



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 AM GMT

PDB ID : 2QMH  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

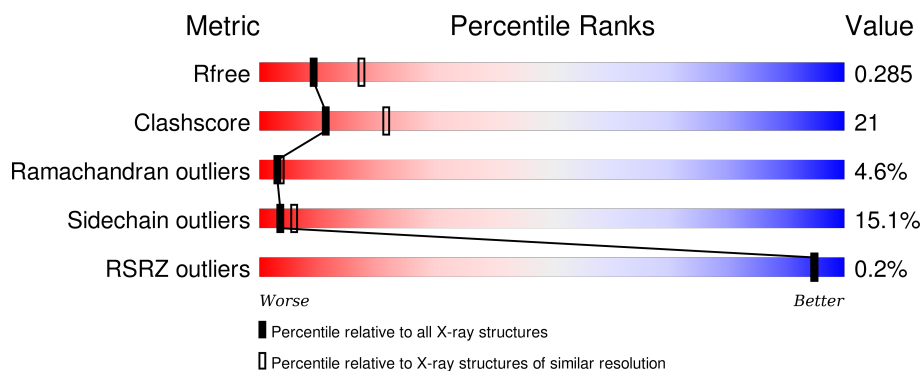
# 1 Overall quality at a glance i

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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 2328 (2.60-2.60)                                      |
| Clashscore            | 102246                      | 2679 (2.60-2.60)                                      |
| Ramachandran outliers | 100387                      | 2635 (2.60-2.60)                                      |
| Sidechain outliers    | 100360                      | 2635 (2.60-2.60)                                      |
| RSRZ outliers         | 91569                       | 2334 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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    | <div> <div style="width: 46%; background-color: red;"></div> <div style="width: 24%; background-color: orange;"></div> <div style="width: 7%; background-color: yellow;"></div> <div style="width: 21%; background-color: green;"></div> </div> |
| 1   | B     | 205    | <div> <div style="width: 55%; background-color: red;"></div> <div style="width: 27%; background-color: orange;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 12%; background-color: green;"></div> </div> |
| 1   | C     | 205    | <div> <div style="width: 50%; background-color: red;"></div> <div style="width: 24%; background-color: orange;"></div> <div style="width: 6%; background-color: yellow;"></div> <div style="width: 20%; background-color: green;"></div> </div> |
| 1   | D     | 205    | <div> <div style="width: 54%; background-color: red;"></div> <div style="width: 25%; background-color: orange;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 12%; background-color: green;"></div> </div> |
| 1   | E     | 205    | <div> <div style="width: 41%; background-color: red;"></div> <div style="width: 33%; background-color: orange;"></div> <div style="width: 6%; background-color: yellow;"></div> <div style="width: 20%; background-color: green;"></div> </div> |

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| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|---|
| 1   | F     | 205    | <div><div></div><div>38%33%6%22%</div></div>  |
| 1   | G     | 205    | <div><div></div><div>42%26%9%22%</div></div>  |
| 1   | H     | 205    | <div><div></div><div>55%22%10%13%</div></div> |
| 1   | I     | 205    | <div><div></div><div>43%27%6%22%</div></div>  |
| 1   | J     | 205    | <div><div></div><div>54%23%9%13%</div></div>  |
| 1   | K     | 205    | <div><div></div><div>40%30%8%21%</div></div>  |
| 1   | L     | 205    | <div><div></div><div>%47%22%8%21%</div></div> |

## 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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     | 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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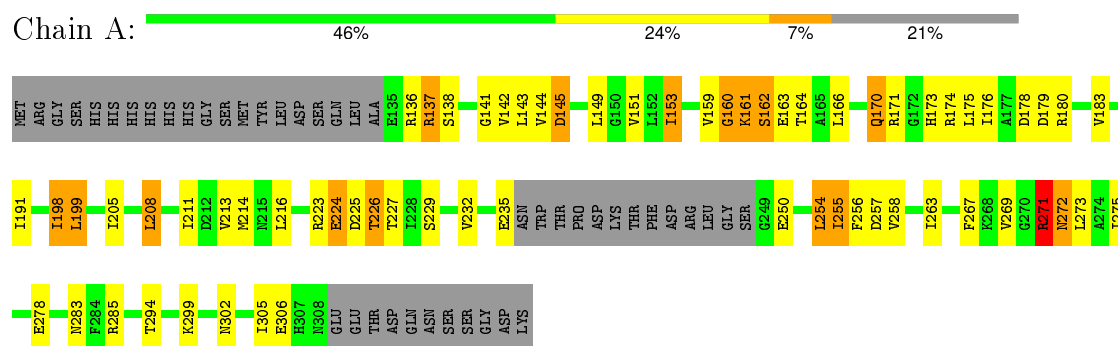
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2   | B     | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 2   | C     | 3        | Total<br>3  | 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       |

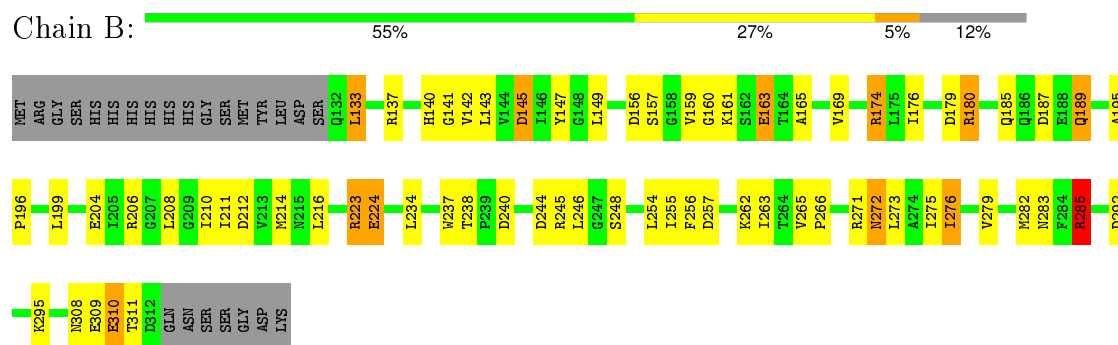
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

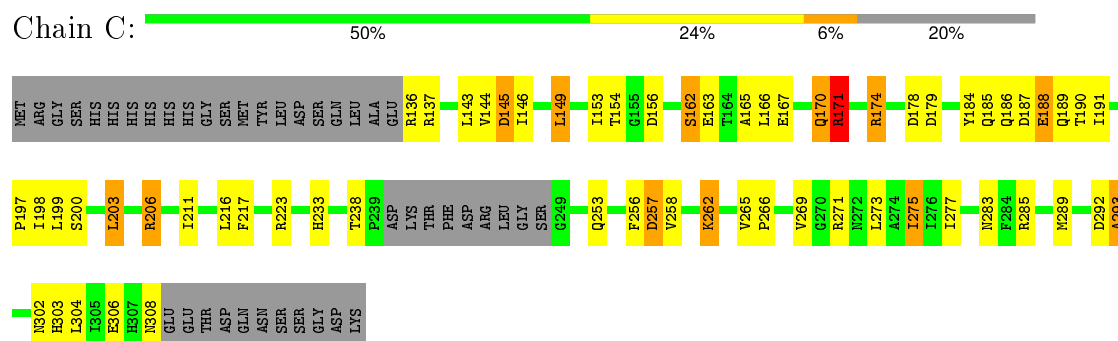
- Molecule 1: HPr kinase/phosphorylase



- Molecule 1: HPr kinase/phosphorylase



- Molecule 1: HPr kinase/phosphorylase



[illegible]

Chain E:

| Amino Acid | Category |
|------------|----------|
| Y184       | Green    |
| I263       | Green    |
| T264       | Green    |
| I265       | Green    |
| V265       | Green    |
| P266       | Green    |
| P267       | Green    |
| K268       | Green    |
| V269       | Green    |
| G270       | Green    |
| R271       | Green    |
| N272       | Green    |
| L273       | Green    |
| L274       | Green    |
| I275       | Green    |
| L276       | Green    |
| I277       | Green    |
| E278       | Green    |
| N283       | Green    |
| R284       | Green    |
| K285       | Green    |
| A286       | Green    |
| K287       | Green    |
| S288       | Green    |
| N289       | Green    |
| D292       | Green    |
| A293       | Green    |
| T294       | Green    |
| E298       | Green    |
| K299       | Green    |
| L304       | Green    |
| L305       | Green    |
| E309       | Green    |
| GLU        | Green    |
| THR        | Green    |
| ASP        | Green    |
| GLN        | Green    |
| GLU        | Green    |
| ASN        | Green    |
| SER        | Green    |
| SER        | Green    |
| GLY        | Green    |
| ASP        | Green    |
| LVS        | Green    |
| I185       | Yellow   |
| I186       | Yellow   |
| I187       | Yellow   |
| I188       | Yellow   |
| I189       | Yellow   |
| T190       | Yellow   |
| I191       | Yellow   |
| P196       | Yellow   |
| P197       | Yellow   |
| I198       | Yellow   |
| L199       | Yellow   |
| S200       | Yellow   |
| H201       | Yellow   |
| L202       | Yellow   |
| L203       | Yellow   |
| E204       | Yellow   |
| L205       | Yellow   |
| L208       | Yellow   |
| G209       | Yellow   |
| L210       | Yellow   |
| L211       | Yellow   |
| D212       | Yellow   |
| L216       | Yellow   |
| F217       | Yellow   |
| G220       | Yellow   |
| R223       | Yellow   |
| T226       | Yellow   |
| S229       | Yellow   |
| N236       | Yellow   |
| TRP        | Yellow   |
| THR        | Yellow   |
| PRO        | Yellow   |
| ASP        | Yellow   |
| LVS        | Yellow   |
| THR        | Yellow   |
| PHE        | Yellow   |
| ASP        | Yellow   |
| ARG        | Yellow   |
| LEU        | Yellow   |
| GLY        | Yellow   |
| S248       | Yellow   |
| G249       | Yellow   |
| E250       | Yellow   |
| Q251       | Yellow   |
| L254       | Yellow   |
| L255       | Yellow   |
| F256       | Yellow   |
| D257       | Yellow   |
| V262       | Yellow   |
| MET        | Orange   |
| ARG        | Orange   |
| GLY        | Orange   |
| SER        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| HIS        | Orange   |
| GLY        | Orange   |
| SER        | Orange   |
| MET        | Orange   |
| THR        | Orange   |
| LEU        | Orange   |
| ASP        | Orange   |
| SER        | Orange   |
| SER        | Orange   |
| GLN        | Orange   |
| LEU        | Orange   |
| ALA        | Orange   |
| E135       | Orange   |
| R136       | Orange   |
| R137       | Orange   |
| S138       | Orange   |
| M139       | Orange   |
| V142       | Orange   |
| L143       | Orange   |
| W144       | Orange   |
| D145       | Orange   |
| L149       | Orange   |
| I153       | Orange   |
| D156       | Orange   |
| V159       | Orange   |
| K161       | Orange   |
| S162       | Orange   |
| E163       | Orange   |
| L164       | Orange   |
| A165       | Orange   |
| L166       | Orange   |
| Q170       | Orange   |
| R171       | Orange   |
| G172       | Orange   |
| H173       | Orange   |
| R174       | Orange   |
| L175       | Orange   |
| L176       | Orange   |
| L177       | Orange   |
| D178       | Orange   |
| D179       | Orange   |
| R180       | Orange   |
| V181       | Orange   |
| D182       | Orange   |
| V182       | Orange   |

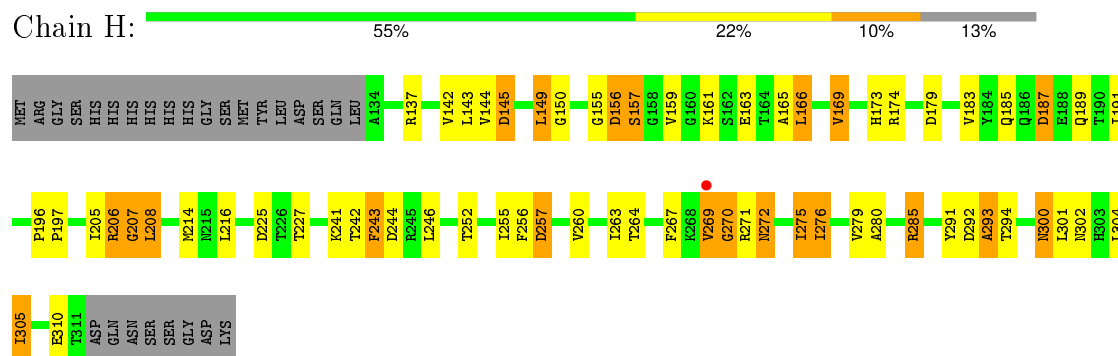
[illegible]

Chain G:

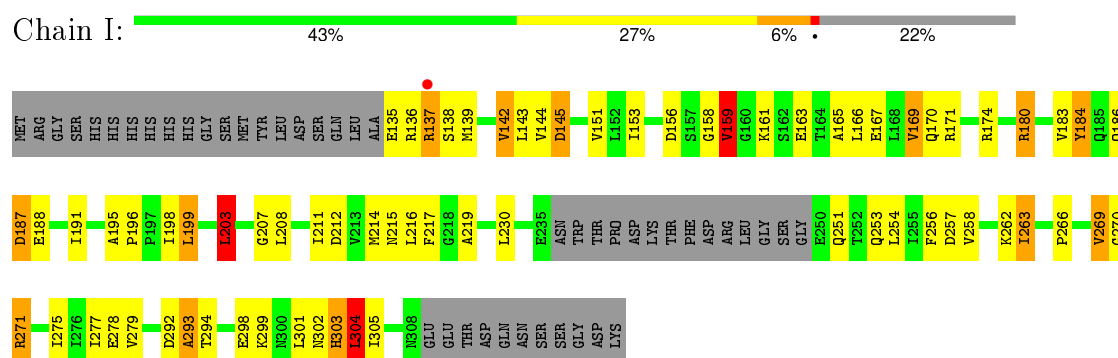
42% 26% 9% 22%

| Amino Acid | Category |
|------------|----------|
| Q185       | Green    |
| V269       | Green    |
| G186       | Green    |
| D270       | Green    |
| R271       | Green    |
| E188       | Green    |
| N272       | Green    |
| I275       | Green    |
| I276       | Green    |
| V279       | Green    |
| P196       | Green    |
| N282       | Green    |
| N283       | Green    |
| A286       | Green    |
| K287       | Green    |
| S288       | Green    |
| N289       | Green    |
| D292       | Green    |
| A293       | Green    |
| E298       | Green    |
| L304       | Green    |
| I305       | Green    |
| E306       | Green    |
| H307       | Green    |
| N308       | Green    |
| GLU        | Green    |
| GLU        | Green    |
| THR        | Green    |
| ASP        | Green    |
| GLN        | Green    |
| ASN        | Green    |
| SER        | Green    |
| SER        | Green    |
| GLY        | Green    |
| ASP        | Green    |
| LYS        | Green    |
| D187       | Yellow   |
| E188       | Yellow   |
| I189       | Yellow   |
| T190       | Yellow   |
| I191       | Yellow   |
| V192       | Yellow   |
| P197       | Yellow   |
| I198       | Yellow   |
| L199       | Yellow   |
| S200       | Yellow   |
| L203       | Yellow   |
| E204       | Yellow   |
| T205       | Yellow   |
| R206       | Yellow   |
| G207       | Yellow   |
| L208       | Yellow   |
| T211       | Yellow   |
| D212       | Yellow   |
| N215       | Yellow   |
| L216       | Yellow   |
| F217       | Yellow   |
| G220       | Yellow   |
| T226       | Yellow   |
| T227       | Yellow   |
| T228       | Yellow   |
| S229       | Yellow   |
| E236       | Yellow   |
| ASN        | Yellow   |
| TRP        | Yellow   |
| THR        | Yellow   |
| PRO        | Yellow   |
| ASP        | Yellow   |
| LYS        | Yellow   |
| THR        | Yellow   |
| PHE        | Yellow   |
| ASP        | Yellow   |
| ARG        | Yellow   |
| LEU        | Yellow   |
| GLY        | Yellow   |
| SER        | Yellow   |
| GLY        | Yellow   |
| E250       | Yellow   |
| Q251       | Yellow   |
| L254       | Yellow   |
| F256       | Yellow   |
| V268       | Yellow   |
| E135       | Orange   |
| R136       | Orange   |
| R137       | Orange   |
| S138       | Orange   |
| G141       | Orange   |
| V142       | Orange   |
| L143       | Orange   |
| V144       | Orange   |
| D145       | Orange   |
| I146       | Orange   |
| I147       | Orange   |
| G148       | Orange   |
| L149       | Orange   |
| G155       | Orange   |
| D156       | Orange   |
| S157       | Orange   |
| G158       | Orange   |
| V159       | Orange   |
| G160       | Orange   |
| K161       | Orange   |
| S162       | Orange   |
| E163       | Orange   |
| L166       | Orange   |
| Q170       | Orange   |
| H173       | Orange   |
| R174       | Orange   |
| L175       | Orange   |
| I176       | Orange   |
| A177       | Orange   |
| D178       | Orange   |
| D179       | Orange   |
| R180       | Orange   |
| V183       | Orange   |
| Y184       | Orange   |
| MET        | Grey     |
| ARG        | Grey     |
| GLY        | Grey     |
| SER        | Grey     |
| HIS        | Grey     |
| HIS        | Grey     |
| HIS        | Grey     |
| HIS        | Grey     |
| HIS        | Grey     |
| GLY        | Grey     |
| GLY        | Grey     |
| SER        | Grey     |
| MET        | Grey     |
| TVR        | Grey     |
| LEU        | Grey     |
| ASP        | Grey     |
| SER        | Grey     |
| GLN        | Grey     |
| LEU        | Grey     |
| ALA        | Grey     |
| G155       | Grey     |
| D156       | Grey     |
| S157       | Grey     |
| G158       | Grey     |
| V159       | Grey     |
| G160       | Grey     |
| K161       | Grey     |
| S162       | Grey     |
| E163       | Grey     |
| L166       | Grey     |
| Q170       | Grey     |
| H173       | Grey     |
| R174       | Grey     |
| L175       | Grey     |
| I176       | Grey     |
| A177       | Grey     |
| D178       | Grey     |
| D179       | Grey     |
| R180       | Grey     |
| V183       | Grey     |
| Y184       | Grey     |

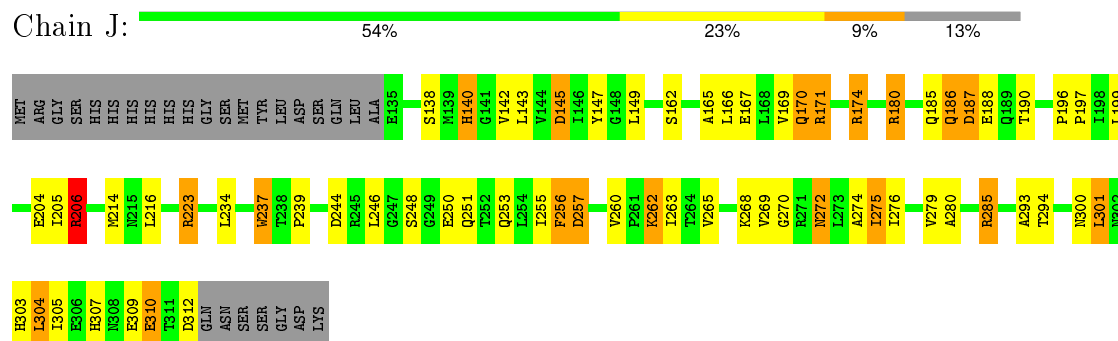
- Molecule 1: HPr kinase/phosphorylase



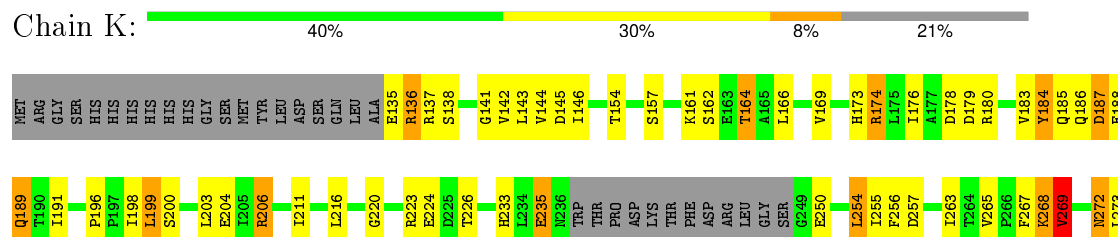
- Molecule 1: HPr kinase/phosphorylase

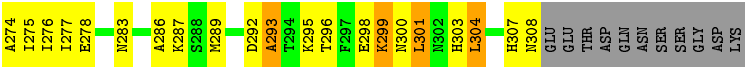


- Molecule 1: HPr kinase/phosphorylase

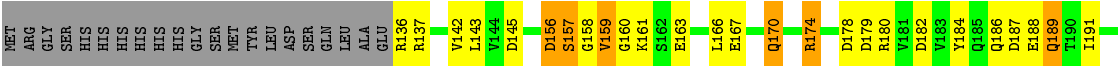


- Molecule 1: HPr kinase/phosphorylase





● Molecule 1: HPr kinase/phosphorylase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 69.06 Å   106.37 Å   106.49 Å<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>82.2 (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 2.59 Å)  | 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 (5.28%)  | DCC              |
| 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> ) | 0.30 , 12.7   | EDS              |
| 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          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$   | Xtriage          |
| Outliers  | 0 of 80370 reflections  | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$    | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.85         | 0/1259         | 0.96        | 1/1703 (0.1%)   |
| 1   | B     | 0.93         | 2/1427 (0.1%)  | 0.97        | 5/1934 (0.3%)   |
| 1   | C     | 0.85         | 0/1289         | 0.95        | 4/1747 (0.2%)   |
| 1   | D     | 0.94         | 0/1427         | 1.01        | 6/1934 (0.3%)   |
| 1   | E     | 0.83         | 0/1282         | 0.97        | 3/1734 (0.2%)   |
| 1   | F     | 0.85         | 0/1252         | 0.91        | 2/1695 (0.1%)   |
| 1   | G     | 0.86         | 0/1255         | 0.94        | 2/1698 (0.1%)   |
| 1   | H     | 0.94         | 0/1402         | 0.99        | 4/1900 (0.2%)   |
| 1   | I     | 0.79         | 1/1255 (0.1%)  | 0.88        | 2/1698 (0.1%)   |
| 1   | J     | 0.91         | 0/1405         | 1.03        | 6/1904 (0.3%)   |
| 1   | K     | 0.84         | 0/1267         | 0.92        | 0/1714          |
| 1   | L     | 0.84         | 1/1263 (0.1%)  | 0.95        | 1/1709 (0.1%)   |
| All | All   | 0.87         | 4/15783 (0.0%) | 0.96        | 36/21370 (0.2%) |

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 (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | L     | 206 | ARG  | CB-CG  | 5.35 | 1.67        | 1.52     |
| 1   | B     | 163 | GLU  | CG-CD  | 5.10 | 1.59        | 1.51     |
| 1   | I     | 217 | PHE  | CE1-CZ | 5.08 | 1.47        | 1.37     |
| 1   | B     | 224 | GLU  | CB-CG  | 5.04 | 1.61        | 1.52     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | B     | 149 | LEU  | CA-CB-CG   | 10.25 | 138.87      | 115.30   |
| 1   | C     | 171 | ARG  | NE-CZ-NH2  | -8.34 | 116.13      | 120.30   |
| 1   | D     | 285 | ARG  | NE-CZ-NH2  | -8.24 | 116.18      | 120.30   |
| 1   | J     | 285 | ARG  | NE-CZ-NH2  | -7.67 | 116.47      | 120.30   |
| 1   | E     | 285 | ARG  | NE-CZ-NH2  | -7.59 | 116.51      | 120.30   |
| 1   | J     | 166 | LEU  | CB-CG-CD2  | -7.57 | 98.13       | 111.00   |
| 1   | I     | 203 | LEU  | CA-CB-CG   | 7.54  | 132.65      | 115.30   |
| 1   | F     | 149 | LEU  | CA-CB-CG   | 7.14  | 131.72      | 115.30   |
| 1   | D     | 285 | ARG  | NE-CZ-NH1  | 7.07  | 123.84      | 120.30   |
| 1   | H     | 285 | ARG  | NE-CZ-NH1  | 6.91  | 123.75      | 120.30   |
| 1   | L     | 203 | LEU  | CA-CB-CG   | 6.83  | 131.00      | 115.30   |
| 1   | H     | 285 | ARG  | NE-CZ-NH2  | -6.38 | 117.11      | 120.30   |
| 1   | I     | 145 | ASP  | CB-CG-OD2  | 6.17  | 123.85      | 118.30   |
| 1   | F     | 145 | ASP  | CB-CG-OD2  | 6.09  | 123.78      | 118.30   |
| 1   | J     | 285 | ARG  | NE-CZ-NH1  | 6.07  | 123.34      | 120.30   |
| 1   | D     | 149 | LEU  | CA-CB-CG   | 6.00  | 129.11      | 115.30   |
| 1   | B     | 285 | ARG  | NE-CZ-NH1  | 5.81  | 123.21      | 120.30   |
| 1   | H     | 166 | LEU  | CB-CG-CD2  | -5.69 | 101.32      | 111.00   |
| 1   | C     | 171 | ARG  | NE-CZ-NH1  | 5.64  | 123.12      | 120.30   |
| 1   | A     | 199 | LEU  | CA-CB-CG   | 5.64  | 128.27      | 115.30   |
| 1   | C     | 149 | LEU  | CA-CB-CG   | 5.61  | 128.21      | 115.30   |
| 1   | E     | 292 | ASP  | CB-CG-OD2  | 5.58  | 123.32      | 118.30   |
| 1   | D     | 246 | LEU  | CB-CG-CD1  | -5.55 | 101.57      | 111.00   |
| 1   | G     | 203 | LEU  | CA-CB-CG   | 5.47  | 127.89      | 115.30   |
| 1   | B     | 223 | ARG  | NE-CZ-NH2  | -5.38 | 117.61      | 120.30   |
| 1   | D     | 246 | LEU  | CA-CB-CG   | 5.24  | 127.34      | 115.30   |
| 1   | J     | 275 | ILE  | CG1-CB-CG2 | -5.23 | 99.89       | 111.40   |
| 1   | B     | 149 | LEU  | CB-CG-CD1  | -5.23 | 102.12      | 111.00   |
| 1   | H     | 149 | LEU  | CA-CB-CG   | 5.21  | 127.29      | 115.30   |
| 1   | E     | 212 | ASP  | CB-CG-OD2  | 5.19  | 122.97      | 118.30   |
| 1   | B     | 285 | ARG  | NE-CZ-NH2  | -5.17 | 117.71      | 120.30   |
| 1   | D     | 208 | LEU  | CA-CB-CG   | 5.14  | 127.11      | 115.30   |
| 1   | J     | 223 | ARG  | NE-CZ-NH2  | -5.13 | 117.73      | 120.30   |
| 1   | G     | 254 | LEU  | CA-CB-CG   | 5.11  | 127.05      | 115.30   |
| 1   | C     | 145 | ASP  | CB-CG-OD2  | 5.07  | 122.86      | 118.30   |
| 1   | J     | 171 | ARG  | NE-CZ-NH2  | -5.04 | 117.78      | 120.30   |

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     | 60      | 0            |
| 1   | B     | 1405  | 0        | 1415     | 54      | 0            |
| 1   | C     | 1269  | 0        | 1292     | 49      | 0            |
| 1   | D     | 1405  | 0        | 1415     | 58      | 0            |
| 1   | E     | 1265  | 0        | 1285     | 64      | 0            |
| 1   | F     | 1235  | 0        | 1258     | 69      | 0            |
| 1   | G     | 1238  | 0        | 1265     | 56      | 0            |
| 1   | H     | 1380  | 0        | 1392     | 53      | 0            |
| 1   | I     | 1238  | 0        | 1265     | 53      | 0            |
| 1   | J     | 1383  | 0        | 1391     | 49      | 0            |
| 1   | K     | 1250  | 0        | 1274     | 70      | 0            |
| 1   | L     | 1246  | 0        | 1271     | 59      | 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            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 3     | 0        | 0        | 0       | 0            |
| All | All   | 15591 | 0        | 15791    | 646     | 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 21.

All (646) 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:HD2  | 1:L:206:ARG:H    | 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              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:206:ARG:HD3  | 1:C:206:ARG:H    | 1.24                     | 0.99              |
| 1:I:137:ARG:HG2  | 1:I:138:SER:H    | 1.30                     | 0.96              |
| 1:G:267:PHE:CE2  | 1:G:271:ARG:HB3  | 2.00                     | 0.96              |
| 1:G:198:ILE:HG13 | 1:G:199:LEU:N    | 1.83                     | 0.94              |
| 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: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:L:235:GLU:O    | 1:L:267:PHE:HB3  | 1.74                     | 0.87              |
| 1:A:223:ARG:O    | 1:A:224:GLU:CB   | 2.23                     | 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: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              |
| 1:B:140:HIS:CE1  | 1:B:180:ARG:NH1  | 2.48                     | 0.81              |
| 1:L:272:ASN:OD1  | 1:L:275:ILE:HG12 | 1.81                     | 0.81              |
| 1:A:205:ILE:HB   | 1:A:208:LEU:HD11 | 1.60                     | 0.81              |
| 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:HH21 | 1:K:206:ARG:HG2  | 1.49                     | 0.78              |
| 1:L:211:ILE:HD13 | 1:L:216:LEU:HD12 | 1.66                     | 0.77              |
| 1:F:272:ASN:C    | 1:F:272:ASN:HD22 | 1.88                     | 0.77              |
| 1:C:206:ARG:CD   | 1:C:206:ARG:H    | 1.92                     | 0.77              |
| 1:K:211:ILE:HG22 | 1:L:283:ASN:ND2  | 2.00                     | 0.77              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:K:191:ILE:CD1  | 1:K:255:ILE:HB   | 2.16                     | 0.75              |
| 1:F:292:ASP:O    | 1:F:293:ALA:HB3  | 1.86                     | 0.75              |
| 1:K:136:ARG:CG   | 1:K:136:ARG:HH11 | 1.99                     | 0.75              |
| 1:I:303:HIS:C    | 1:I:305:ILE:H    | 1.90                     | 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:HG2  | 1:K:189:GLN:O    | 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: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:K:254:LEU:CD2  | 1:K:257:ASP:HA   | 2.20                     | 0.72              |
| 1:J:216:LEU:HD21 | 1:K:283:ASN:HD22 | 1.53                     | 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:D:253:GLN:HB2  | 1:D:262:LYS:HZ1  | 1.54                     | 0.71              |
| 1:B:271:ARG:HD2  | 1:C:163:GLU:OE1  | 1.90                     | 0.71              |
| 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:H:291:TYR:HB3  | 1:I:215:ASN:ND2  | 2.08                     | 0.69              |
| 1:E:185:GLN:OE1  | 1:E:256:PHE:HB3  | 1.93                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:A:272:ASN:C    | 1:A:272:ASN:HD22 | 1.97                     | 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: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:I:203:LEU:HD22 | 1:I:211:ILE:CD1  | 2.26                     | 0.66              |
| 1:E:198:ILE:CG1  | 1:E:199:LEU:N    | 2.59                     | 0.66              |
| 1:K:180:ARG:NH2  | 1:K:199:LEU:CD1  | 2.59                     | 0.66              |
| 1:H:302:ASN:CA   | 1:H:305:ILE:HG22 | 2.24                     | 0.66              |
| 1:C:292:ASP:O    | 1:C:293:ALA:HB3  | 1.96                     | 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:K:183:VAL:O    | 1:K:184:TYR:HB3  | 1.95                     | 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              |
| 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:I:137:ARG:HG2  | 1:I:138:SER:N    | 2.09                     | 0.65              |
| 1:C:154:THR:O    | 1:C:233:HIS:HA   | 1.97                     | 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:H:302:ASN:HA   | 1:H:305:ILE:CG2  | 2.24                     | 0.64              |
| 1:B:271:ARG:HG3  | 1:B:272:ASN:N    | 2.12                     | 0.64              |
| 1:K:154:THR:O    | 1:K:233:HIS:HA   | 1.97                     | 0.63              |
| 1:G:286:ALA:HA   | 1:G:289:MET:HE2  | 1.79                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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: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:B:256:PHE:O    | 1:B:257:ASP:HB2  | 1.98                     | 0.62              |
| 1:A:305:ILE:HG22 | 1:A:306:GLU:HG3  | 1.80                     | 0.62              |
| 1:E:170:GLN:HG2  | 1:E:217:PHE:CE2  | 2.34                     | 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:K:185:GLN:HE21 | 1:K:188:GLU:HA   | 1.65                     | 0.61              |
| 1:H:272:ASN:C    | 1:H:272:ASN:HD22 | 2.02                     | 0.61              |
| 1:H:191:ILE:CD1  | 1:H:255:ILE:HB   | 2.31                     | 0.61              |
| 1:E:188:GLU:O    | 1:E:189:GLN:HG2  | 2.01                     | 0.61              |
| 1:K:166:LEU:HD21 | 1:L:279:VAL:HG21 | 1.83                     | 0.61              |
| 1:F:137:ARG:HB2  | 1:F:256:PHE:CE1  | 2.36                     | 0.61              |
| 1:K:180:ARG:NH2  | 1:K:199:LEU:HD13 | 2.15                     | 0.61              |
| 1:C:136:ARG:HA   | 1:C:256:PHE:CZ   | 2.35                     | 0.61              |
| 1:D:309:GLU:C    | 1:D:311:THR:H    | 2.04                     | 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:H:144:VAL:HG22 | 1:H:145:ASP:N    | 2.15                     | 0.60              |
| 1:B:234:LEU:HD23 | 1:B:265:VAL:HG23 | 1.83                     | 0.60              |
| 1:G:180:ARG:HH21 | 1:G:199:LEU:HD13 | 1.66                     | 0.60              |
| 1:D:237:TRP:HZ3  | 1:D:239:PRO:HB3  | 1.66                     | 0.60              |
| 1:F:214:MET:HG3  | 1:F:222:VAL:HG21 | 1.82                     | 0.60              |
| 1:G:292:ASP:O    | 1:G:293:ALA:HB3  | 2.01                     | 0.60              |
| 1:D:301:LEU:O    | 1:D:305:ILE:HG13 | 2.02                     | 0.60              |
| 1:I:303:HIS:C    | 1:I:305:ILE:N    | 2.54                     | 0.60              |
| 1:J:246:LEU:HD13 | 1:J:248:SER:OG   | 2.02                     | 0.60              |
| 1:G:157:SER:O    | 1:G:160:GLY:HA3  | 2.01                     | 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:H:159:VAL:HG12 | 1:H:267:PHE:CD2  | 2.37                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 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:K:185:GLN:NE2  | 1:K:188:GLU:HA   | 2.18                     | 0.58              |
| 1:J:272:ASN:OD1  | 1:J:275:ILE:HG12 | 2.02                     | 0.58              |
| 1:F:156:ASP:CG   | 1:F:157:SER:H    | 2.05                     | 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:HG3  | 1:K:136:ARG:HH11 | 1.68                     | 0.58              |
| 1:K:198:ILE:HG22 | 1:K:199:LEU:N    | 2.19                     | 0.58              |
| 1:K:206:ARG:HG2  | 1:K:206:ARG:NH2  | 2.15                     | 0.58              |
| 1:A:136:ARG:HG2  | 1:A:137:ARG:H    | 1.68                     | 0.58              |
| 1:G:272:ASN:O    | 1:G:276:ILE:HG12 | 2.03                     | 0.58              |
| 1:D:244:ASP:OD2  | 1:D:246:LEU:O    | 2.21                     | 0.58              |
| 1:H:263:ILE:CD1  | 1:I:207:GLY:O    | 2.51                     | 0.58              |
| 1:E:272:ASN:O    | 1:E:276:ILE:HG12 | 2.03                     | 0.58              |
| 1:J:256:PHE:O    | 1:J:257:ASP:CB   | 2.46                     | 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:E:272:ASN:C    | 1:E:272:ASN:HD22 | 2.08                     | 0.57              |
| 1:H:300:ASN:HB2  | 1:I:199:LEU:HD21 | 1.86                     | 0.57              |
| 1:B:145:ASP:CG   | 1:B:174:ARG:HH21 | 2.08                     | 0.57              |
| 1:D:242:THR:HG23 | 1:D:243:PHE:N    | 2.18                     | 0.57              |
| 1:A:216:LEU:HD21 | 1:C:283:ASN:HD22 | 1.69                     | 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:I:211:ILE:C    | 1:I:211:ILE:HD12 | 2.25                     | 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:B:271:ARG:CD   | 1:C:163:GLU:OE1  | 2.52                     | 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:NH1  | 1:K:136:ARG:CG   | 2.66                     | 0.56              |
| 1:L:267:PHE:HD1  | 1:L:267:PHE:C    | 2.09                     | 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:L:272:ASN:CG   | 1:L:275:ILE:HG12 | 2.26                     | 0.56              |
| 1:E:143:LEU:HD13 | 1:E:176:ILE:HB   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:178:ASP:OD2  | 1:A:179:ASP:N    | 2.39                     | 0.56              |
| 1:C:206:ARG:HD3  | 1:C:206:ARG:N    | 2.08                     | 0.56              |
| 1:B:187:ASP:C    | 1:B:187:ASP:OD2  | 2.45                     | 0.56              |
| 1:G:185:GLN:OE1  | 1:G:256:PHE:HB3  | 2.06                     | 0.56              |
| 1:D:149:LEU:HD22 | 1:D:229:SER:CB   | 2.36                     | 0.55              |
| 1:K:307:HIS:ND1  | 1:K:307:HIS:O    | 2.38                     | 0.55              |
| 1:F:159:VAL:HG13 | 1:F:159:VAL:O    | 2.06                     | 0.55              |
| 1:B:309:GLU:C    | 1:B:311:THR:H    | 2.08                     | 0.55              |
| 1:B:279:VAL:HG21 | 1:C:166:LEU:HD21 | 1.88                     | 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:B:204:GLU:OE1  | 1:B:206:ARG:HG3  | 2.06                     | 0.55              |
| 1:L:160:GLY:HA3  | 1:L:206:ARG:HH22 | 1.70                     | 0.55              |
| 1:A:176:ILE:HD11 | 1:A:226:THR:OG1  | 2.06                     | 0.55              |
| 1:B:137:ARG:NH1  | 1:B:255:ILE:HA   | 2.19                     | 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:H:207:GLY:O    | 1:H:208:LEU:HB2  | 2.07                     | 0.55              |
| 1:D:185:GLN:OE1  | 1:D:256:PHE:O    | 2.24                     | 0.54              |
| 1:K:199:LEU:H    | 1:K:199:LEU:HD12 | 1.73                     | 0.54              |
| 1:C:256:PHE:O    | 1:C:257:ASP:CB   | 2.55                     | 0.54              |
| 1:D:237:TRP:CZ3  | 1:D:239:PRO:HB3  | 2.42                     | 0.54              |
| 1:A:211:ILE:HD12 | 1:A:216:LEU:HD12 | 1.89                     | 0.54              |
| 1:L:174:ARG:HG2  | 1:L:223:ARG:HB2  | 1.90                     | 0.54              |
| 1:I:163:GLU:OE2  | 1:I:163:GLU:N    | 2.38                     | 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: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:D:196:PRO:HG2  | 1:D:199:LEU:HD12 | 1.89                     | 0.54              |
| 1:G:180:ARG:HH21 | 1:G:199:LEU:HD11 | 1.73                     | 0.54              |
| 1:E:136:ARG:HH11 | 1:E:136:ARG:HG3  | 1.71                     | 0.54              |
| 1:H:155:GLY:O    | 1:H:159:VAL:HG21 | 2.08                     | 0.54              |
| 1:D:263:ILE:CG2  | 1:D:264:THR:N    | 2.70                     | 0.54              |
| 1:L:256:PHE:O    | 1:L:257:ASP:CB   | 2.54                     | 0.54              |
| 1:F:235:GLU:HB3  | 1:F:266:PRO:HA   | 1.89                     | 0.54              |
| 1:F:235:GLU:O    | 1:F:236:ASN:HB3  | 2.08                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:303:HIS:HD2  | 1:K:308:ASN:CA   | 2.15                     | 0.53              |
| 1:J:255:ILE:HD12 | 1:J:260:VAL:HG21 | 1.90                     | 0.53              |
| 1:G:191:ILE:HG22 | 1:G:228:ILE:HB   | 1.90                     | 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              |
| 1:G:145:ASP:C    | 1:G:145:ASP:OD2  | 2.46                     | 0.53              |
| 1:G:267:PHE:CD2  | 1:G:271:ARG:HB3  | 2.41                     | 0.53              |
| 1:L:254:LEU:HD21 | 1:L:257:ASP:HA   | 1.90                     | 0.53              |
| 1:G:180:ARG:NH2  | 1:G:199:LEU:HD13 | 2.24                     | 0.53              |
| 1:L:272:ASN:OD1  | 1:L:275:ILE:CG1  | 2.52                     | 0.53              |
| 1:F:292:ASP:O    | 1:F:293:ALA:CB   | 2.50                     | 0.53              |
| 1:K:136:ARG:HG2  | 1:K:136:ARG:HH11 | 1.71                     | 0.53              |
| 1:D:308:ASN:HA   | 1:F:180:ARG:HH21 | 1.73                     | 0.53              |
| 1:L:267:PHE:C    | 1:L:267:PHE:CD1  | 2.82                     | 0.53              |
| 1:F:266:PRO:HG2  | 1:F:271:ARG:HH12 | 1.72                     | 0.53              |
| 1:C:189:GLN:HG3  | 1:C:190:THR:OG1  | 2.09                     | 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:D:300:ASN:HD22 | 1:D:303:HIS:HD2  | 1.56                     | 0.53              |
| 1:C:273:LEU:O    | 1:C:277:ILE:HG13 | 2.08                     | 0.53              |
| 1:I:171:ARG:HE   | 1:I:278:GLU:CD   | 2.12                     | 0.53              |
| 1:K:184:TYR:HD1  | 1:K:185:GLN:O    | 1.92                     | 0.52              |
| 1:F:272:ASN:C    | 1:F:272:ASN:ND2  | 2.57                     | 0.52              |
| 1:D:166:LEU:HD13 | 1:D:203:LEU:HD13 | 1.91                     | 0.52              |
| 1:G:141:GLY:HA2  | 1:G:161:LYS:HE3  | 1.90                     | 0.52              |
| 1:H:272:ASN:ND2  | 1:H:272:ASN:C    | 2.63                     | 0.52              |
| 1:A:254:LEU:HD12 | 1:A:257:ASP:HA   | 1.91                     | 0.52              |
| 1:D:156:ASP:N    | 1:D:156:ASP:OD2  | 2.38                     | 0.52              |
| 1:A:145:ASP:C    | 1:A:145:ASP:OD1  | 2.46                     | 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:D:162:SER:OG   | 1:D:178:ASP:OD2  | 2.25                     | 0.52              |
| 1:E:198:ILE:HG13 | 1:E:199:LEU:H    | 1.74                     | 0.52              |
| 1:A:254:LEU:HA   | 1:A:258:VAL:O    | 2.09                     | 0.52              |
| 1:J:244:ASP:OD1  | 1:J:246:LEU:O    | 2.26                     | 0.52              |
| 1:K:145:ASP:OD2  | 1:K:145:ASP:C    | 2.48                     | 0.52              |
| 1:E:145:ASP:C    | 1:E:145:ASP:OD2  | 2.47                     | 0.52              |
| 1:A:143:LEU:HG   | 1:A:176:ILE:HD12 | 1.91                     | 0.52              |
| 1:L:268:LYS:O    | 1:L:269:VAL:O    | 2.28                     | 0.52              |
| 1:G:188:GLU:O    | 1:G:189:GLN:HB3  | 2.09                     | 0.52              |
| 1:F:273:LEU:O    | 1:F:277:ILE:HG13 | 2.10                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:161:LYS:O    | 1:D:164:THR:HB   | 2.09                     | 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:J:171:ARG:HH22 | 1:J:275:ILE:CD1  | 2.23                     | 0.52              |
| 1:G:272:ASN:C    | 1:G:272:ASN:HD22 | 2.13                     | 0.52              |
| 1:H:275:ILE:CG2  | 1:H:276:ILE:HD13 | 2.39                     | 0.52              |
| 1:F:149:LEU:HD22 | 1:F:229:SER:HB2  | 1.93                     | 0.51              |
| 1:A:183:VAL:HG23 | 1:A:191:ILE:HG23 | 1.91                     | 0.51              |
| 1:J:279:VAL:HG21 | 1:L:166:LEU:HD21 | 1.92                     | 0.51              |
| 1:K:187:ASP:OD2  | 1:K:188:GLU:N    | 2.43                     | 0.51              |
| 1:G:163:GLU:O    | 1:G:166:LEU:HB3  | 2.10                     | 0.51              |
| 1:J:275:ILE:HD11 | 1:L:167:GLU:OE2  | 2.11                     | 0.51              |
| 1:E:149:LEU:HD21 | 1:E:229:SER:HB2  | 1.91                     | 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:A:272:ASN:C    | 1:A:272:ASN:ND2  | 2.64                     | 0.51              |
| 1:A:214:MET:HE3  | 1:F:215:ASN:HD22 | 1.76                     | 0.51              |
| 1:I:153:ILE:HD13 | 1:I:277:ILE:HD13 | 1.93                     | 0.51              |
| 1:G:170:GLN:OE1  | 1:G:170:GLN:HA   | 2.11                     | 0.51              |
| 1:B:145:ASP:OD2  | 1:B:174:ARG:NH2  | 2.44                     | 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:H:269:VAL:HG23 | 1:H:270:GLY:N    | 2.26                     | 0.50              |
| 1:H:155:GLY:O    | 1:H:159:VAL:CG2  | 2.59                     | 0.50              |
| 1:A:142:VAL:HG12 | 1:A:144:VAL:HG13 | 1.93                     | 0.50              |
| 1:A:159:VAL:O    | 1:A:159:VAL:HG13 | 2.11                     | 0.50              |
| 1:E:216:LEU:HD21 | 1:F:283:ASN:HD22 | 1.77                     | 0.50              |
| 1:B:189:GLN:N    | 1:B:189:GLN:HE21 | 2.09                     | 0.50              |
| 1:L:156:ASP:HA   | 1:L:161:LYS:HZ2  | 1.74                     | 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:C:188:GLU:N    | 1:C:188:GLU:OE1  | 2.44                     | 0.50              |
| 1:J:246:LEU:HD22 | 1:J:294:THR:HG23 | 1.94                     | 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:I:302:ASN:C    | 1:I:304:LEU:H    | 2.15                     | 0.50              |
| 1:I:302:ASN:C    | 1:I:304:LEU:N    | 2.65                     | 0.50              |
| 1:L:159:VAL:HG12 | 1:L:267:PHE:CZ   | 2.47                     | 0.50              |
| 1:K:204:GLU:O    | 1:K:206:ARG:NH2  | 2.45                     | 0.50              |
| 1:H:157:SER:C    | 1:H:159:VAL:H    | 2.15                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:142:VAL:HG21 | 1:L:161:LYS:HB3  | 1.94                     | 0.49              |
| 1:I:212:ASP:OD1  | 1:I:215:ASN:HB2  | 2.12                     | 0.49              |
| 1:A:198:ILE:HD13 | 1:A:199:LEU:N    | 2.25                     | 0.49              |
| 1:H:191:ILE:HD13 | 1:H:255:ILE:HB   | 1.94                     | 0.49              |
| 1:G:159:VAL:O    | 1:G:160:GLY:O    | 2.29                     | 0.49              |
| 1:A:223:ARG:NH1  | 1:A:226:THR:CG2  | 2.74                     | 0.49              |
| 1:E:198:ILE:C    | 1:E:198:ILE:HD12 | 2.32                     | 0.49              |
| 1:I:151:VAL:HG22 | 1:I:230:LEU:HD23 | 1.93                     | 0.49              |
| 1:B:282:MET:HB3  | 1:C:216:LEU:HD22 | 1.95                     | 0.49              |
| 1:K:286:ALA:HA   | 1:K:289:MET:HE2  | 1.94                     | 0.49              |
| 1:D:242:THR:CG2  | 1:D:243:PHE:N    | 2.75                     | 0.49              |
| 1:C:174:ARG:HG2  | 1:C:223:ARG:HB2  | 1.95                     | 0.49              |
| 1:A:153:ILE:HA   | 1:A:232:VAL:O    | 2.10                     | 0.49              |
| 1:J:205:ILE:HG22 | 1:J:205:ILE:O    | 2.13                     | 0.49              |
| 1:G:286:ALA:HA   | 1:G:289:MET:CE   | 2.41                     | 0.49              |
| 1:D:237:TRP:HZ2  | 1:F:206:ARG:HH12 | 1.60                     | 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:I:180:ARG:HD2  | 1:I:196:PRO:HG3  | 1.94                     | 0.49              |
| 1:E:170:GLN:HG2  | 1:E:217:PHE:HE2  | 1.77                     | 0.49              |
| 1:B:308:ASN:O    | 1:B:311:THR:OG1  | 2.20                     | 0.49              |
| 1:D:156:ASP:O    | 1:D:159:VAL:HG22 | 2.13                     | 0.49              |
| 1:D:292:ASP:OD2  | 1:D:292:ASP:O    | 2.31                     | 0.48              |
| 1:L:158:GLY:O    | 1:L:159:VAL:C    | 2.52                     | 0.48              |
| 1:H:242:THR:O    | 1:H:243:PHE:O    | 2.31                     | 0.48              |
| 1:J:185:GLN:OE1  | 1:J:256:PHE:O    | 2.30                     | 0.48              |
| 1:H:275:ILE:HG22 | 1:H:276:ILE:HD13 | 1.94                     | 0.48              |
| 1:E:156:ASP:HB3  | 1:E:161:LYS:HZ3  | 1.77                     | 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:E:286:ALA:HA   | 1:E:289:MET:HE2  | 1.95                     | 0.48              |
| 1:L:137:ARG:NH2  | 1:L:256:PHE:H    | 2.11                     | 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:E:163:GLU:O    | 1:E:166:LEU:HB3  | 2.13                     | 0.48              |
| 1:K:136:ARG:HG2  | 1:K:136:ARG:NH1  | 2.28                     | 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:G:211:ILE:C    | 1:G:211:ILE:HD12 | 2.33                     | 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              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:140:HIS:HD2  | 1:F:141:GLY:N    | 2.12                     | 0.48              |
| 1:I:214:MET:HG2  | 1:I:214:MET:O    | 2.12                     | 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:L:195:ALA:HA   | 1:L:196:PRO:HD2  | 1.65                     | 0.47              |
| 1:D:145:ASP:CG   | 1:D:174:ARG:HH21 | 2.16                     | 0.47              |
| 1:F:171:ARG:HE   | 1:F:278:GLU:CD   | 2.17                     | 0.47              |
| 1:G:304:LEU:HD22 | 1:G:304:LEU:HA   | 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:I:195:ALA:HA   | 1:I:196:PRO:HD2  | 1.63                     | 0.47              |
| 1:H:150:GLY:HA3  | 1:H:227:THR:O    | 2.15                     | 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:I:203:LEU:CD2  | 1:I:211:ILE:HD11 | 2.39                     | 0.47              |
| 1:F:272:ASN:HD21 | 1:F:275:ILE:H    | 1.57                     | 0.47              |
| 1:L:292:ASP:O    | 1:L:293:ALA:CB   | 2.63                     | 0.47              |
| 1:D:279:VAL:O    | 1:D:280:ALA:C    | 2.50                     | 0.47              |
| 1:E:211:ILE:C    | 1:E:211:ILE:HD12 | 2.35                     | 0.47              |
| 1:H:244:ASP:OD1  | 1:H:246:LEU:O    | 2.32                     | 0.47              |
| 1:E:254:LEU:HD23 | 1:E:257:ASP:HA   | 1.97                     | 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:F:166:LEU:O    | 1:F:169:VAL:HG22 | 2.15                     | 0.47              |
| 1:L:235:GLU:O    | 1:L:267:PHE:CB   | 2.54                     | 0.46              |
| 1:L:166:LEU:HD13 | 1:L:203:LEU:HD21 | 1.97                     | 0.46              |
| 1:A:160:GLY:O    | 1:A:162:SER:N    | 2.48                     | 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:K:272:ASN:HD22 | 1:K:272:ASN:C    | 2.17                     | 0.46              |
| 1:C:184:TYR:HD1  | 1:C:185:GLN:O    | 1.98                     | 0.46              |
| 1:B:262:LYS:HG2  | 1:B:263:ILE:N    | 2.29                     | 0.46              |
| 1:B:176:ILE:O    | 1:B:195:ALA:HB2  | 2.16                     | 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:H:255:ILE:HD12 | 1:H:260:VAL:HG21 | 1.97                     | 0.46              |
| 1:D:237:TRP:HZ3  | 1:D:239:PRO:CA   | 2.29                     | 0.46              |
| 1:L:234:LEU:HD22 | 1:L:273:LEU:HD13 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:253:GLN:CB   | 1:I:262:LYS:HD2  | 2.46                     | 0.46              |
| 1:F:307:HIS:ND1  | 1:F:308:ASN:N    | 2.64                     | 0.46              |
| 1:G:283:ASN:HD22 | 1:H:216:LEU:HD21 | 1.80                     | 0.46              |
| 1:H:269:VAL:C    | 1:H:271:ARG:H    | 2.19                     | 0.46              |
| 1:F:275:ILE:O    | 1:F:279:VAL:HG23 | 2.15                     | 0.46              |
| 1:D:191:ILE:CD1  | 1:D:260:VAL:CG2  | 2.93                     | 0.46              |
| 1:A:163:GLU:OE1  | 1:C:271:ARG:HB2  | 2.16                     | 0.46              |
| 1:D:145:ASP:O    | 1:D:173:HIS:HB3  | 2.16                     | 0.46              |
| 1:H:285:ARG:NH1  | 2:H:325:HOH:O    | 2.47                     | 0.46              |
| 1:K:178:ASP:CG   | 1:K:203:LEU:HD23 | 2.36                     | 0.46              |
| 1:I:269:VAL:O    | 1:I:271:ARG:N    | 2.48                     | 0.46              |
| 1:E:248:SER:HB2  | 1:E:249:GLY:H    | 1.60                     | 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:F:157:SER:O    | 1:F:158:GLY:C    | 2.54                     | 0.46              |
| 1:C:162:SER:HB3  | 1:C:178:ASP:OD1  | 2.16                     | 0.46              |
| 1:F:145:ASP:CG   | 1:F:174:ARG:HH21 | 2.20                     | 0.45              |
| 1:G:196:PRO:O    | 1:G:200:SER:HB2  | 2.16                     | 0.45              |
| 1:K:301:LEU:HD23 | 1:K:301:LEU:HA   | 1.69                     | 0.45              |
| 1:H:205:ILE:O    | 1:H:206:ARG:C    | 2.55                     | 0.45              |
| 1:A:183:VAL:HG23 | 1:A:191:ILE:CG2  | 2.46                     | 0.45              |
| 1:K:183:VAL:HG23 | 1:K:256:PHE:HE1  | 1.82                     | 0.45              |
| 1:G:170:GLN:OE1  | 1:G:217:PHE:HE2  | 1.98                     | 0.45              |
| 1:B:212:ASP:OD2  | 1:B:212:ASP:C    | 2.55                     | 0.45              |
| 1:H:137:ARG:HG3  | 1:H:256:PHE:HZ   | 1.75                     | 0.45              |
| 1:A:198:ILE:C    | 1:A:198:ILE:HD13 | 2.37                     | 0.45              |
| 1:L:142:VAL:CG2  | 1:L:161:LYS:HB3  | 2.46                     | 0.45              |
| 1:H:142:VAL:HG11 | 1:H:165:ALA:HB2  | 1.98                     | 0.45              |
| 1:G:279:VAL:HA   | 1:G:282:MET:CE   | 2.47                     | 0.45              |
| 1:G:212:ASP:HB3  | 1:G:215:ASN:HB3  | 1.99                     | 0.45              |
| 1:L:203:LEU:HD22 | 1:L:211:ILE:HG13 | 1.99                     | 0.45              |
| 1:E:184:TYR:HA   | 1:E:256:PHE:HE1  | 1.80                     | 0.45              |
| 1:J:145:ASP:OD2  | 1:J:145:ASP:C    | 2.55                     | 0.45              |
| 1:H:187:ASP:OD2  | 1:H:187:ASP:C    | 2.55                     | 0.45              |
| 1:L:251:GLN:HB3  | 1:L:252:THR:H    | 1.54                     | 0.45              |
| 1:H:185:GLN:OE1  | 1:H:256:PHE:O    | 2.35                     | 0.45              |
| 1:H:292:ASP:O    | 1:H:293:ALA:C    | 2.55                     | 0.45              |
| 1:E:156:ASP:HB3  | 1:E:161:LYS:HZ2  | 1.81                     | 0.45              |
| 1:G:159:VAL:HG11 | 1:G:206:ARG:HG3  | 1.98                     | 0.45              |
| 1:B:279:VAL:HG13 | 1:C:216:LEU:HD13 | 1.99                     | 0.45              |
| 1:E:251:GLN:HE21 | 1:E:262:LYS:HD3  | 1.82                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:211:ILE:HD13 | 1:E:216:LEU:HD12 | 1.98                     | 0.45              |
| 1:E:174:ARG:CD   | 1:E:220:GLY:O    | 2.64                     | 0.45              |
| 1:C:144:VAL:HG23 | 1:C:146:ILE:HG13 | 1.99                     | 0.45              |
| 1:H:225:ASP:OD2  | 1:H:225:ASP:C    | 2.55                     | 0.45              |
| 1:I:263:ILE:O    | 1:I:263:ILE:HG13 | 2.17                     | 0.45              |
| 1:A:149:LEU:HD11 | 1:A:229:SER:CB   | 2.47                     | 0.45              |
| 1:J:279:VAL:O    | 1:J:280:ALA:C    | 2.54                     | 0.45              |
| 1:G:145:ASP:O    | 1:G:173:HIS:HB3  | 2.16                     | 0.45              |
| 1:E:149:LEU:CD2  | 1:E:229:SER:HB2  | 2.47                     | 0.45              |
| 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:C:171:ARG:HG2  | 1:C:171:ARG:HH11 | 1.82                     | 0.44              |
| 1:E:136:ARG:HG3  | 1:E:136:ARG:NH1  | 2.32                     | 0.44              |
| 1:J:145:ASP:CG   | 1:J:174:ARG:HH21 | 2.20                     | 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:I:216:LEU:HA   | 1:I:216:LEU:HD23 | 1.74                     | 0.44              |
| 1:F:154:THR:O    | 1:F:233:HIS:HA   | 2.17                     | 0.44              |
| 1:J:196:PRO:O    | 1:J:197:PRO:C    | 2.55                     | 0.44              |
| 1:F:272:ASN:CG   | 1:F:275:ILE:HG12 | 2.38                     | 0.44              |
| 1:A:267:PHE:HE1  | 1:A:271:ARG:HB3  | 1.82                     | 0.44              |
| 1:H:145:ASP:OD2  | 1:H:145:ASP:C    | 2.55                     | 0.44              |
| 1:F:235:GLU:O    | 1:F:236:ASN:CB   | 2.65                     | 0.44              |
| 1:G:287:LYS:HE3  | 1:G:287:LYS:HB2  | 1.89                     | 0.44              |
| 1:J:140:HIS:CD2  | 1:J:180:ARG:HH11 | 2.36                     | 0.44              |
| 1:G:157:SER:O    | 1:G:160:GLY:CA   | 2.64                     | 0.44              |
| 1:G:157:SER:O    | 1:G:160:GLY:N    | 2.50                     | 0.44              |
| 1:G:204:GLU:O    | 1:G:206:ARG:NH1  | 2.51                     | 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:J:162:SER:O    | 1:J:165:ALA:HB3  | 2.17                     | 0.44              |
| 1:I:180:ARG:HD2  | 1:I:196:PRO:HB3  | 1.98                     | 0.44              |
| 1:G:279:VAL:HA   | 1:G:282:MET:HE3  | 2.00                     | 0.44              |
| 1:F:290:GLY:O    | 1:F:291:TYR:C    | 2.56                     | 0.44              |
| 1:I:211:ILE:O    | 1:I:211:ILE:HD12 | 2.16                     | 0.44              |
| 1:F:254:LEU:HA   | 1:F:258:VAL:O    | 2.18                     | 0.44              |
| 1:I:137:ARG:H    | 1:I:256:PHE:HZ   | 1.65                     | 0.44              |
| 1:A:226:THR:HB   | 1:A:227:THR:O    | 2.17                     | 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              |
| 1:B:137:ARG:HB2  | 1:B:256:PHE:CZ   | 2.53                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:185:GLN:HG2  | 1:F:186:GLN:H    | 1.83                     | 0.44              |
| 1:E:184:TYR:HD1  | 1:E:185:GLN:O    | 2.01                     | 0.43              |
| 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:H:270:GLY:O    | 1:I:159:VAL:HG11 | 2.18                     | 0.43              |
| 1:G:184:TYR:HA   | 1:G:256:PHE:HE1  | 1.83                     | 0.43              |
| 1:J:272:ASN:HD21 | 1:J:274:ALA:HB3  | 1.83                     | 0.43              |
| 1:F:139:MET:HE3  | 1:F:183:VAL:HG21 | 2.00                     | 0.43              |
| 1:F:253:GLN:HB2  | 1:F:262:LYS:HD2  | 1.99                     | 0.43              |
| 1:E:138:SER:HB2  | 1:E:182:ASP:OD1  | 2.19                     | 0.43              |
| 1:A:223:ARG:O    | 1:A:224:GLU:HB3  | 2.14                     | 0.43              |
| 1:J:301:LEU:HD23 | 1:J:305:ILE:HD11 | 2.00                     | 0.43              |
| 1:F:179:ASP:O    | 1:F:180:ARG:C    | 2.56                     | 0.43              |
| 1:A:175:LEU:CD2  | 1:A:213:VAL:HG21 | 2.48                     | 0.43              |
| 1:K:304:LEU:O    | 1:K:304:LEU:HD22 | 2.18                     | 0.43              |
| 1:H:145:ASP:O    | 1:H:173:HIS:HB3  | 2.17                     | 0.43              |
| 1:F:156:ASP:O    | 1:F:161:LYS:NZ   | 2.51                     | 0.43              |
| 1:B:309:GLU:C    | 1:B:311:THR:N    | 2.70                     | 0.43              |
| 1:H:280:ALA:HB2  | 1:I:208:LEU:HD21 | 2.00                     | 0.43              |
| 1:I:203:LEU:HD23 | 1:I:203:LEU:C    | 2.39                     | 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:J:187:ASP:OD2  | 1:J:187:ASP:C    | 2.57                     | 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:K:295:LYS:O    | 1:K:299:LYS:HB2  | 2.18                     | 0.43              |
| 1:F:184:TYR:O    | 1:F:184:TYR:HD1  | 2.02                     | 0.43              |
| 1:C:203:LEU:C    | 1:C:203:LEU:HD23 | 2.39                     | 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:279:VAL:HG21 | 1:C:166:LEU:CD2  | 2.49                     | 0.43              |
| 1:F:143:LEU:HD13 | 1:F:176:ILE:HB   | 2.01                     | 0.43              |
| 1:D:269:VAL:O    | 1:D:269:VAL:HG23 | 2.19                     | 0.43              |
| 1:F:292:ASP:HB3  | 1:F:295:LYS:HB2  | 2.01                     | 0.43              |
| 1:D:275:ILE:O    | 1:D:279:VAL:HG23 | 2.18                     | 0.43              |
| 1:J:171:ARG:HH22 | 1:J:275:ILE:HD11 | 1.83                     | 0.42              |
| 1:D:242:THR:HG23 | 1:D:243:PHE:H    | 1.81                     | 0.42              |
| 1:H:263:ILE:HG13 | 1:H:264:THR:N    | 2.34                     | 0.42              |
| 1:B:246:LEU:HD13 | 1:B:248:SER:OG   | 2.19                     | 0.42              |
| 1:J:145:ASP:OD1  | 1:J:223:ARG:NH1  | 2.50                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:136:ARG:HG3  | 1:L:184:TYR:HB3  | 2.01                     | 0.42              |
| 1:I:136:ARG:HG3  | 1:I:184:TYR:HB3  | 2.02                     | 0.42              |
| 1:K:196:PRO:HG3  | 1:K:199:LEU:HB2  | 2.00                     | 0.42              |
| 1:F:161:LYS:O    | 1:F:164:THR:HB   | 2.19                     | 0.42              |
| 1:E:145:ASP:O    | 1:E:173:HIS:HB3  | 2.20                     | 0.42              |
| 1:K:296:THR:O    | 1:K:299:LYS:HB3  | 2.19                     | 0.42              |
| 1:G:178:ASP:CG   | 1:G:203:LEU:HD12 | 2.39                     | 0.42              |
| 1:E:196:PRO:CG   | 1:E:199:LEU:HB2  | 2.49                     | 0.42              |
| 1:E:149:LEU:HD23 | 1:E:149:LEU:HA   | 1.85                     | 0.42              |
| 1:L:178:ASP:O    | 1:L:179:ASP:C    | 2.58                     | 0.42              |
| 1:F:263:ILE:CG2  | 1:F:264:THR:N    | 2.82                     | 0.42              |
| 1:K:283:ASN:O    | 1:K:287:LYS:HB2  | 2.19                     | 0.42              |
| 1:F:265:VAL:HA   | 1:F:266:PRO:HD2  | 1.86                     | 0.42              |
| 1:E:156:ASP:N    | 1:E:161:LYS:HZ2  | 2.16                     | 0.42              |
| 1:C:153:ILE:CD1  | 1:C:277:ILE:HD13 | 2.48                     | 0.42              |
| 1:K:141:GLY:HA2  | 1:K:161:LYS:HE3  | 2.02                     | 0.42              |
| 1:H:196:PRO:O    | 1:H:197:PRO:C    | 2.58                     | 0.42              |
| 1:K:268:LYS:HG3  | 1:K:269:VAL:N    | 2.34                     | 0.42              |
| 1:G:183:VAL:HG12 | 1:G:184:TYR:N    | 2.34                     | 0.42              |
| 1:B:275:ILE:HD12 | 1:C:167:GLU:HA   | 2.02                     | 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:L:137:ARG:HB2  | 1:L:256:PHE:CE1  | 2.55                     | 0.42              |
| 1:F:140:HIS:CD2  | 1:F:141:GLY:N    | 2.88                     | 0.42              |
| 1:D:205:ILE:O    | 1:D:206:ARG:C    | 2.58                     | 0.42              |
| 1:A:183:VAL:CG2  | 1:A:191:ILE:HG23 | 2.49                     | 0.41              |
| 1:F:272:ASN:HD21 | 1:F:274:ALA:CB   | 2.23                     | 0.41              |
| 1:I:156:ASP:HA   | 1:I:161:LYS:NZ   | 2.36                     | 0.41              |
| 1:F:185:GLN:OE1  | 1:F:256:PHE:HB3  | 2.20                     | 0.41              |
| 1:L:178:ASP:O    | 1:L:180:ARG:N    | 2.53                     | 0.41              |
| 1:B:310:GLU:O    | 1:B:310:GLU:HG3  | 2.20                     | 0.41              |
| 1:F:156:ASP:CG   | 1:F:157:SER:N    | 2.73                     | 0.41              |
| 1:D:212:ASP:OD2  | 1:D:212:ASP:C    | 2.59                     | 0.41              |
| 1:G:174:ARG:CD   | 1:G:220:GLY:O    | 2.68                     | 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              |
| 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:HG2  | 1:K:250:GLU:H    | 1.56                     | 0.41              |
| 1:G:198:ILE:HG23 | 1:G:199:LEU:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:180:ARG:HH21 | 1:E:199:LEU:HD12 | 1.84                     | 0.41              |
| 1:K:187:ASP:CG   | 1:K:189:GLN:H    | 2.24                     | 0.41              |
| 1:E:304:LEU:O    | 1:E:304:LEU:HD12 | 2.20                     | 0.41              |
| 1:F:152:LEU:HB3  | 1:F:231:ILE:HG12 | 2.01                     | 0.41              |
| 1:D:292:ASP:CG   | 1:D:295:LYS:HG3  | 2.40                     | 0.41              |
| 1:G:158:GLY:C    | 1:G:160:GLY:H    | 2.24                     | 0.41              |
| 1:C:253:GLN:HB2  | 1:C:262:LYS:HZ2  | 1.86                     | 0.41              |
| 1:L:191:ILE:HD12 | 1:L:260:VAL:HG21 | 2.03                     | 0.41              |
| 1:F:179:ASP:CG   | 1:F:180:ARG:HG2  | 2.41                     | 0.41              |
| 1:D:203:LEU:C    | 1:D:203:LEU:HD23 | 2.41                     | 0.41              |
| 1:A:145:ASP:O    | 1:A:173:HIS:HB3  | 2.21                     | 0.41              |
| 1:K:176:ILE:N    | 1:K:176:ILE:HD12 | 2.35                     | 0.41              |
| 1:A:153:ILE:H    | 1:A:153:ILE:HG12 | 1.76                     | 0.41              |
| 1:E:174:ARG:HH11 | 1:E:174:ARG:HD3  | 1.69                     | 0.41              |
| 1:F:139:MET:CE   | 1:F:183:VAL:HG21 | 2.50                     | 0.41              |
| 1:E:267:PHE:CE2  | 1:E:271:ARG:HB2  | 2.55                     | 0.41              |
| 1:K:174:ARG:CD   | 1:K:220:GLY:O    | 2.68                     | 0.41              |
| 1:D:309:GLU:C    | 1:D:311:THR:N    | 2.72                     | 0.41              |
| 1:D:196:PRO:O    | 1:D:197:PRO:C    | 2.57                     | 0.41              |
| 1:L:184:TYR:C    | 1:L:184:TYR:CD1  | 2.94                     | 0.41              |
| 1:I:139:MET:SD   | 1:I:183:VAL:HG21 | 2.61                     | 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:L:216:LEU:HD23 | 1:L:216:LEU:HA   | 1.84                     | 0.41              |
| 1:B:254:LEU:HD23 | 1:B:255:ILE:N    | 2.35                     | 0.41              |
| 1:E:191:ILE:HA   | 1:E:191:ILE:HD13 | 1.94                     | 0.41              |
| 1:J:171:ARG:NH2  | 1:J:275:ILE:CD1  | 2.84                     | 0.41              |
| 1:B:275:ILE:CG2  | 1:B:276:ILE:N    | 2.83                     | 0.41              |
| 1:I:186:GLN:O    | 1:I:187:ASP:C    | 2.59                     | 0.41              |
| 1:K:272:ASN:HD22 | 1:K:273:LEU:N    | 2.19                     | 0.41              |
| 1:C:171:ARG:NH1  | 1:C:171:ARG:HG2  | 2.36                     | 0.41              |
| 1:J:145:ASP:OD2  | 1:J:174:ARG:NH2  | 2.54                     | 0.41              |
| 1:D:268:LYS:O    | 1:D:269:VAL:C    | 2.59                     | 0.41              |
| 1:J:149:LEU:C    | 1:J:149:LEU:HD23 | 2.41                     | 0.41              |
| 1:L:265:VAL:HA   | 1:L:266:PRO:HD2  | 1.93                     | 0.41              |
| 1:C:303:HIS:O    | 1:C:303:HIS:ND1  | 2.54                     | 0.41              |
| 1:H:166:LEU:HD12 | 1:H:166:LEU:HA   | 1.71                     | 0.41              |
| 1:K:224:GLU:HA   | 1:K:224:GLU:OE2  | 2.20                     | 0.41              |
| 1:E:143:LEU:HD13 | 1:E:176:ILE:CB   | 2.51                     | 0.41              |
| 1:L:199:LEU:HA   | 1:L:199:LEU:HD23 | 1.87                     | 0.41              |
| 1:F:170:GLN:HG2  | 1:F:217:PHE:HE2  | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:273:LEU:HD23 | 1:B:273:LEU:HA   | 1.88                     | 0.41              |
| 1:G:235:GLU:O    | 1:G:267:PHE:HB3  | 2.21                     | 0.40              |
| 1:B:256:PHE:O    | 1:B:257:ASP:CB   | 2.64                     | 0.40              |
| 1:D:166:LEU:HA   | 1:D:166:LEU:HD12 | 1.87                     | 0.40              |
| 1:A:254:LEU:CD1  | 1:A:257:ASP:HA   | 2.51                     | 0.40              |
| 1:I:253:GLN:HB3  | 1:I:262:LYS:HD2  | 2.03                     | 0.40              |
| 1:D:206:ARG:O    | 1:E:271:ARG:NH2  | 2.49                     | 0.40              |
| 1:E:178:ASP:CB   | 1:E:203:LEU:HD23 | 2.51                     | 0.40              |
| 1:C:136:ARG:CA   | 1:C:256:PHE:HZ   | 2.30                     | 0.40              |
| 1:I:214:MET:CE   | 1:I:219:ALA:HB2  | 2.51                     | 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:L:156:ASP:O    | 1:L:157:SER:O    | 2.40                     | 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:J:268:LYS:O    | 1:J:270:GLY:N    | 2.54                     | 0.40              |
| 1:I:166:LEU:HD13 | 1:I:203:LEU:HD21 | 2.02                     | 0.40              |
| 1:F:166:LEU:HD13 | 1:F:203:LEU:HD23 | 2.04                     | 0.40              |
| 1:H:279:VAL:O    | 1:H:280:ALA:C    | 2.58                     | 0.40              |
| 1:F:285:ARG:O    | 1:F:289:MET:HG3  | 2.22                     | 0.40              |
| 1:B:292:ASP:CG   | 1:B:295:LYS:HD3  | 2.41                     | 0.40              |
| 1:B:145:ASP:CG   | 1:B:174:ARG:NH2  | 2.74                     | 0.40              |
| 1:B:283:ASN:HA   | 1:C:216:LEU:HD21 | 2.04                     | 0.40              |
| 1:C:171:ARG:CG   | 1:C:171:ARG:HH11 | 2.34                     | 0.40              |
| 1:L:212:ASP:HB3  | 1:L:215:ASN:HB2  | 2.03                     | 0.40              |
| 1:J:170:GLN:HE21 | 1:J:170:GLN:HA   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 1   | A     | 157/205 (77%)   | 127 (81%)  | 23 (15%)  | 7 (4%)   | 3           | 4  |
| 1   | B     | 179/205 (87%)   | 161 (90%)  | 16 (9%)   | 2 (1%)   | 17          | 36 |
| 1   | C     | 160/205 (78%)   | 140 (88%)  | 12 (8%)   | 8 (5%)   | 3           | 3  |
| 1   | D     | 179/205 (87%)   | 155 (87%)  | 17 (10%)  | 7 (4%)   | 4           | 5  |
| 1   | E     | 160/205 (78%)   | 132 (82%)  | 23 (14%)  | 5 (3%)   | 5           | 8  |
| 1   | F     | 156/205 (76%)   | 142 (91%)  | 10 (6%)   | 4 (3%)   | 7           | 11 |
| 1   | G     | 156/205 (76%)   | 130 (83%)  | 14 (9%)   | 12 (8%)  | 1           | 1  |
| 1   | H     | 176/205 (86%)   | 149 (85%)  | 17 (10%)  | 10 (6%)  | 2           | 2  |
| 1   | I     | 156/205 (76%)   | 134 (86%)  | 11 (7%)   | 11 (7%)  | 1           | 1  |
| 1   | J     | 176/205 (86%)   | 151 (86%)  | 18 (10%)  | 7 (4%)   | 4           | 4  |
| 1   | K     | 158/205 (77%)   | 129 (82%)  | 20 (13%)  | 9 (6%)   | 2           | 2  |
| 1   | L     | 157/205 (77%)   | 130 (83%)  | 19 (12%)  | 8 (5%)   | 2           | 3  |
| All | All   | 1970/2460 (80%) | 1680 (85%) | 200 (10%) | 90 (5%)  | 3           | 3  |

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%) | 113 (84%) | 22 (16%) | 3           | 5 |
| 1   | B     | 153/174 (88%) | 132 (86%) | 21 (14%) | 4           | 8 |
| 1   | C     | 138/174 (79%) | 118 (86%) | 20 (14%) | 4           | 6 |
| 1   | D     | 153/174 (88%) | 130 (85%) | 23 (15%) | 3           | 6 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |   |
|-----|-------|-----------------|------------|-----------|-------------|---|
| 1   | E     | 138/174 (79%)   | 117 (85%)  | 21 (15%)  | 3           | 6 |
| 1   | F     | 135/174 (78%)   | 115 (85%)  | 20 (15%)  | 4           | 6 |
| 1   | G     | 135/174 (78%)   | 116 (86%)  | 19 (14%)  | 4           | 7 |
| 1   | H     | 150/174 (86%)   | 128 (85%)  | 22 (15%)  | 4           | 6 |
| 1   | I     | 135/174 (78%)   | 115 (85%)  | 20 (15%)  | 4           | 6 |
| 1   | J     | 151/174 (87%)   | 127 (84%)  | 24 (16%)  | 3           | 5 |
| 1   | K     | 136/174 (78%)   | 112 (82%)  | 24 (18%)  | 2           | 3 |
| 1   | L     | 136/174 (78%)   | 116 (85%)  | 20 (15%)  | 4           | 6 |
| All | All   | 1695/2088 (81%) | 1439 (85%) | 256 (15%) | 3           | 6 |

All (256) 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     | 174 | ARG  |
| 1   | A     | 198 | ILE  |
| 1   | A     | 208 | LEU  |
| 1   | A     | 250 | GLU  |
| 1   | A     | 254 | LEU  |
| 1   | A     | 255 | ILE  |
| 1   | A     | 263 | ILE  |
| 1   | A     | 271 | ARG  |
| 1   | A     | 272 | ASN  |
| 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  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 169 | VAL  |
| 1   | B     | 174 | ARG  |
| 1   | B     | 179 | ASP  |
| 1   | B     | 180 | ARG  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 208 | LEU  |
| 1   | B     | 210 | ILE  |
| 1   | B     | 214 | MET  |
| 1   | B     | 223 | ARG  |
| 1   | B     | 224 | GLU  |
| 1   | B     | 237 | TRP  |
| 1   | B     | 238 | THR  |
| 1   | B     | 240 | ASP  |
| 1   | B     | 245 | ARG  |
| 1   | B     | 272 | ASN  |
| 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     | 170 | GLN  |
| 1   | C     | 171 | ARG  |
| 1   | C     | 174 | ARG  |
| 1   | C     | 187 | ASP  |
| 1   | C     | 188 | GLU  |
| 1   | C     | 198 | ILE  |
| 1   | C     | 199 | LEU  |
| 1   | C     | 203 | LEU  |
| 1   | C     | 206 | ARG  |
| 1   | C     | 238 | THR  |
| 1   | C     | 262 | LYS  |
| 1   | C     | 265 | VAL  |
| 1   | C     | 269 | VAL  |
| 1   | C     | 275 | ILE  |
| 1   | C     | 306 | GLU  |
| 1   | C     | 308 | ASN  |
| 1   | D     | 132 | GLN  |
| 1   | D     | 133 | LEU  |
| 1   | D     | 137 | ARG  |
| 1   | D     | 143 | LEU  |
| 1   | D     | 156 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 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     | 285 | ARG  |
| 1   | E     | 143 | LEU  |
| 1   | E     | 145 | ASP  |
| 1   | E     | 149 | LEU  |
| 1   | E     | 153 | ILE  |
| 1   | E     | 164 | THR  |
| 1   | E     | 174 | ARG  |
| 1   | E     | 186 | GLN  |
| 1   | E     | 198 | ILE  |
| 1   | E     | 208 | LEU  |
| 1   | E     | 210 | ILE  |
| 1   | E     | 226 | THR  |
| 1   | E     | 248 | SER  |
| 1   | E     | 263 | ILE  |
| 1   | E     | 265 | VAL  |
| 1   | E     | 272 | ASN  |
| 1   | E     | 275 | ILE  |
| 1   | E     | 283 | ASN  |
| 1   | E     | 287 | LYS  |
| 1   | E     | 294 | THR  |
| 1   | E     | 298 | GLU  |
| 1   | E     | 299 | LYS  |
| 1   | F     | 143 | LEU  |
| 1   | F     | 144 | VAL  |
| 1   | F     | 145 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 149 | LEU  |
| 1   | F     | 170 | GLN  |
| 1   | F     | 174 | ARG  |
| 1   | F     | 184 | TYR  |
| 1   | F     | 187 | ASP  |
| 1   | F     | 189 | GLN  |
| 1   | F     | 198 | ILE  |
| 1   | F     | 199 | LEU  |
| 1   | F     | 202 | LEU  |
| 1   | F     | 208 | LEU  |
| 1   | F     | 214 | MET  |
| 1   | F     | 215 | ASN  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 250 | GLU  |
| 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     | 157 | SER  |
| 1   | G     | 174 | ARG  |
| 1   | G     | 191 | ILE  |
| 1   | G     | 198 | ILE  |
| 1   | G     | 229 | SER  |
| 1   | G     | 269 | VAL  |
| 1   | G     | 272 | ASN  |
| 1   | G     | 275 | ILE  |
| 1   | G     | 288 | SER  |
| 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     | 149 | LEU  |
| 1   | H     | 156 | ASP  |
| 1   | H     | 163 | GLU  |
| 1   | H     | 169 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 174 | ARG  |
| 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     | 300 | ASN  |
| 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     | 174 | ARG  |
| 1   | I     | 180 | ARG  |
| 1   | I     | 184 | TYR  |
| 1   | I     | 198 | ILE  |
| 1   | I     | 199 | LEU  |
| 1   | I     | 203 | LEU  |
| 1   | I     | 254 | LEU  |
| 1   | I     | 257 | ASP  |
| 1   | I     | 263 | ILE  |
| 1   | I     | 271 | ARG  |
| 1   | I     | 301 | LEU  |
| 1   | I     | 304 | LEU  |
| 1   | J     | 138 | SER  |
| 1   | J     | 140 | HIS  |
| 1   | J     | 143 | LEU  |
| 1   | J     | 145 | ASP  |
| 1   | J     | 169 | VAL  |
| 1   | J     | 170 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 174 | ARG  |
| 1   | J     | 180 | ARG  |
| 1   | J     | 186 | GLN  |
| 1   | J     | 187 | ASP  |
| 1   | J     | 188 | GLU  |
| 1   | J     | 206 | ARG  |
| 1   | J     | 214 | MET  |
| 1   | J     | 237 | TRP  |
| 1   | J     | 250 | GLU  |
| 1   | J     | 251 | GLN  |
| 1   | J     | 256 | PHE  |
| 1   | J     | 262 | LYS  |
| 1   | J     | 263 | ILE  |
| 1   | J     | 272 | ASN  |
| 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     | 162 | SER  |
| 1   | K     | 164 | THR  |
| 1   | K     | 169 | VAL  |
| 1   | K     | 174 | ARG  |
| 1   | K     | 179 | ASP  |
| 1   | K     | 186 | GLN  |
| 1   | K     | 187 | ASP  |
| 1   | K     | 189 | GLN  |
| 1   | K     | 206 | ARG  |
| 1   | K     | 223 | ARG  |
| 1   | K     | 235 | GLU  |
| 1   | K     | 254 | LEU  |
| 1   | K     | 263 | ILE  |
| 1   | K     | 265 | VAL  |
| 1   | K     | 268 | LYS  |
| 1   | K     | 269 | VAL  |
| 1   | K     | 272 | ASN  |
| 1   | K     | 275 | ILE  |
| 1   | K     | 298 | GLU  |
| 1   | K     | 299 | LYS  |
| 1   | K     | 304 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 143 | LEU  |
| 1   | L     | 145 | ASP  |
| 1   | L     | 159 | VAL  |
| 1   | L     | 170 | GLN  |
| 1   | L     | 174 | ARG  |
| 1   | L     | 182 | ASP  |
| 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     | 256 | PHE  |
| 1   | L     | 265 | VAL  |
| 1   | L     | 267 | PHE  |
| 1   | L     | 272 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 189 | GLN  |
| 1   | A     | 215 | ASN  |
| 1   | A     | 233 | HIS  |
| 1   | A     | 272 | ASN  |
| 1   | A     | 283 | ASN  |
| 1   | B     | 140 | HIS  |
| 1   | B     | 189 | GLN  |
| 1   | B     | 272 | ASN  |
| 1   | B     | 283 | ASN  |
| 1   | C     | 283 | ASN  |
| 1   | D     | 201 | HIS  |
| 1   | D     | 272 | ASN  |
| 1   | D     | 283 | ASN  |
| 1   | D     | 300 | ASN  |
| 1   | D     | 303 | HIS  |
| 1   | E     | 201 | HIS  |
| 1   | E     | 251 | GLN  |
| 1   | E     | 272 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 283 | ASN  |
| 1   | E     | 300 | ASN  |
| 1   | F     | 140 | HIS  |
| 1   | F     | 215 | ASN  |
| 1   | F     | 251 | GLN  |
| 1   | F     | 272 | ASN  |
| 1   | F     | 283 | ASN  |
| 1   | G     | 140 | HIS  |
| 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  |
| 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     | 272 | ASN  |
| 1   | K     | 283 | ASN  |
| 1   | K     | 300 | ASN  |
| 1   | K     | 303 | HIS  |
| 1   | L     | 186 | GLN  |
| 1   | L     | 272 | ASN  |
| 1   | L     | 283 | ASN  |
| 1   | L     | 300 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2 |     | OWAB(Å²) | Q<0.9           |   |
|-----|-------|-----------------|--------|---------|-----|----------|-----------------|---|
| 1   | A     | 161/205 (78%)   | -0.27  | 0       | 100 | 100      | 23, 53, 79, 88  | 0 |
| 1   | B     | 181/205 (88%)   | -0.30  | 0       | 100 | 100      | 22, 44, 85, 98  | 0 |
| 1   | C     | 164/205 (80%)   | -0.20  | 0       | 100 | 100      | 30, 54, 89, 102 | 0 |
| 1   | D     | 181/205 (88%)   | -0.26  | 0       | 100 | 100      | 23, 43, 85, 101 | 0 |
| 1   | E     | 164/205 (80%)   | -0.33  | 0       | 100 | 100      | 27, 51, 78, 91  | 0 |
| 1   | F     | 160/205 (78%)   | -0.23  | 0       | 100 | 100      | 32, 52, 89, 98  | 0 |
| 1   | G     | 160/205 (78%)   | -0.24  | 1 (0%)  | 90  | 88       | 23, 51, 78, 84  | 0 |
| 1   | H     | 178/205 (86%)   | -0.32  | 1 (0%)  | 90  | 88       | 21, 43, 81, 101 | 0 |
| 1   | I     | 160/205 (78%)   | -0.24  | 1 (0%)  | 90  | 88       | 33, 54, 86, 97  | 0 |
| 1   | J     | 178/205 (86%)   | -0.26  | 0       | 100 | 100      | 23, 43, 82, 100 | 0 |
| 1   | K     | 162/205 (79%)   | -0.31  | 0       | 100 | 100      | 21, 52, 78, 82  | 0 |
| 1   | L     | 161/205 (78%)   | -0.18  | 2 (1%)  | 81  | 77       | 30, 54, 87, 106 | 0 |
| All | All   | 2010/2460 (81%) | -0.26  | 5 (0%)  | 95  | 95       | 21, 50, 85, 106 | 0 |

All (5) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 250 | GLU  | 3.2  |
| 1   | L     | 308 | ASN  | 2.8  |
| 1   | G     | 208 | LEU  | 2.7  |
| 1   | H     | 269 | VAL  | 2.6  |
| 1   | I     | 137 | ARG  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.