240 | ASP  |
| 1   | B     | 262 | LYS  |
| 1   | B     | 263 | ILE  |
| 1   | B     | 269 | VAL  |
| 1   | B     | 271 | ARG  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 275 | ILE  |
| 1   | B     | 276 | ILE  |
| 1   | B     | 285 | ARG  |
| 1   | C     | 143 | LEU  |
| 1   | C     | 145 | ASP  |
| 1   | C     | 149 | LEU  |
| 1   | C     | 162 | SER  |
| 1   | C     | 164 | THR  |
| 1   | C     | 167 | GLU  |
| 1   | C     | 170 | GLN  |
| 1   | C     | 171 | ARG  |
| 1   | C     | 188 | GLU  |
| 1   | C     | 198 | ILE  |
| 1   | C     | 199 | LEU  |
| 1   | C     | 203 | LEU  |
| 1   | C     | 206 | ARG  |
| 1   | C     | 228 | ILE  |
| 1   | C     | 235 | GLU  |
| 1   | C     | 238 | THR  |
| 1   | C     | 262 | LYS  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 269 | VAL  |
| 1   | C     | 275 | ILE  |
| 1   | C     | 287 | LYS  |
| 1   | C     | 306 | GLU  |
| 1   | C     | 308 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 132 | GLN  |
| 1   | D     | 133 | LEU  |
| 1   | D     | 137 | ARG  |
| 1   | D     | 143 | LEU  |
| 1   | D     | 145 | ASP  |
| 1   | D     | 146 | ILE  |
| 1   | D     | 156 | ASP  |
| 1   | D     | 169 | VAL  |
| 1   | D     | 174 | ARG  |
| 1   | D     | 176 | ILE  |
| 1   | D     | 189 | GLN  |
| 1   | D     | 197 | PRO  |
| 1   | D     | 204 | GLU  |
| 1   | D     | 206 | ARG  |
| 1   | D     | 214 | MET  |
| 1   | D     | 237 | TRP  |
| 1   | D     | 242 | THR  |
| 1   | D     | 251 | GLN  |
| 1   | D     | 262 | LYS  |
| 1   | D     | 271 | ARG  |
| 1   | D     | 272 | ASN  |
| 1   | D     | 273 | LEU  |
| 1   | D     | 275 | ILE  |
| 1   | D     | 276 | ILE  |
| 1   | D     | 277 | ILE  |
| 1   | D     | 285 | ARG  |
| 1   | D     | 299 | LYS  |
| 1   | E     | 143 | LEU  |
| 1   | E     | 145 | ASP  |
| 1   | E     | 149 | LEU  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 164 | THR  |
| 1   | E     | 169 | VAL  |
| 1   | E     | 174 | ARG  |
| 1   | E     | 183 | VAL  |
| 1   | E     | 198 | ILE  |
| 1   | E     | 208 | LEU  |
| 1   | E     | 210 | ILE  |
| 1   | E     | 211 | ILE  |
| 1   | E     | 226 | THR  |
| 1   | E     | 248 | SER  |
| 1   | E     | 263 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 265 | VAL  |
| 1   | E     | 272 | ASN  |
| 1   | E     | 275 | ILE  |
| 1   | E     | 283 | ASN  |
| 1   | E     | 294 | THR  |
| 1   | E     | 298 | GLU  |
| 1   | F     | 143 | LEU  |
| 1   | F     | 144 | VAL  |
| 1   | F     | 145 | ASP  |
| 1   | F     | 149 | LEU  |
| 1   | F     | 170 | GLN  |
| 1   | F     | 174 | ARG  |
| 1   | F     | 187 | ASP  |
| 1   | F     | 189 | GLN  |
| 1   | F     | 191 | ILE  |
| 1   | F     | 198 | ILE  |
| 1   | F     | 199 | LEU  |
| 1   | F     | 202 | LEU  |
| 1   | F     | 208 | LEU  |
| 1   | F     | 211 | ILE  |
| 1   | F     | 214 | MET  |
| 1   | F     | 215 | ASN  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 272 | ASN  |
| 1   | F     | 304 | LEU  |
| 1   | F     | 306 | GLU  |
| 1   | G     | 138 | SER  |
| 1   | G     | 143 | LEU  |
| 1   | G     | 145 | ASP  |
| 1   | G     | 149 | LEU  |
| 1   | G     | 156 | ASP  |
| 1   | G     | 161 | LYS  |
| 1   | G     | 164 | THR  |
| 1   | G     | 169 | VAL  |
| 1   | G     | 191 | ILE  |
| 1   | G     | 198 | ILE  |
| 1   | G     | 205 | ILE  |
| 1   | G     | 229 | SER  |
| 1   | G     | 265 | VAL  |
| 1   | G     | 269 | VAL  |
| 1   | G     | 275 | ILE  |
| 1   | G     | 288 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 298 | GLU  |
| 1   | G     | 304 | LEU  |
| 1   | G     | 305 | ILE  |
| 1   | G     | 306 | GLU  |
| 1   | G     | 307 | HIS  |
| 1   | H     | 143 | LEU  |
| 1   | H     | 145 | ASP  |
| 1   | H     | 146 | ILE  |
| 1   | H     | 149 | LEU  |
| 1   | H     | 156 | ASP  |
| 1   | H     | 163 | GLU  |
| 1   | H     | 169 | VAL  |
| 1   | H     | 179 | ASP  |
| 1   | H     | 183 | VAL  |
| 1   | H     | 187 | ASP  |
| 1   | H     | 189 | GLN  |
| 1   | H     | 206 | ARG  |
| 1   | H     | 214 | MET  |
| 1   | H     | 252 | THR  |
| 1   | H     | 272 | ASN  |
| 1   | H     | 275 | ILE  |
| 1   | H     | 276 | ILE  |
| 1   | H     | 301 | LEU  |
| 1   | H     | 304 | LEU  |
| 1   | H     | 305 | ILE  |
| 1   | H     | 310 | GLU  |
| 1   | I     | 135 | GLU  |
| 1   | I     | 142 | VAL  |
| 1   | I     | 143 | LEU  |
| 1   | I     | 144 | VAL  |
| 1   | I     | 145 | ASP  |
| 1   | I     | 159 | VAL  |
| 1   | I     | 169 | VAL  |
| 1   | I     | 170 | GLN  |
| 1   | I     | 180 | ARG  |
| 1   | I     | 198 | ILE  |
| 1   | I     | 199 | LEU  |
| 1   | I     | 200 | SER  |
| 1   | I     | 203 | LEU  |
| 1   | I     | 254 | LEU  |
| 1   | I     | 257 | ASP  |
| 1   | I     | 263 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 271 | ARG  |
| 1   | I     | 275 | ILE  |
| 1   | I     | 287 | LYS  |
| 1   | I     | 301 | LEU  |
| 1   | I     | 303 | HIS  |
| 1   | I     | 304 | LEU  |
| 1   | J     | 143 | LEU  |
| 1   | J     | 145 | ASP  |
| 1   | J     | 169 | VAL  |
| 1   | J     | 170 | GLN  |
| 1   | J     | 174 | ARG  |
| 1   | J     | 180 | ARG  |
| 1   | J     | 186 | GLN  |
| 1   | J     | 187 | ASP  |
| 1   | J     | 188 | GLU  |
| 1   | J     | 210 | ILE  |
| 1   | J     | 214 | MET  |
| 1   | J     | 237 | TRP  |
| 1   | J     | 238 | THR  |
| 1   | J     | 240 | ASP  |
| 1   | J     | 250 | GLU  |
| 1   | J     | 251 | GLN  |
| 1   | J     | 254 | LEU  |
| 1   | J     | 256 | PHE  |
| 1   | J     | 262 | LYS  |
| 1   | J     | 263 | ILE  |
| 1   | J     | 265 | VAL  |
| 1   | J     | 276 | ILE  |
| 1   | J     | 277 | ILE  |
| 1   | J     | 296 | THR  |
| 1   | J     | 301 | LEU  |
| 1   | J     | 304 | LEU  |
| 1   | J     | 307 | HIS  |
| 1   | J     | 312 | ASP  |
| 1   | K     | 135 | GLU  |
| 1   | K     | 136 | ARG  |
| 1   | K     | 143 | LEU  |
| 1   | K     | 145 | ASP  |
| 1   | K     | 162 | SER  |
| 1   | K     | 164 | THR  |
| 1   | K     | 169 | VAL  |
| 1   | K     | 179 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 186 | GLN  |
| 1   | K     | 187 | ASP  |
| 1   | K     | 189 | GLN  |
| 1   | K     | 191 | ILE  |
| 1   | K     | 206 | ARG  |
| 1   | K     | 208 | LEU  |
| 1   | K     | 223 | ARG  |
| 1   | K     | 235 | GLU  |
| 1   | K     | 250 | GLU  |
| 1   | K     | 254 | LEU  |
| 1   | K     | 263 | ILE  |
| 1   | K     | 265 | VAL  |
| 1   | K     | 269 | VAL  |
| 1   | K     | 275 | ILE  |
| 1   | K     | 298 | GLU  |
| 1   | K     | 299 | LYS  |
| 1   | K     | 304 | LEU  |
| 1   | L     | 143 | LEU  |
| 1   | L     | 145 | ASP  |
| 1   | L     | 159 | VAL  |
| 1   | L     | 169 | VAL  |
| 1   | L     | 170 | GLN  |
| 1   | L     | 179 | ASP  |
| 1   | L     | 182 | ASP  |
| 1   | L     | 183 | VAL  |
| 1   | L     | 186 | GLN  |
| 1   | L     | 188 | GLU  |
| 1   | L     | 189 | GLN  |
| 1   | L     | 198 | ILE  |
| 1   | L     | 203 | LEU  |
| 1   | L     | 206 | ARG  |
| 1   | L     | 208 | LEU  |
| 1   | L     | 211 | ILE  |
| 1   | L     | 215 | ASN  |
| 1   | L     | 230 | LEU  |
| 1   | L     | 235 | GLU  |
| 1   | L     | 254 | LEU  |
| 1   | L     | 256 | PHE  |
| 1   | L     | 263 | ILE  |
| 1   | L     | 265 | VAL  |
| 1   | L     | 267 | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 140 | HIS  |
| 1   | A     | 170 | GLN  |
| 1   | A     | 189 | GLN  |
| 1   | A     | 215 | ASN  |
| 1   | A     | 283 | ASN  |
| 1   | A     | 307 | HIS  |
| 1   | B     | 132 | GLN  |
| 1   | B     | 140 | HIS  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 251 | GLN  |
| 1   | B     | 283 | ASN  |
| 1   | B     | 300 | ASN  |
| 1   | B     | 307 | HIS  |
| 1   | B     | 308 | ASN  |
| 1   | C     | 170 | GLN  |
| 1   | C     | 283 | ASN  |
| 1   | D     | 251 | GLN  |
| 1   | D     | 283 | ASN  |
| 1   | D     | 300 | ASN  |
| 1   | D     | 303 | HIS  |
| 1   | D     | 307 | HIS  |
| 1   | E     | 251 | GLN  |
| 1   | E     | 272 | ASN  |
| 1   | E     | 283 | ASN  |
| 1   | E     | 300 | ASN  |
| 1   | F     | 140 | HIS  |
| 1   | F     | 215 | ASN  |
| 1   | F     | 272 | ASN  |
| 1   | F     | 283 | ASN  |
| 1   | G     | 140 | HIS  |
| 1   | G     | 186 | GLN  |
| 1   | G     | 201 | HIS  |
| 1   | G     | 272 | ASN  |
| 1   | G     | 283 | ASN  |
| 1   | G     | 300 | ASN  |
| 1   | H     | 189 | GLN  |
| 1   | H     | 272 | ASN  |
| 1   | H     | 283 | ASN  |
| 1   | I     | 140 | HIS  |
| 1   | I     | 186 | GLN  |
| 1   | I     | 215 | ASN  |
| 1   | I     | 233 | HIS  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 251 | GLN  |
| 1   | I     | 300 | ASN  |
| 1   | J     | 140 | HIS  |
| 1   | J     | 170 | GLN  |
| 1   | J     | 186 | GLN  |
| 1   | J     | 272 | ASN  |
| 1   | J     | 283 | ASN  |
| 1   | J     | 303 | HIS  |
| 1   | K     | 140 | HIS  |
| 1   | K     | 272 | ASN  |
| 1   | K     | 283 | ASN  |
| 1   | K     | 300 | ASN  |
| 1   | K     | 308 | ASN  |
| 1   | L     | 186 | GLN  |
| 1   | L     | 201 | HIS  |
| 1   | L     | 272 | ASN  |
| 1   | L     | 283 | ASN  |
| 1   | L     | 300 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 161/205 (78%)   | -1.55  | 0 100 100 | 23, 53, 79, 88        | 0     |
| 1   | B     | 181/205 (88%)   | -1.54  | 0 100 100 | 22, 44, 85, 98        | 0     |
| 1   | C     | 164/205 (80%)   | -1.48  | 0 100 100 | 30, 54, 89, 102       | 0     |
| 1   | D     | 181/205 (88%)   | -1.51  | 0 100 100 | 23, 43, 85, 101       | 0     |
| 1   | E     | 164/205 (80%)   | -1.53  | 0 100 100 | 27, 51, 78, 91        | 0     |
| 1   | F     | 160/205 (78%)   | -1.52  | 0 100 100 | 32, 52, 89, 98        | 0     |
| 1   | G     | 160/205 (78%)   | -1.52  | 0 100 100 | 23, 51, 78, 84        | 0     |
| 1   | H     | 178/205 (86%)   | -1.55  | 0 100 100 | 21, 43, 81, 101       | 0     |
| 1   | I     | 160/205 (78%)   | -1.49  | 0 100 100 | 33, 54, 86, 97        | 0     |
| 1   | J     | 178/205 (86%)   | -1.54  | 0 100 100 | 23, 43, 82, 100       | 0     |
| 1   | K     | 162/205 (79%)   | -1.54  | 0 100 100 | 21, 52, 78, 82        | 0     |
| 1   | L     | 161/205 (78%)   | -1.51  | 0 100 100 | 30, 54, 87, 106       | 0     |
| All | All   | 2010/2460 (81%) | -1.52  | 0 100 100 | 21, 50, 85, 106       | 0     |

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

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.