



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 AM UTC

PDB ID : 3GMH / pdb\_00003gmh  
Title : Crystal Structure of the Mad2 Dimer  
Authors : Ozkan, E.; Luo, X.; Machius, M.; Yu, H.; Deisenhofer, J.  
Deposited on : 2009-03-13  
Resolution : 3.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

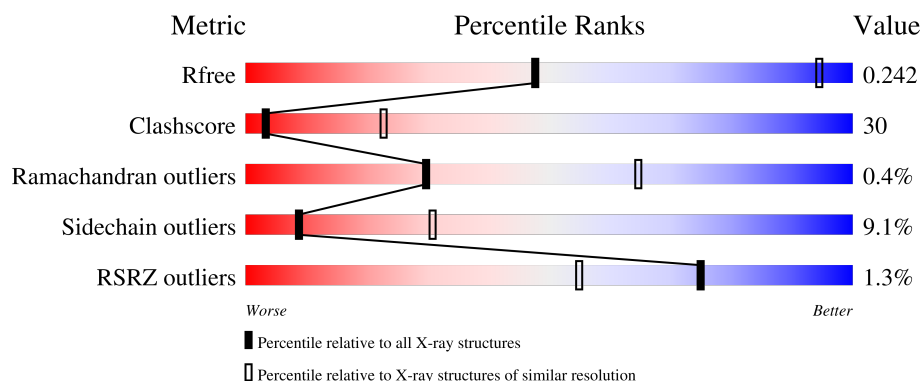
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.95 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1046 (4.16-3.76)                                      |
| Clashscore            | 190562                      | 1019 (4.14-3.78)                                      |
| Ramachandran outliers | 187476                      | 1031 (4.16-3.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (4.16-3.76)                                      |
| RSRZ outliers         | 180081                      | 1046 (4.16-3.76)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | A     | 207    | <div> <div>53%</div> <div>37%</div> <div>7%</div> </div>                              |
| 1   | B     | 207    | <div> <div>2%</div> <div>42%</div> <div>42%</div> <div>6%</div> <div>11%</div> </div> |
| 1   | C     | 207    | <div> <div>53%</div> <div>36%</div> <div>5%</div> <div>6%</div> </div>                |
| 1   | D     | 207    | <div> <div>%</div> <div>45%</div> <div>38%</div> <div>7%</div> <div>10%</div> </div>  |
| 1   | E     | 207    | <div> <div>2%</div> <div>53%</div> <div>35%</div> <div>9%</div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 207    |                  |
| 1   | G     | 207    |                  |
| 1   | H     | 207    |                  |
| 1   | I     | 207    |                  |
| 1   | J     | 207    |                  |
| 1   | K     | 207    |                  |
| 1   | L     | 207    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | SO4  | A     | 207 | -         | -        | X       | -                |
| 2   | SO4  | C     | 206 | -         | -        | X       | -                |
| 2   | SO4  | E     | 206 | -         | -        | X       | -                |
| 2   | SO4  | K     | 206 | -         | -        | X       | -                |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18301 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 Mitotic spindle assembly checkpoint protein MAD2A.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 193      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1561  | 1003 | 253 | 301 | 4 |         |         |       |
| 1   | B     | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1495  | 965  | 240 | 286 | 4 |         |         |       |
| 1   | C     | 195      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1576  | 1012 | 256 | 304 | 4 |         |         |       |
| 1   | D     | 187      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1515  | 977  | 246 | 288 | 4 |         |         |       |
| 1   | E     | 188      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1522  | 981  | 245 | 292 | 4 |         |         |       |
| 1   | F     | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1495  | 965  | 240 | 286 | 4 |         |         |       |
| 1   | G     | 187      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1518  | 978  | 246 | 290 | 4 |         |         |       |
| 1   | H     | 186      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1505  | 971  | 243 | 287 | 4 |         |         |       |
| 1   | I     | 188      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 983  | 247 | 291 | 4 |         |         |       |
| 1   | J     | 185      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1495  | 965  | 240 | 286 | 4 |         |         |       |
| 1   | K     | 188      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1525  | 983  | 247 | 291 | 4 |         |         |       |
| 1   | L     | 187      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1509  | 974  | 243 | 288 | 4 |         |         |       |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -1      | MET      | -      | expression tag | UNP Q13257 |
| A     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| A     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| A     | 2       | SER      | -      | expression tag | UNP Q13257 |
| A     | 3       | HIS      | -      | expression tag | UNP Q13257 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| A     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| A     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| A     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| A     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| A     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| A     | 10      | SER      | -      | expression tag | UNP Q13257 |
| B     | -1      | MET      | -      | expression tag | UNP Q13257 |
| B     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| B     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| B     | 2       | SER      | -      | expression tag | UNP Q13257 |
| B     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| B     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| B     | 10      | SER      | -      | expression tag | UNP Q13257 |
| C     | -1      | MET      | -      | expression tag | UNP Q13257 |
| C     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| C     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| C     | 2       | SER      | -      | expression tag | UNP Q13257 |
| C     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| C     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| C     | 10      | SER      | -      | expression tag | UNP Q13257 |
| D     | -1      | MET      | -      | expression tag | UNP Q13257 |
| D     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| D     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| D     | 2       | SER      | -      | expression tag | UNP Q13257 |
| D     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| D     | 9       | GLY      | -      | expression tag | UNP Q13257 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | 10      | SER      | -      | expression tag | UNP Q13257 |
| E     | -1      | MET      | -      | expression tag | UNP Q13257 |
| E     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| E     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| E     | 2       | SER      | -      | expression tag | UNP Q13257 |
| E     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| E     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| E     | 10      | SER      | -      | expression tag | UNP Q13257 |
| F     | -1      | MET      | -      | expression tag | UNP Q13257 |
| F     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| F     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| F     | 2       | SER      | -      | expression tag | UNP Q13257 |
| F     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| F     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| F     | 10      | SER      | -      | expression tag | UNP Q13257 |
| G     | -1      | MET      | -      | expression tag | UNP Q13257 |
| G     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| G     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| G     | 2       | SER      | -      | expression tag | UNP Q13257 |
| G     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| G     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| G     | 10      | SER      | -      | expression tag | UNP Q13257 |
| H     | -1      | MET      | -      | expression tag | UNP Q13257 |
| H     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| H     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| H     | 2       | SER      | -      | expression tag | UNP Q13257 |
| H     | 3       | HIS      | -      | expression tag | UNP Q13257 |

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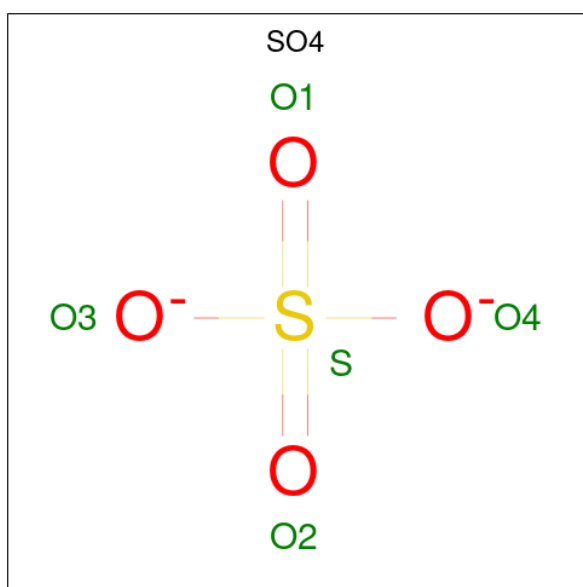
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| H     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| H     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| H     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| H     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| H     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| H     | 10      | SER      | -      | expression tag | UNP Q13257 |
| I     | -1      | MET      | -      | expression tag | UNP Q13257 |
| I     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| I     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| I     | 2       | SER      | -      | expression tag | UNP Q13257 |
| I     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| I     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| I     | 10      | SER      | -      | expression tag | UNP Q13257 |
| J     | -1      | MET      | -      | expression tag | UNP Q13257 |
| J     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| J     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| J     | 2       | SER      | -      | expression tag | UNP Q13257 |
| J     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| J     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| J     | 10      | SER      | -      | expression tag | UNP Q13257 |
| K     | -1      | MET      | -      | expression tag | UNP Q13257 |
| K     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| K     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| K     | 2       | SER      | -      | expression tag | UNP Q13257 |
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| K     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| K     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| K     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| K     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| K     | 9       | GLY      | -      | expression tag | UNP Q13257 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | 10      | SER      | -      | expression tag | UNP Q13257 |
| L     | -1      | MET      | -      | expression tag | UNP Q13257 |
| L     | 0       | ARG      | -      | expression tag | UNP Q13257 |
| L     | 1       | GLY      | -      | expression tag | UNP Q13257 |
| L     | 2       | SER      | -      | expression tag | UNP Q13257 |
| L     | 3       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 4       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 5       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 6       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 7       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 8       | HIS      | -      | expression tag | UNP Q13257 |
| L     | 9       | GLY      | -      | expression tag | UNP Q13257 |
| L     | 10      | SER      | -      | expression tag | UNP Q13257 |

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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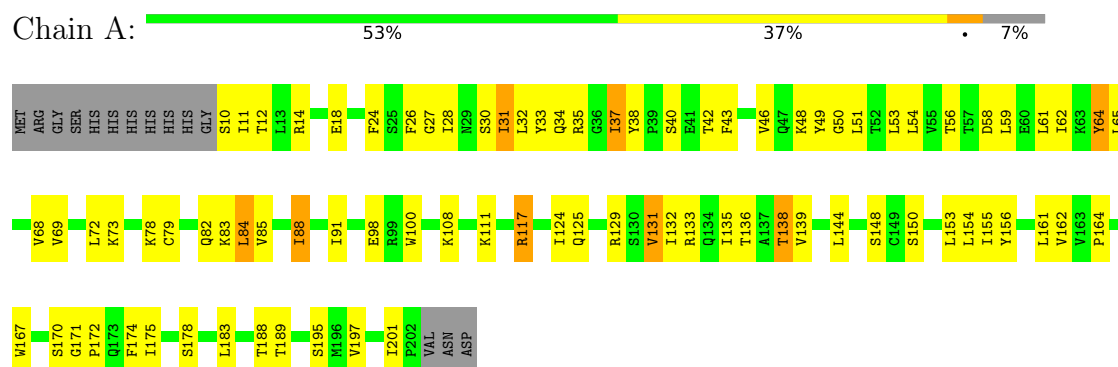
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

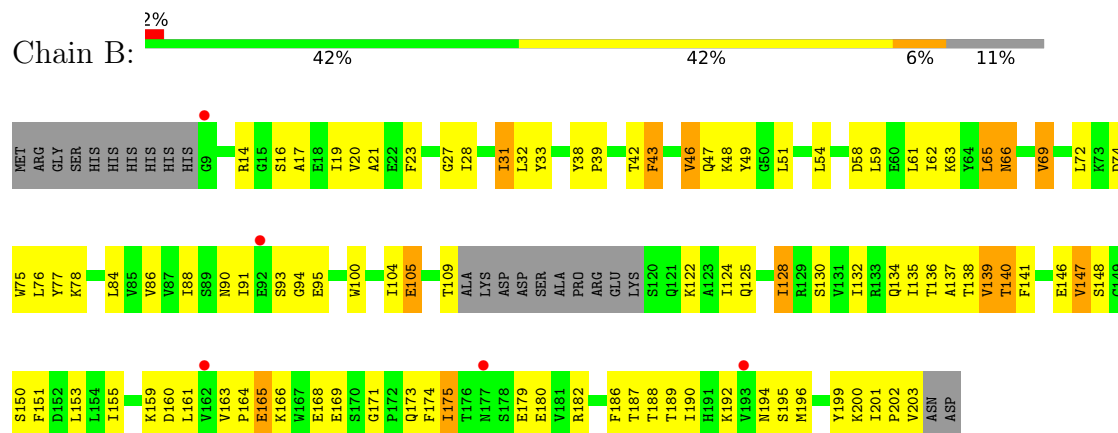
### 3 Residue-property plots

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

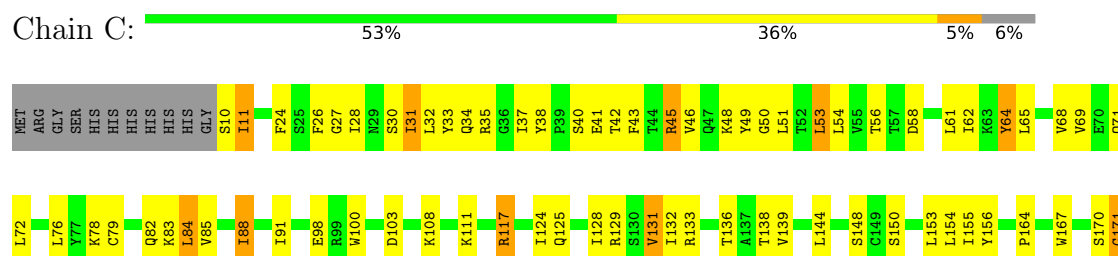
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A

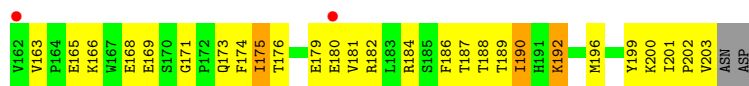
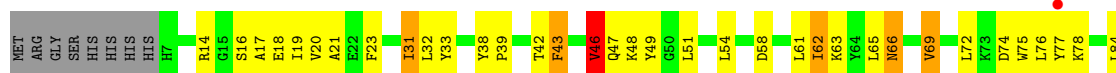


- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A

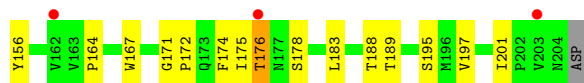
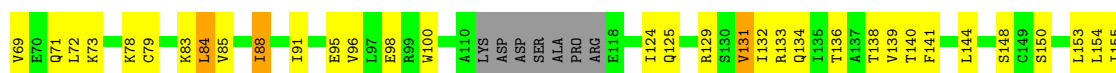
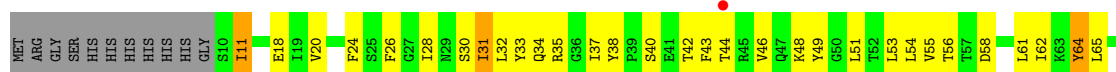




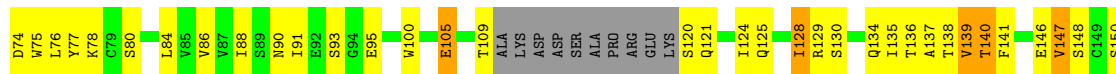
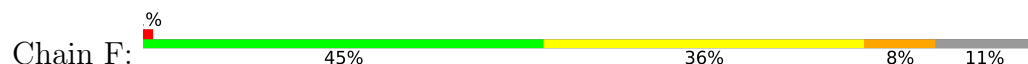
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A

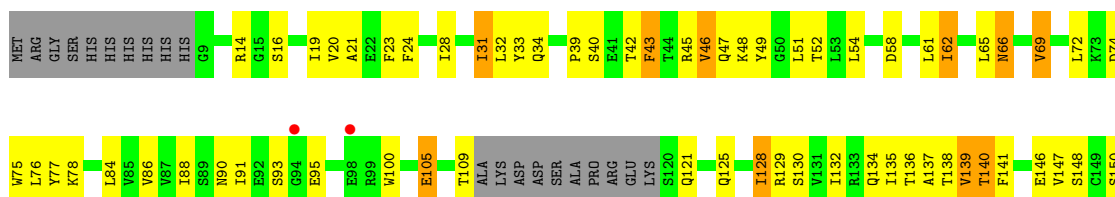


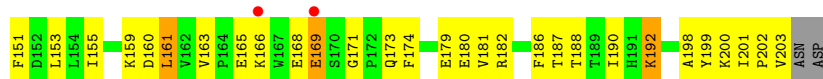
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



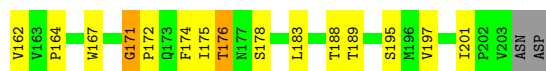
- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



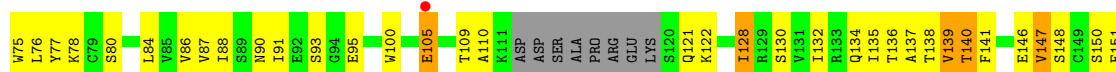




- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



- Molecule 1: Mitotic spindle assembly checkpoint protein MAD2A



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 124.83Å 104.92Å 157.75Å<br>90.00° 97.57° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 49.73 – 3.95<br>49.73 – 3.95                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (49.73-3.95)<br>99.5 (49.73-3.95)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.17                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.33 (at 3.88Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine)                                      | Depositor        |
| R, $R_{free}$                                                           | 0.218 , 0.251<br>0.208 , 0.242                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1781 reflections (4.99%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 115.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.497                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 129.6                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 18301                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 156.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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     | 0.49         | 0/1589      | 0.91        | 2/2155 (0.1%)   |
| 1   | B     | 0.61         | 0/1521      | 0.91        | 1/2063 (0.0%)   |
| 1   | C     | 0.47         | 0/1604      | 0.91        | 2/2176 (0.1%)   |
| 1   | D     | 0.62         | 0/1543      | 0.94        | 3/2093 (0.1%)   |
| 1   | E     | 0.43         | 0/1548      | 0.87        | 2/2099 (0.1%)   |
| 1   | F     | 0.49         | 0/1521      | 0.87        | 1/2063 (0.0%)   |
| 1   | G     | 0.41         | 0/1544      | 0.87        | 2/2092 (0.1%)   |
| 1   | H     | 0.46         | 0/1532      | 0.86        | 1/2078 (0.0%)   |
| 1   | I     | 0.46         | 0/1551      | 0.88        | 2/2102 (0.1%)   |
| 1   | J     | 0.45         | 0/1521      | 0.88        | 3/2063 (0.1%)   |
| 1   | K     | 0.43         | 0/1551      | 0.89        | 2/2102 (0.1%)   |
| 1   | L     | 0.52         | 0/1535      | 0.92        | 3/2081 (0.1%)   |
| All | All   | 0.49         | 0/18560     | 0.89        | 24/25167 (0.1%) |

There are no bond length outliers.

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | D     | 161 | LEU  | N-CA-C | 7.27 | 119.57      | 108.52   |
| 1   | J     | 161 | LEU  | N-CA-C | 7.16 | 119.40      | 108.52   |
| 1   | F     | 161 | LEU  | N-CA-C | 6.95 | 119.09      | 108.52   |
| 1   | K     | 171 | GLY  | CA-C-N | 6.67 | 126.45      | 119.05   |
| 1   | K     | 171 | GLY  | C-N-CA | 6.67 | 126.45      | 119.05   |
| 1   | A     | 171 | GLY  | CA-C-N | 6.65 | 126.43      | 119.05   |
| 1   | A     | 171 | GLY  | C-N-CA | 6.65 | 126.43      | 119.05   |
| 1   | G     | 171 | GLY  | CA-C-N | 6.46 | 126.22      | 119.05   |
| 1   | G     | 171 | GLY  | C-N-CA | 6.46 | 126.22      | 119.05   |
| 1   | E     | 171 | GLY  | CA-C-N | 6.44 | 126.20      | 119.05   |
| 1   | E     | 171 | GLY  | C-N-CA | 6.44 | 126.20      | 119.05   |
| 1   | C     | 171 | GLY  | CA-C-N | 6.41 | 125.83      | 118.85   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 171 | GLY  | C-N-CA | 6.41  | 125.83      | 118.85   |
| 1   | I     | 171 | GLY  | CA-C-N | 6.27  | 126.01      | 119.05   |
| 1   | I     | 171 | GLY  | C-N-CA | 6.27  | 126.01      | 119.05   |
| 1   | H     | 87  | VAL  | N-CA-C | 5.51  | 114.30      | 106.53   |
| 1   | L     | 87  | VAL  | N-CA-C | 5.33  | 114.04      | 106.53   |
| 1   | B     | 94  | GLY  | N-CA-C | -5.22 | 107.47      | 114.25   |
| 1   | D     | 46  | VAL  | CA-C-N | -5.22 | 115.37      | 122.93   |
| 1   | D     | 46  | VAL  | C-N-CA | -5.22 | 115.37      | 122.93   |
| 1   | J     | 46  | VAL  | CA-C-N | -5.16 | 115.89      | 123.00   |
| 1   | J     | 46  | VAL  | C-N-CA | -5.16 | 115.89      | 123.00   |
| 1   | L     | 110 | ALA  | N-CA-C | 5.14  | 116.79      | 108.26   |
| 1   | L     | 165 | GLU  | N-CA-C | -5.03 | 106.98      | 113.01   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1561  | 0        | 1581     | 93      | 0            |
| 1   | B     | 1495  | 0        | 1517     | 100     | 0            |
| 1   | C     | 1576  | 0        | 1596     | 95      | 0            |
| 1   | D     | 1515  | 0        | 1531     | 99      | 0            |
| 1   | E     | 1522  | 0        | 1544     | 86      | 0            |
| 1   | F     | 1495  | 0        | 1517     | 103     | 0            |
| 1   | G     | 1518  | 0        | 1542     | 88      | 0            |
| 1   | H     | 1505  | 0        | 1524     | 104     | 0            |
| 1   | I     | 1525  | 0        | 1551     | 156     | 0            |
| 1   | J     | 1495  | 0        | 1517     | 109     | 0            |
| 1   | K     | 1525  | 0        | 1551     | 87      | 0            |
| 1   | L     | 1509  | 0        | 1535     | 105     | 0            |
| 2   | A     | 10    | 0        | 0        | 3       | 0            |
| 2   | B     | 5     | 0        | 0        | 0       | 0            |
| 2   | C     | 10    | 0        | 0        | 2       | 0            |
| 2   | D     | 5     | 0        | 0        | 0       | 0            |
| 2   | E     | 5     | 0        | 0        | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | G     | 5     | 0        | 0        | 1       | 0            |
| 2   | H     | 5     | 0        | 0        | 0       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | K     | 5     | 0        | 0        | 2       | 0            |
| 2   | L     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 18301 | 0        | 18506    | 1119    | 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 30.

All (1119) 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:I:35:ARG:NH2   | 1:I:145:LEU:HD11 | 1.46                     | 1.27              |
| 1:H:171:GLY:HA3  | 1:H:188:THR:O    | 1.60                     | 1.01              |
| 1:F:23:PHE:HE1   | 1:F:128:ILE:HG12 | 1.28                     | 0.97              |
| 1:I:34:GLN:HB3   | 1:I:139:VAL:HG21 | 1.43                     | 0.97              |
| 1:B:63:LYS:HE2   | 1:H:63:LYS:HE2   | 1.49                     | 0.95              |
| 1:L:171:GLY:HA3  | 1:L:188:THR:O    | 1.69                     | 0.93              |
| 1:I:35:ARG:HE    | 1:I:88:ILE:HD12  | 1.31                     | 0.93              |
| 1:D:23:PHE:HE1   | 1:D:128:ILE:HG12 | 1.35                     | 0.92              |
| 1:J:16:SER:HB2   | 1:J:109:THR:HG21 | 1.52                     | 0.90              |
| 1:H:16:SER:HB2   | 1:H:109:THR:HG21 | 1.53                     | 0.90              |
| 1:J:23:PHE:HE1   | 1:J:128:ILE:HG12 | 1.36                     | 0.90              |
| 1:F:16:SER:HB2   | 1:F:109:THR:HG21 | 1.54                     | 0.90              |
| 1:H:23:PHE:HE1   | 1:H:128:ILE:HG12 | 1.38                     | 0.89              |
| 1:B:23:PHE:HE1   | 1:B:128:ILE:HG12 | 1.35                     | 0.89              |
| 1:I:35:ARG:NH2   | 1:I:145:LEU:CD1  | 2.36                     | 0.89              |
| 1:L:16:SER:HB2   | 1:L:109:THR:HG21 | 1.54                     | 0.88              |
| 1:D:16:SER:HB2   | 1:D:109:THR:HG21 | 1.55                     | 0.88              |
| 1:L:23:PHE:HE1   | 1:L:128:ILE:HG12 | 1.38                     | 0.88              |
| 1:K:32:LEU:HD22  | 1:K:37:ILE:HG21  | 1.55                     | 0.87              |
| 1:A:32:LEU:HD22  | 1:A:37:ILE:HG21  | 1.57                     | 0.87              |
| 1:I:144:LEU:HD23 | 1:J:129:ARG:HH21 | 1.39                     | 0.87              |
| 1:I:35:ARG:CZ    | 1:I:98:GLU:OE2   | 2.23                     | 0.87              |
| 1:B:16:SER:HB2   | 1:B:109:THR:HG21 | 1.55                     | 0.86              |
| 1:C:32:LEU:HD22  | 1:C:37:ILE:HG21  | 1.58                     | 0.85              |
| 1:D:122:LYS:HD3  | 1:K:41:GLU:HG3   | 1.57                     | 0.84              |
| 1:E:32:LEU:HD22  | 1:E:37:ILE:HG21  | 1.57                     | 0.84              |
| 1:J:90:ASN:HB3   | 1:J:93:SER:HB3   | 1.60                     | 0.84              |
| 1:I:35:ARG:CZ    | 1:I:98:GLU:CD    | 2.51                     | 0.84              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:32:LEU:HD22  | 1:G:37:ILE:HG21  | 1.58                     | 0.83              |
| 1:L:90:ASN:HB3   | 1:L:93:SER:HB3   | 1.60                     | 0.83              |
| 1:B:90:ASN:HB3   | 1:B:93:SER:HB3   | 1.60                     | 0.83              |
| 1:I:35:ARG:HG2   | 1:I:35:ARG:HH11  | 1.44                     | 0.83              |
| 1:D:173:GLN:HB2  | 1:D:187:THR:HG22 | 1.60                     | 0.83              |
| 1:I:35:ARG:HH22  | 1:I:145:LEU:HD11 | 1.43                     | 0.83              |
| 1:B:200:LYS:HB3  | 1:B:202:PRO:HD3  | 1.61                     | 0.83              |
| 1:D:90:ASN:HB3   | 1:D:93:SER:HB3   | 1.59                     | 0.83              |
| 1:I:138:THR:HA   | 1:I:141:PHE:CE1  | 2.14                     | 0.82              |
| 1:I:144:LEU:CD2  | 1:J:129:ARG:HH21 | 1.93                     | 0.82              |
| 1:B:173:GLN:HB2  | 1:B:187:THR:HG22 | 1.60                     | 0.81              |
| 1:L:48:LYS:HG2   | 1:L:49:TYR:CD1   | 2.15                     | 0.81              |
| 1:F:90:ASN:HB3   | 1:F:93:SER:HB3   | 1.61                     | 0.81              |
| 1:D:200:LYS:HB3  | 1:D:202:PRO:HD3  | 1.62                     | 0.80              |
| 1:D:171:GLY:HA3  | 1:D:188:THR:O    | 1.81                     | 0.80              |
| 1:I:35:ARG:NH1   | 1:I:35:ARG:HB3   | 1.96                     | 0.80              |
| 1:F:23:PHE:CE1   | 1:F:128:ILE:HG12 | 2.16                     | 0.80              |
| 1:J:173:GLN:HB2  | 1:J:187:THR:HG22 | 1.64                     | 0.80              |
| 1:I:38:TYR:HB3   | 1:I:39:PRO:CD    | 2.12                     | 0.80              |
| 1:J:200:LYS:HB3  | 1:J:202:PRO:HD3  | 1.64                     | 0.80              |
| 1:E:172:PRO:HB2  | 1:E:174:PHE:CE1  | 2.17                     | 0.79              |
| 1:F:173:GLN:HB2  | 1:F:187:THR:HG22 | 1.65                     | 0.79              |
| 1:H:75:TRP:CH2   | 1:H:190:ILE:HD11 | 2.17                     | 0.79              |
| 1:I:124:ILE:HD13 | 1:I:188:THR:HG22 | 1.63                     | 0.79              |
| 1:A:124:ILE:HD13 | 1:A:188:THR:HG22 | 1.61                     | 0.79              |
| 1:B:48:LYS:HG2   | 1:B:49:TYR:CD1   | 2.17                     | 0.79              |
| 1:H:91:ILE:HD13  | 1:H:150:SER:HB3  | 1.64                     | 0.79              |
| 1:H:200:LYS:HB3  | 1:H:202:PRO:HD3  | 1.63                     | 0.79              |
| 1:J:91:ILE:HD13  | 1:J:150:SER:HB3  | 1.63                     | 0.79              |
| 1:C:124:ILE:HD13 | 1:C:188:THR:HG22 | 1.64                     | 0.79              |
| 1:A:26:PHE:CE1   | 1:A:48:LYS:HG2   | 2.18                     | 0.79              |
| 1:D:48:LYS:HG2   | 1:D:49:TYR:CD1   | 2.18                     | 0.79              |
| 1:I:133:ARG:HD3  | 1:J:34:GLN:HA    | 1.65                     | 0.79              |
| 1:G:124:ILE:HD13 | 1:G:188:THR:HG22 | 1.65                     | 0.79              |
| 1:B:171:GLY:HA3  | 1:B:188:THR:O    | 1.83                     | 0.78              |
| 1:E:65:LEU:O     | 1:E:69:VAL:HG23  | 1.83                     | 0.78              |
| 1:H:90:ASN:HB3   | 1:H:93:SER:HB3   | 1.63                     | 0.78              |
| 1:L:91:ILE:HD13  | 1:L:150:SER:HB3  | 1.65                     | 0.78              |
| 1:C:49:TYR:O     | 1:C:129:ARG:HD3  | 1.84                     | 0.78              |
| 1:I:133:ARG:CD   | 1:J:34:GLN:HA    | 2.14                     | 0.78              |
| 1:E:26:PHE:CE1   | 1:E:48:LYS:HG2   | 2.19                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:49:TYR:O     | 1:E:129:ARG:HD3  | 1.83                     | 0.77              |
| 1:F:91:ILE:HD13  | 1:F:150:SER:HB3  | 1.67                     | 0.77              |
| 1:K:124:ILE:HD13 | 1:K:188:THR:HG22 | 1.66                     | 0.77              |
| 1:G:26:PHE:CE1   | 1:G:48:LYS:HG2   | 2.19                     | 0.77              |
| 1:B:46:VAL:HA    | 1:H:46:VAL:HA    | 1.66                     | 0.77              |
| 1:I:34:GLN:CB    | 1:I:139:VAL:HG21 | 2.13                     | 0.77              |
| 1:C:10:SER:HA    | 1:C:117:ARG:O    | 1.85                     | 0.76              |
| 1:G:37:ILE:HD11  | 1:G:88:ILE:HD13  | 1.67                     | 0.76              |
| 1:K:172:PRO:HB2  | 1:K:174:PHE:CE1  | 2.21                     | 0.76              |
| 1:L:75:TRP:CH2   | 1:L:190:ILE:HD11 | 2.19                     | 0.76              |
| 1:E:124:ILE:HD13 | 1:E:188:THR:HG22 | 1.67                     | 0.76              |
| 1:G:170:SER:O    | 1:J:198:ALA:HB3  | 1.84                     | 0.76              |
| 1:H:48:LYS:HG2   | 1:H:49:TYR:CD1   | 2.20                     | 0.76              |
| 1:K:26:PHE:CE1   | 1:K:48:LYS:HG2   | 2.21                     | 0.76              |
| 1:A:56:THR:HG21  | 1:A:61:LEU:HD23  | 1.68                     | 0.76              |
| 1:A:72:LEU:HD11  | 1:A:155:ILE:HD11 | 1.68                     | 0.76              |
| 1:F:47:GLN:HB3   | 1:I:146:GLU:C    | 2.11                     | 0.76              |
| 1:A:37:ILE:HD11  | 1:A:88:ILE:HD13  | 1.68                     | 0.76              |
| 1:F:120:SER:HB2  | 1:I:58:ASP:CG    | 2.11                     | 0.76              |
| 1:C:26:PHE:CE1   | 1:C:48:LYS:HG2   | 2.19                     | 0.75              |
| 1:E:56:THR:HG21  | 1:E:61:LEU:HD23  | 1.69                     | 0.75              |
| 1:K:56:THR:HG21  | 1:K:61:LEU:HD23  | 1.66                     | 0.75              |
| 1:I:51:LEU:HD22  | 1:J:40:SER:OG    | 1.86                     | 0.75              |
| 1:J:171:GLY:HA3  | 1:J:188:THR:O    | 1.86                     | 0.75              |
| 1:B:75:TRP:CH2   | 1:B:190:ILE:HD11 | 2.21                     | 0.75              |
| 1:J:48:LYS:HG2   | 1:J:49:TYR:CD1   | 2.20                     | 0.75              |
| 1:J:75:TRP:CH2   | 1:J:190:ILE:HD11 | 2.20                     | 0.75              |
| 1:A:10:SER:HA    | 1:A:117:ARG:O    | 1.87                     | 0.75              |
| 1:I:10:SER:HA    | 1:I:117:ARG:O    | 1.87                     | 0.75              |
| 1:K:49:TYR:O     | 1:K:129:ARG:HD3  | 1.87                     | 0.75              |
| 1:I:49:TYR:O     | 1:I:129:ARG:HD3  | 1.86                     | 0.74              |
| 1:F:171:GLY:HA3  | 1:F:188:THR:O    | 1.87                     | 0.74              |
| 1:A:129:ARG:NH2  | 2:A:207:SO4:O3   | 2.21                     | 0.74              |
| 1:A:49:TYR:O     | 1:A:129:ARG:HD3  | 1.87                     | 0.74              |
| 1:C:41:GLU:HG3   | 1:L:122:LYS:HD3  | 1.68                     | 0.74              |
| 1:D:75:TRP:CH2   | 1:D:190:ILE:HD11 | 2.23                     | 0.74              |
| 1:E:26:PHE:HE1   | 1:E:48:LYS:HG2   | 1.53                     | 0.74              |
| 1:I:35:ARG:NE    | 1:I:98:GLU:OE2   | 2.21                     | 0.74              |
| 1:D:91:ILE:HD13  | 1:D:150:SER:HB3  | 1.69                     | 0.74              |
| 1:L:62:ILE:O     | 1:L:66:ASN:HB2   | 1.88                     | 0.73              |
| 1:D:33:TYR:HB2   | 1:D:43:PHE:CE2   | 2.23                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:49:TYR:O     | 1:G:129:ARG:HD3  | 1.85                     | 0.73              |
| 1:L:75:TRP:CD1   | 1:L:161:LEU:HD21 | 2.22                     | 0.73              |
| 1:G:56:THR:HG21  | 1:G:61:LEU:HD23  | 1.69                     | 0.73              |
| 1:G:26:PHE:HE1   | 1:G:48:LYS:HG2   | 1.54                     | 0.73              |
| 1:I:140:THR:HB   | 1:J:52:THR:O     | 1.89                     | 0.73              |
| 1:F:75:TRP:CH2   | 1:F:190:ILE:HD11 | 2.23                     | 0.73              |
| 1:G:65:LEU:O     | 1:G:69:VAL:HG23  | 1.89                     | 0.73              |
| 1:C:37:ILE:HD11  | 1:C:88:ILE:HD13  | 1.71                     | 0.73              |
| 1:C:72:LEU:HD11  | 1:C:155:ILE:HD11 | 1.69                     | 0.73              |
| 1:G:72:LEU:HD11  | 1:G:155:ILE:HD11 | 1.71                     | 0.73              |
| 1:G:10:SER:HA    | 1:G:117:ARG:O    | 1.88                     | 0.72              |
| 1:I:26:PHE:CE1   | 1:I:48:LYS:HG2   | 2.24                     | 0.72              |
| 1:I:136:THR:O    | 1:I:139:VAL:HG12 | 1.89                     | 0.72              |
| 1:K:10:SER:HA    | 1:K:117:ARG:O    | 1.88                     | 0.72              |
| 1:C:38:TYR:CE1   | 1:C:61:LEU:HD22  | 2.24                     | 0.72              |
| 1:B:33:TYR:HB2   | 1:B:43:PHE:CE2   | 2.25                     | 0.72              |
| 1:G:154:LEU:HD22 | 1:J:199:TYR:O    | 1.89                     | 0.72              |
| 1:J:23:PHE:CE1   | 1:J:128:ILE:HG12 | 2.24                     | 0.72              |
| 1:I:65:LEU:O     | 1:I:69:VAL:HG23  | 1.89                     | 0.72              |
| 1:E:37:ILE:HD11  | 1:E:88:ILE:HD13  | 1.71                     | 0.72              |
| 1:H:201:ILE:HG22 | 1:H:201:ILE:O    | 1.90                     | 0.72              |
| 1:I:35:ARG:HH11  | 1:I:35:ARG:CG    | 2.02                     | 0.72              |
| 1:D:201:ILE:HG22 | 1:D:201:ILE:O    | 1.89                     | 0.71              |
| 1:E:72:LEU:HD11  | 1:E:155:ILE:HD11 | 1.71                     | 0.71              |
| 1:H:198:ALA:HB3  | 1:I:170:SER:O    | 1.91                     | 0.71              |
| 1:I:35:ARG:HH21  | 1:I:145:LEU:HD11 | 1.52                     | 0.71              |
| 1:J:62:ILE:O     | 1:J:66:ASN:HB2   | 1.90                     | 0.71              |
| 1:K:65:LEU:O     | 1:K:69:VAL:HG23  | 1.91                     | 0.71              |
| 1:G:38:TYR:CE1   | 1:G:61:LEU:HD22  | 2.25                     | 0.71              |
| 1:A:26:PHE:HE1   | 1:A:48:LYS:HG2   | 1.55                     | 0.71              |
| 1:B:201:ILE:HG22 | 1:B:201:ILE:O    | 1.90                     | 0.71              |
| 1:H:201:ILE:HD11 | 1:I:167:TRP:CZ3  | 2.25                     | 0.71              |
| 1:I:134:GLN:O    | 1:I:138:THR:HG23 | 1.91                     | 0.71              |
| 1:H:201:ILE:HG12 | 1:I:167:TRP:CZ3  | 2.25                     | 0.71              |
| 1:F:47:GLN:HG3   | 1:F:47:GLN:O     | 1.91                     | 0.71              |
| 1:I:72:LEU:HD11  | 1:I:155:ILE:HD11 | 1.73                     | 0.71              |
| 1:C:26:PHE:HE1   | 1:C:48:LYS:HG2   | 1.54                     | 0.71              |
| 1:E:38:TYR:CE1   | 1:E:61:LEU:HD22  | 2.26                     | 0.70              |
| 1:I:35:ARG:CZ    | 1:I:35:ARG:HB3   | 2.21                     | 0.70              |
| 1:K:72:LEU:HD11  | 1:K:155:ILE:HD11 | 1.73                     | 0.70              |
| 1:A:59:LEU:HD21  | 1:E:55:VAL:HG21  | 1.72                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:62:ILE:O     | 1:F:66:ASN:HB2   | 1.91                     | 0.70              |
| 1:C:58:ASP:O     | 1:C:62:ILE:HG13  | 1.92                     | 0.70              |
| 1:J:201:ILE:O    | 1:J:201:ILE:HG22 | 1.90                     | 0.70              |
| 1:B:63:LYS:CE    | 1:H:63:LYS:HE2   | 2.20                     | 0.70              |
| 1:C:33:TYR:CE1   | 1:C:54:LEU:HD22  | 2.27                     | 0.70              |
| 1:D:62:ILE:O     | 1:D:66:ASN:HB2   | 1.91                     | 0.70              |
| 1:K:26:PHE:HE1   | 1:K:48:LYS:HG2   | 1.56                     | 0.70              |
| 1:L:23:PHE:CE1   | 1:L:128:ILE:HG12 | 2.26                     | 0.70              |
| 1:F:47:GLN:NE2   | 1:I:38:TYR:HE2   | 1.90                     | 0.70              |
| 1:F:147:VAL:HG23 | 1:F:148:SER:O    | 1.92                     | 0.70              |
| 1:D:42:THR:HB    | 1:D:43:PHE:CD1   | 2.27                     | 0.69              |
| 1:J:147:VAL:HG23 | 1:J:148:SER:O    | 1.92                     | 0.69              |
| 1:C:65:LEU:O     | 1:C:69:VAL:HG23  | 1.92                     | 0.69              |
| 1:B:62:ILE:O     | 1:B:66:ASN:HB2   | 1.92                     | 0.69              |
| 1:B:147:VAL:HG23 | 1:B:148:SER:O    | 1.91                     | 0.69              |
| 1:J:33:TYR:HB2   | 1:J:43:PHE:CE2   | 2.27                     | 0.69              |
| 1:D:23:PHE:CE1   | 1:D:128:ILE:HG12 | 2.23                     | 0.69              |
| 1:G:170:SER:N    | 1:J:198:ALA:O    | 2.23                     | 0.69              |
| 1:I:144:LEU:CD2  | 1:J:129:ARG:NH2  | 2.55                     | 0.69              |
| 1:F:42:THR:HB    | 1:F:43:PHE:CD1   | 2.28                     | 0.68              |
| 1:H:201:ILE:HG12 | 1:I:167:TRP:CE3  | 2.28                     | 0.68              |
| 1:H:62:ILE:O     | 1:H:66:ASN:HB2   | 1.92                     | 0.68              |
| 1:I:56:THR:HG21  | 1:I:61:LEU:HD23  | 1.73                     | 0.68              |
| 1:D:147:VAL:HG23 | 1:D:148:SER:O    | 1.94                     | 0.68              |
| 1:I:34:GLN:HG2   | 1:J:45:ARG:HH22  | 1.57                     | 0.68              |
| 1:K:37:ILE:HD11  | 1:K:88:ILE:HD13  | 1.73                     | 0.68              |
| 1:K:38:TYR:CE1   | 1:K:61:LEU:HD22  | 2.29                     | 0.68              |
| 1:B:23:PHE:CE1   | 1:B:128:ILE:HG12 | 2.23                     | 0.68              |
| 1:H:42:THR:HB    | 1:H:43:PHE:CD1   | 2.29                     | 0.68              |
| 1:C:56:THR:HG21  | 1:C:61:LEU:HD23  | 1.74                     | 0.68              |
| 1:E:31:ILE:O     | 1:E:35:ARG:HG2   | 1.94                     | 0.68              |
| 1:H:147:VAL:HG23 | 1:H:148:SER:O    | 1.94                     | 0.68              |
| 1:B:48:LYS:HG2   | 1:B:49:TYR:CE1   | 2.29                     | 0.67              |
| 1:B:63:LYS:HE2   | 1:H:63:LYS:CE    | 2.23                     | 0.67              |
| 1:L:48:LYS:HG2   | 1:L:49:TYR:CE1   | 2.28                     | 0.67              |
| 1:I:34:GLN:OE1   | 1:I:136:THR:HG23 | 1.93                     | 0.67              |
| 1:I:35:ARG:NH2   | 1:I:98:GLU:CD    | 2.52                     | 0.67              |
| 1:D:42:THR:HB    | 1:D:43:PHE:HD1   | 1.58                     | 0.67              |
| 1:I:133:ARG:HD3  | 1:J:33:TYR:O     | 1.93                     | 0.67              |
| 1:I:172:PRO:HB2  | 1:I:174:PHE:CE1  | 2.29                     | 0.67              |
| 1:F:49:TYR:CE2   | 1:F:124:ILE:HG21 | 2.29                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:74:ASP:O     | 1:H:77:TYR:HD2   | 1.77                     | 0.67              |
| 1:H:168:GLU:HB2  | 1:H:170:SER:O    | 1.95                     | 0.67              |
| 1:D:63:LYS:HG3   | 1:L:59:LEU:HD21  | 1.74                     | 0.67              |
| 1:K:83:LYS:HB2   | 1:K:156:TYR:HB2  | 1.76                     | 0.67              |
| 1:L:74:ASP:O     | 1:L:77:TYR:HD2   | 1.78                     | 0.67              |
| 1:E:141:PHE:HA   | 1:F:129:ARG:HG2  | 1.76                     | 0.67              |
| 1:I:167:TRP:H    | 1:I:167:TRP:CD1  | 2.12                     | 0.67              |
| 1:F:42:THR:HB    | 1:F:43:PHE:HD1   | 1.59                     | 0.67              |
| 1:G:31:ILE:O     | 1:G:35:ARG:HG2   | 1.95                     | 0.67              |
| 1:L:42:THR:HB    | 1:L:43:PHE:CD1   | 2.29                     | 0.67              |
| 1:L:147:VAL:HG23 | 1:L:148:SER:O    | 1.94                     | 0.67              |
| 1:B:91:ILE:HD13  | 1:B:150:SER:HB3  | 1.76                     | 0.66              |
| 1:H:33:TYR:HB2   | 1:H:43:PHE:CE2   | 2.29                     | 0.66              |
| 1:I:34:GLN:HG2   | 1:J:45:ARG:NH2   | 2.10                     | 0.66              |
| 1:A:129:ARG:NH1  | 2:A:207:SO4:O2   | 2.29                     | 0.66              |
| 1:B:42:THR:HB    | 1:B:43:PHE:CD1   | 2.31                     | 0.66              |
| 1:D:122:LYS:HA   | 1:K:41:GLU:HB2   | 1.76                     | 0.66              |
| 1:K:31:ILE:O     | 1:K:35:ARG:HG2   | 1.96                     | 0.66              |
| 1:I:144:LEU:HD23 | 1:J:129:ARG:NH2  | 2.10                     | 0.66              |
| 1:G:167:TRP:CZ3  | 1:J:201:ILE:HD11 | 2.30                     | 0.66              |
| 1:I:58:ASP:O     | 1:I:62:ILE:HG13  | 1.95                     | 0.66              |
| 1:J:130:SER:O    | 1:J:134:GLN:HG3  | 1.96                     | 0.66              |
| 1:F:26:PHE:HE1   | 1:F:49:TYR:HE1   | 1.44                     | 0.66              |
| 1:C:167:TRP:CD1  | 1:C:167:TRP:H    | 2.14                     | 0.66              |
| 1:F:74:ASP:O     | 1:F:77:TYR:HD2   | 1.78                     | 0.66              |
| 1:L:42:THR:HB    | 1:L:43:PHE:HD1   | 1.61                     | 0.66              |
| 1:D:48:LYS:HG2   | 1:D:49:TYR:CE1   | 2.31                     | 0.66              |
| 1:E:83:LYS:HB2   | 1:E:156:TYR:HB2  | 1.77                     | 0.66              |
| 1:E:167:TRP:H    | 1:E:167:TRP:CD1  | 2.12                     | 0.66              |
| 1:H:146:GLU:HA   | 1:H:182:ARG:NH2  | 2.11                     | 0.66              |
| 1:H:201:ILE:CD1  | 1:I:167:TRP:CZ3  | 2.78                     | 0.66              |
| 1:K:58:ASP:O     | 1:K:62:ILE:HG13  | 1.96                     | 0.66              |
| 1:H:42:THR:HB    | 1:H:43:PHE:HD1   | 1.60                     | 0.66              |
| 1:I:26:PHE:HE1   | 1:I:48:LYS:HG2   | 1.60                     | 0.66              |
| 1:B:74:ASP:O     | 1:B:77:TYR:HD2   | 1.79                     | 0.66              |
| 1:F:130:SER:O    | 1:F:134:GLN:HG3  | 1.95                     | 0.66              |
| 1:A:65:LEU:O     | 1:A:69:VAL:HG23  | 1.96                     | 0.65              |
| 1:E:172:PRO:CB   | 1:E:174:PHE:CE1  | 2.79                     | 0.65              |
| 1:A:38:TYR:CE1   | 1:A:61:LEU:HD22  | 2.30                     | 0.65              |
| 1:I:141:PHE:O    | 1:J:129:ARG:HD3  | 1.96                     | 0.65              |
| 1:J:146:GLU:HA   | 1:J:182:ARG:NH2  | 2.12                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:172:PRO:HB2  | 1:C:174:PHE:CE1  | 2.31                     | 0.65              |
| 1:G:167:TRP:H    | 1:G:167:TRP:CD1  | 2.14                     | 0.65              |
| 1:G:172:PRO:HB2  | 1:G:174:PHE:CE1  | 2.31                     | 0.65              |
| 1:J:42:THR:HB    | 1:J:43:PHE:CD1   | 2.32                     | 0.65              |
| 1:B:130:SER:O    | 1:B:134:GLN:HG3  | 1.97                     | 0.65              |
| 1:L:146:GLU:HA   | 1:L:182:ARG:NH2  | 2.11                     | 0.65              |
| 1:B:146:GLU:HA   | 1:B:182:ARG:NH2  | 2.12                     | 0.65              |
| 1:G:58:ASP:O     | 1:G:62:ILE:HG13  | 1.95                     | 0.65              |
| 1:A:167:TRP:CD1  | 1:A:167:TRP:H    | 2.11                     | 0.65              |
| 1:E:58:ASP:O     | 1:E:62:ILE:HG13  | 1.97                     | 0.65              |
| 1:H:23:PHE:CE1   | 1:H:128:ILE:HG12 | 2.26                     | 0.65              |
| 1:K:167:TRP:H    | 1:K:167:TRP:CD1  | 2.15                     | 0.65              |
| 1:B:42:THR:HB    | 1:B:43:PHE:HD1   | 1.62                     | 0.64              |
| 1:F:33:TYR:HB2   | 1:F:43:PHE:CE2   | 2.32                     | 0.64              |
| 1:H:48:LYS:HG2   | 1:H:49:TYR:CE1   | 2.32                     | 0.64              |
| 1:B:63:LYS:NZ    | 1:H:63:LYS:CE    | 2.60                     | 0.64              |
| 1:K:33:TYR:CE1   | 1:K:54:LEU:HD22  | 2.32                     | 0.64              |
| 1:L:33:TYR:HB2   | 1:L:43:PHE:CE2   | 2.32                     | 0.64              |
| 1:B:63:LYS:CE    | 1:H:63:LYS:CE    | 2.75                     | 0.64              |
| 1:H:130:SER:O    | 1:H:134:GLN:HG3  | 1.97                     | 0.64              |
| 1:D:74:ASP:O     | 1:D:77:TYR:HD2   | 1.79                     | 0.64              |
| 1:D:130:SER:O    | 1:D:134:GLN:HG3  | 1.97                     | 0.64              |
| 1:L:168:GLU:HB2  | 1:L:170:SER:O    | 1.96                     | 0.64              |
| 1:A:83:LYS:HB2   | 1:A:156:TYR:HB2  | 1.80                     | 0.64              |
| 1:D:46:VAL:HA    | 1:L:46:VAL:HA    | 1.80                     | 0.64              |
| 1:L:130:SER:O    | 1:L:134:GLN:HG3  | 1.98                     | 0.64              |
| 1:H:163:VAL:HG22 | 1:H:190:ILE:HD12 | 1.79                     | 0.64              |
| 1:I:83:LYS:HB2   | 1:I:156:TYR:HB2  | 1.79                     | 0.64              |
| 1:A:172:PRO:HB2  | 1:A:174:PHE:CE1  | 2.32                     | 0.64              |
| 1:F:146:GLU:HA   | 1:F:182:ARG:NH2  | 2.12                     | 0.64              |
| 1:I:36:GLY:O     | 1:I:37:ILE:HG22  | 1.97                     | 0.64              |
| 1:J:42:THR:HB    | 1:J:43:PHE:HD1   | 1.63                     | 0.63              |
| 1:F:168:GLU:O    | 1:F:169:GLU:HB3  | 1.98                     | 0.63              |
| 1:J:74:ASP:O     | 1:J:77:TYR:HD2   | 1.79                     | 0.63              |
| 1:C:31:ILE:O     | 1:C:35:ARG:HG2   | 1.99                     | 0.63              |
| 1:A:129:ARG:HH12 | 1:A:133:ARG:NH2  | 1.97                     | 0.63              |
| 1:A:33:TYR:CE1   | 1:A:54:LEU:HD22  | 2.34                     | 0.63              |
| 1:A:58:ASP:O     | 1:A:62:ILE:HG13  | 1.97                     | 0.63              |
| 1:G:83:LYS:HB2   | 1:G:156:TYR:HB2  | 1.81                     | 0.62              |
| 1:J:168:GLU:O    | 1:J:169:GLU:HB3  | 1.98                     | 0.62              |
| 1:E:33:TYR:CE1   | 1:E:54:LEU:HD22  | 2.34                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:34:GLN:HB3   | 1:I:139:VAL:CG2  | 2.27                     | 0.62              |
| 1:C:72:LEU:HD11  | 1:C:155:ILE:CD1  | 2.29                     | 0.62              |
| 1:C:129:ARG:NH2  | 2:C:206:SO4:O4   | 2.30                     | 0.62              |
| 1:D:146:GLU:HA   | 1:D:182:ARG:NH2  | 2.14                     | 0.62              |
| 1:I:33:TYR:CE1   | 1:I:54:LEU:HD22  | 2.33                     | 0.62              |
| 1:I:51:LEU:HD21  | 1:I:129:ARG:HG2  | 1.82                     | 0.62              |
| 1:J:48:LYS:HG2   | 1:J:49:TYR:CE1   | 2.34                     | 0.62              |
| 1:K:30:SER:O     | 1:K:34:GLN:HG3   | 1.99                     | 0.62              |
| 1:L:163:VAL:HG22 | 1:L:190:ILE:HD12 | 1.80                     | 0.62              |
| 1:I:85:VAL:HB    | 1:I:154:LEU:HB2  | 1.82                     | 0.62              |
| 1:A:72:LEU:HD11  | 1:A:155:ILE:CD1  | 2.30                     | 0.61              |
| 1:B:63:LYS:CE    | 1:H:63:LYS:NZ    | 2.63                     | 0.61              |
| 1:G:51:LEU:HD21  | 1:G:129:ARG:HG2  | 1.82                     | 0.61              |
| 1:C:33:TYR:CZ    | 1:C:54:LEU:HD22  | 2.35                     | 0.61              |
| 1:B:165:GLU:H    | 1:B:165:GLU:CD   | 2.09                     | 0.61              |
| 1:A:31:ILE:O     | 1:A:35:ARG:HG2   | 2.00                     | 0.61              |
| 1:C:83:LYS:HB2   | 1:C:156:TYR:HB2  | 1.83                     | 0.61              |
| 1:F:165:GLU:CD   | 1:F:165:GLU:H    | 2.07                     | 0.61              |
| 1:H:168:GLU:O    | 1:H:169:GLU:HB3  | 2.01                     | 0.61              |
| 1:E:51:LEU:HD21  | 1:E:129:ARG:HG2  | 1.83                     | 0.61              |
| 1:L:168:GLU:O    | 1:L:169:GLU:HB3  | 2.00                     | 0.61              |
| 1:D:179:GLU:CD   | 1:D:180:GLU:H    | 2.09                     | 0.60              |
| 1:E:33:TYR:CD2   | 1:E:54:LEU:HD13  | 2.35                     | 0.60              |
| 1:K:172:PRO:CB   | 1:K:174:PHE:CE1  | 2.83                     | 0.60              |
| 1:I:35:ARG:NE    | 1:I:88:ILE:HD12  | 2.10                     | 0.60              |
| 1:A:85:VAL:HB    | 1:A:154:LEU:HB2  | 1.84                     | 0.60              |
| 1:F:46:VAL:HA    | 1:I:146:GLU:HB2  | 1.81                     | 0.60              |
| 1:G:33:TYR:CE1   | 1:G:54:LEU:HD22  | 2.35                     | 0.60              |
| 1:L:14:ARG:HA    | 1:L:105:GLU:HB3  | 1.84                     | 0.60              |
| 1:C:85:VAL:HB    | 1:C:154:LEU:HB2  | 1.84                     | 0.60              |
| 1:G:129:ARG:HH12 | 1:G:133:ARG:NH2  | 2.00                     | 0.60              |
| 1:G:133:ARG:HD3  | 1:H:33:TYR:O     | 2.02                     | 0.60              |
| 1:D:90:ASN:CG    | 1:D:93:SER:HB2   | 2.27                     | 0.59              |
| 1:L:14:ARG:HB3   | 1:L:105:GLU:HG2  | 1.83                     | 0.59              |
| 1:I:35:ARG:NH1   | 1:I:35:ARG:CB    | 2.64                     | 0.59              |
| 1:J:179:GLU:CD   | 1:J:180:GLU:H    | 2.10                     | 0.59              |
| 1:G:129:ARG:NH1  | 1:G:133:ARG:NH2  | 2.51                     | 0.59              |
| 1:A:100:TRP:CD2  | 1:A:197:VAL:HG23 | 2.37                     | 0.59              |
| 1:L:179:GLU:CD   | 1:L:180:GLU:H    | 2.11                     | 0.59              |
| 1:C:129:ARG:HH12 | 1:C:133:ARG:NH2  | 2.00                     | 0.59              |
| 1:A:30:SER:O     | 1:A:34:GLN:HG3   | 2.03                     | 0.59              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:K:51:LEU:HD21  | 1:K:129:ARG:HG2 | 1.85                     | 0.59              |
| 1:H:201:ILE:CG1  | 1:I:167:TRP:CZ3 | 2.85                     | 0.58              |
| 1:I:72:LEU:HD11  | 1:I:155:ILE:CD1 | 2.33                     | 0.58              |
| 1:I:133:ARG:HD3  | 1:J:34:GLN:CA   | 2.33                     | 0.58              |
| 1:H:64:TYR:HE1   | 1:H:172:PRO:O   | 1.87                     | 0.58              |
| 1:A:59:LEU:HD22  | 1:E:44:THR:HG22 | 1.85                     | 0.58              |
| 1:A:129:ARG:NH1  | 1:A:133:ARG:NH2 | 2.51                     | 0.58              |
| 1:B:43:PHE:HD1   | 1:B:43:PHE:N    | 2.01                     | 0.58              |
| 1:C:33:TYR:CD2   | 1:C:54:LEU:HD13 | 2.38                     | 0.58              |
| 1:B:159:LYS:O    | 1:B:159:LYS:HG3 | 2.02                     | 0.58              |
| 1:A:59:LEU:HD22  | 1:E:44:THR:CG2  | 2.33                     | 0.58              |
| 1:G:72:LEU:HD11  | 1:G:155:ILE:CD1 | 2.33                     | 0.58              |
| 1:B:179:GLU:CD   | 1:B:180:GLU:H   | 2.11                     | 0.58              |
| 1:D:159:LYS:O    | 1:D:159:LYS:HG3 | 2.02                     | 0.58              |
| 1:G:42:THR:HB    | 1:G:43:PHE:CD1  | 2.39                     | 0.58              |
| 1:G:33:TYR:CD2   | 1:G:54:LEU:HD13 | 2.39                     | 0.58              |
| 1:K:33:TYR:CZ    | 1:K:54:LEU:HD22 | 2.38                     | 0.58              |
| 1:D:168:GLU:O    | 1:D:169:GLU:HB3 | 2.03                     | 0.58              |
| 1:G:30:SER:O     | 1:G:34:GLN:HG3  | 2.04                     | 0.58              |
| 1:G:91:ILE:HD13  | 1:G:150:SER:OG  | 2.04                     | 0.58              |
| 1:I:38:TYR:HB3   | 1:I:39:PRO:HD2  | 1.85                     | 0.58              |
| 1:B:200:LYS:HE3  | 1:C:170:SER:OG  | 2.03                     | 0.58              |
| 1:E:72:LEU:HD11  | 1:E:155:ILE:CD1 | 2.33                     | 0.58              |
| 1:D:165:GLU:CD   | 1:D:165:GLU:H   | 2.11                     | 0.58              |
| 1:F:179:GLU:CD   | 1:F:180:GLU:H   | 2.11                     | 0.58              |
| 1:C:91:ILE:HD13  | 1:C:150:SER:OG  | 2.04                     | 0.57              |
| 1:L:162:VAL:HG23 | 1:L:162:VAL:O   | 2.04                     | 0.57              |
| 1:I:91:ILE:HD13  | 1:I:150:SER:OG  | 2.03                     | 0.57              |
| 1:A:91:ILE:HD13  | 1:A:150:SER:OG  | 2.03                     | 0.57              |
| 1:E:91:ILE:HD13  | 1:E:150:SER:OG  | 2.04                     | 0.57              |
| 1:E:133:ARG:HD3  | 1:F:33:TYR:O    | 2.04                     | 0.57              |
| 1:F:14:ARG:HA    | 1:F:105:GLU:HB3 | 1.85                     | 0.57              |
| 1:B:168:GLU:O    | 1:B:169:GLU:HB3 | 2.03                     | 0.57              |
| 1:K:72:LEU:HD11  | 1:K:155:ILE:CD1 | 2.34                     | 0.57              |
| 1:A:33:TYR:CD2   | 1:A:54:LEU:HD13 | 2.39                     | 0.57              |
| 1:B:90:ASN:CG    | 1:B:93:SER:HB2  | 2.30                     | 0.57              |
| 1:B:14:ARG:HA    | 1:B:105:GLU:HB3 | 1.85                     | 0.57              |
| 1:F:159:LYS:O    | 1:F:159:LYS:HG3 | 2.04                     | 0.57              |
| 1:K:91:ILE:HD13  | 1:K:150:SER:OG  | 2.05                     | 0.57              |
| 1:L:168:GLU:C    | 1:L:170:SER:H   | 2.13                     | 0.57              |
| 1:K:64:TYR:CD1   | 1:K:64:TYR:C    | 2.83                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:30:SER:O     | 1:C:34:GLN:HG3   | 2.05                     | 0.56              |
| 1:E:172:PRO:HB3  | 1:E:174:PHE:CZ   | 2.40                     | 0.56              |
| 1:F:49:TYR:CE1   | 1:F:128:ILE:HD11 | 2.40                     | 0.56              |
| 1:J:159:LYS:HG3  | 1:J:159:LYS:O    | 2.03                     | 0.56              |
| 1:G:64:TYR:CD1   | 1:G:64:TYR:C     | 2.83                     | 0.56              |
| 1:H:31:ILE:HD13  | 1:H:100:TRP:CD2  | 2.40                     | 0.56              |
| 1:K:33:TYR:CD2   | 1:K:54:LEU:HD13  | 2.39                     | 0.56              |
| 1:D:91:ILE:CD1   | 1:D:150:SER:HB3  | 2.34                     | 0.56              |
| 1:F:16:SER:O     | 1:F:19:ILE:HG22  | 2.04                     | 0.56              |
| 1:F:88:ILE:HG12  | 1:F:151:PHE:CE1  | 2.40                     | 0.56              |
| 1:H:14:ARG:HA    | 1:H:105:GLU:HB3  | 1.88                     | 0.56              |
| 1:I:144:LEU:HD21 | 1:J:129:ARG:NH2  | 2.20                     | 0.56              |
| 1:K:42:THR:HB    | 1:K:43:PHE:CD1   | 2.40                     | 0.56              |
| 1:F:47:GLN:HB3   | 1:I:146:GLU:O    | 2.05                     | 0.56              |
| 1:H:16:SER:O     | 1:H:19:ILE:HG22  | 2.05                     | 0.56              |
| 1:L:43:PHE:HD1   | 1:L:43:PHE:N     | 2.04                     | 0.56              |
| 1:A:42:THR:HB    | 1:A:43:PHE:CD1   | 2.40                     | 0.56              |
| 1:K:129:ARG:HH12 | 1:K:133:ARG:NH2  | 2.03                     | 0.56              |
| 1:B:43:PHE:CD1   | 1:B:43:PHE:N     | 2.72                     | 0.56              |
| 1:C:129:ARG:NH1  | 1:C:133:ARG:NH2  | 2.54                     | 0.56              |
| 1:D:14:ARG:HA    | 1:D:105:GLU:HB3  | 1.87                     | 0.56              |
| 1:H:8:HIS:CG     | 1:H:9:GLY:H      | 2.24                     | 0.56              |
| 1:I:129:ARG:NH1  | 1:I:133:ARG:NH2  | 2.54                     | 0.56              |
| 1:I:35:ARG:NH1   | 1:I:35:ARG:CG    | 2.64                     | 0.56              |
| 1:H:43:PHE:HD1   | 1:H:43:PHE:N     | 2.04                     | 0.56              |
| 1:H:179:GLU:CD   | 1:H:180:GLU:H    | 2.14                     | 0.56              |
| 1:K:129:ARG:NH1  | 1:K:133:ARG:NH2  | 2.53                     | 0.56              |
| 1:D:43:PHE:HD1   | 1:D:43:PHE:N     | 2.04                     | 0.56              |
| 1:E:129:ARG:HH12 | 1:E:133:ARG:NH2  | 2.04                     | 0.56              |
| 1:G:85:VAL:HB    | 1:G:154:LEU:HB2  | 1.88                     | 0.55              |
| 1:I:31:ILE:HD13  | 1:I:100:TRP:CD2  | 2.41                     | 0.55              |
| 1:I:34:GLN:OE1   | 1:J:45:ARG:NH2   | 2.39                     | 0.55              |
| 1:A:33:TYR:CZ    | 1:A:54:LEU:HD22  | 2.41                     | 0.55              |
| 1:A:133:ARG:HD3  | 1:B:33:TYR:O     | 2.05                     | 0.55              |
| 1:E:33:TYR:CZ    | 1:E:54:LEU:HD22  | 2.41                     | 0.55              |
| 1:E:64:TYR:CD1   | 1:E:64:TYR:C     | 2.83                     | 0.55              |
| 1:F:19:ILE:CG2   | 1:F:20:VAL:N     | 2.70                     | 0.55              |
| 1:H:168:GLU:C    | 1:H:170:SER:H    | 2.13                     | 0.55              |
| 1:I:139:VAL:HG13 | 1:I:140:THR:N    | 2.20                     | 0.55              |
| 1:A:51:LEU:HD21  | 1:A:129:ARG:HG2  | 1.87                     | 0.55              |
| 1:A:64:TYR:CD1   | 1:A:64:TYR:C     | 2.85                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:91:ILE:HG22  | 1:A:148:SER:O    | 2.06                     | 0.55              |
| 1:C:183:LEU:HB2  | 1:C:195:SER:O    | 2.07                     | 0.55              |
| 1:I:172:PRO:CB   | 1:I:174:PHE:CE1  | 2.89                     | 0.55              |
| 1:B:63:LYS:HZ1   | 1:H:63:LYS:HZ1   | 1.55                     | 0.55              |
| 1:F:136:THR:O    | 1:F:139:VAL:HG13 | 2.07                     | 0.55              |
| 1:C:31:ILE:HD13  | 1:C:100:TRP:CD2  | 2.42                     | 0.55              |
| 1:H:173:GLN:HB2  | 1:H:187:THR:HG22 | 1.89                     | 0.55              |
| 1:B:31:ILE:HD13  | 1:B:100:TRP:CD2  | 2.42                     | 0.55              |
| 1:E:129:ARG:NH1  | 1:E:133:ARG:NH2  | 2.55                     | 0.55              |
| 1:I:40:SER:O     | 1:I:43:PHE:O     | 2.25                     | 0.55              |
| 1:K:164:PRO:O    | 1:K:167:TRP:HD1  | 1.89                     | 0.55              |
| 1:I:24:PHE:CE2   | 1:I:84:LEU:HG    | 2.43                     | 0.55              |
| 1:K:85:VAL:HB    | 1:K:154:LEU:HB2  | 1.89                     | 0.55              |
| 1:A:59:LEU:CD2   | 1:E:55:VAL:CG2   | 2.85                     | 0.54              |
| 1:L:31:ILE:HD13  | 1:L:100:TRP:CD2  | 2.42                     | 0.54              |
| 1:A:33:TYR:CE2   | 1:A:54:LEU:HD13  | 2.42                     | 0.54              |
| 1:C:108:LYS:HD2  | 1:C:111:LYS:NZ   | 2.22                     | 0.54              |
| 1:D:43:PHE:CD1   | 1:D:43:PHE:N     | 2.75                     | 0.54              |
| 1:I:64:TYR:CD1   | 1:I:64:TYR:C     | 2.84                     | 0.54              |
| 1:A:164:PRO:O    | 1:A:167:TRP:HD1  | 1.91                     | 0.54              |
| 1:E:164:PRO:O    | 1:E:167:TRP:HD1  | 1.91                     | 0.54              |
| 1:F:31:ILE:HD13  | 1:F:100:TRP:CD2  | 2.43                     | 0.54              |
| 1:A:108:LYS:HD2  | 1:A:111:LYS:NZ   | 2.22                     | 0.54              |
| 1:E:33:TYR:CE2   | 1:E:54:LEU:HD13  | 2.43                     | 0.54              |
| 1:J:31:ILE:HD13  | 1:J:100:TRP:CD2  | 2.43                     | 0.54              |
| 1:A:82:GLN:CD    | 1:D:196:MET:HE1  | 2.32                     | 0.54              |
| 1:E:85:VAL:HB    | 1:E:154:LEU:HB2  | 1.89                     | 0.54              |
| 1:K:31:ILE:HD13  | 1:K:100:TRP:CD2  | 2.43                     | 0.54              |
| 1:F:19:ILE:HG23  | 1:F:20:VAL:N     | 2.23                     | 0.54              |
| 1:E:42:THR:HB    | 1:E:43:PHE:CD1   | 2.42                     | 0.54              |
| 1:G:164:PRO:O    | 1:G:167:TRP:HD1  | 1.91                     | 0.54              |
| 1:L:43:PHE:CD1   | 1:L:43:PHE:N     | 2.74                     | 0.54              |
| 1:E:31:ILE:HD13  | 1:E:100:TRP:CD2  | 2.43                     | 0.54              |
| 1:I:129:ARG:HH12 | 1:I:133:ARG:NH2  | 2.06                     | 0.54              |
| 1:K:100:TRP:CD2  | 1:K:197:VAL:HG23 | 2.42                     | 0.54              |
| 1:C:41:GLU:HB2   | 1:L:122:LYS:HA   | 1.89                     | 0.54              |
| 1:C:64:TYR:CD1   | 1:C:64:TYR:C     | 2.86                     | 0.54              |
| 1:C:164:PRO:O    | 1:C:167:TRP:HD1  | 1.90                     | 0.54              |
| 1:G:167:TRP:HZ3  | 1:J:201:ILE:HD11 | 1.72                     | 0.54              |
| 1:H:19:ILE:CG2   | 1:H:20:VAL:N     | 2.71                     | 0.54              |
| 1:E:30:SER:O     | 1:E:34:GLN:HG3   | 2.08                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:43:PHE:CD1   | 1:H:43:PHE:N     | 2.74                     | 0.53              |
| 1:A:59:LEU:HD21  | 1:E:55:VAL:CG2   | 2.39                     | 0.53              |
| 1:G:33:TYR:CZ    | 1:G:54:LEU:HD22  | 2.43                     | 0.53              |
| 1:I:164:PRO:O    | 1:I:167:TRP:HD1  | 1.92                     | 0.53              |
| 1:C:28:ILE:HD13  | 1:C:153:LEU:HD21 | 1.90                     | 0.53              |
| 1:I:142:LEU:O    | 1:I:143:PRO:C    | 2.51                     | 0.53              |
| 1:A:183:LEU:HB2  | 1:A:195:SER:O    | 2.09                     | 0.53              |
| 1:L:16:SER:O     | 1:L:19:ILE:HG22  | 2.09                     | 0.53              |
| 1:L:90:ASN:CB    | 1:L:93:SER:HB3   | 2.37                     | 0.53              |
| 1:F:91:ILE:CD1   | 1:F:150:SER:HB3  | 2.39                     | 0.53              |
| 1:G:51:LEU:HD21  | 1:G:129:ARG:CG   | 2.38                     | 0.53              |
| 1:K:33:TYR:CE2   | 1:K:54:LEU:HD13  | 2.44                     | 0.53              |
| 1:C:42:THR:HB    | 1:C:43:PHE:CD1   | 2.43                     | 0.53              |
| 1:A:82:GLN:OE1   | 1:D:196:MET:HE1  | 2.08                     | 0.53              |
| 1:F:120:SER:CB   | 1:I:58:ASP:OD1   | 2.57                     | 0.53              |
| 1:I:33:TYR:CZ    | 1:I:54:LEU:HD22  | 2.43                     | 0.53              |
| 1:J:90:ASN:CB    | 1:J:93:SER:HB3   | 2.37                     | 0.53              |
| 1:D:63:LYS:HE2   | 1:L:63:LYS:HE2   | 1.91                     | 0.52              |
| 1:F:47:GLN:HE21  | 1:I:38:TYR:HE2   | 1.56                     | 0.52              |
| 1:I:100:TRP:CD2  | 1:I:197:VAL:HG23 | 2.44                     | 0.52              |
| 1:J:14:ARG:HA    | 1:J:105:GLU:HB3  | 1.91                     | 0.52              |
| 1:G:31:ILE:HD13  | 1:G:100:TRP:CD2  | 2.44                     | 0.52              |
| 1:L:19:ILE:CG2   | 1:L:20:VAL:N     | 2.72                     | 0.52              |
| 1:C:100:TRP:CD2  | 1:C:197:VAL:HG23 | 2.44                     | 0.52              |
| 1:I:34:GLN:CG    | 1:J:45:ARG:HH22  | 2.22                     | 0.52              |
| 1:K:91:ILE:HG22  | 1:K:148:SER:O    | 2.10                     | 0.52              |
| 1:L:175:ILE:HG22 | 1:L:176:THR:N    | 2.24                     | 0.52              |
| 1:A:43:PHE:CD1   | 1:A:43:PHE:N     | 2.77                     | 0.52              |
| 1:A:82:GLN:HB2   | 1:D:196:MET:HE1  | 1.91                     | 0.52              |
| 1:A:82:GLN:HB2   | 1:D:196:MET:CE   | 2.39                     | 0.52              |
| 1:G:54:LEU:N     | 1:G:54:LEU:HD12  | 2.24                     | 0.52              |
| 1:A:172:PRO:CB   | 1:A:174:PHE:CE1  | 2.93                     | 0.52              |
| 1:G:100:TRP:CD2  | 1:G:197:VAL:HG23 | 2.44                     | 0.52              |
| 1:J:43:PHE:CD1   | 1:J:43:PHE:N     | 2.77                     | 0.52              |
| 1:C:43:PHE:CD1   | 1:C:43:PHE:N     | 2.78                     | 0.52              |
| 1:C:129:ARG:NH1  | 2:C:206:SO4:O1   | 2.40                     | 0.52              |
| 1:F:43:PHE:CD1   | 1:F:43:PHE:N     | 2.77                     | 0.52              |
| 1:C:33:TYR:CE2   | 1:C:54:LEU:HD13  | 2.44                     | 0.52              |
| 1:G:49:TYR:HD2   | 1:G:125:GLN:HG3  | 1.75                     | 0.52              |
| 1:I:24:PHE:CD2   | 1:I:84:LEU:HG    | 2.44                     | 0.52              |
| 1:J:43:PHE:HD1   | 1:J:43:PHE:N     | 2.07                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:33:TYR:CD2   | 1:I:54:LEU:HD13  | 2.45                     | 0.52              |
| 1:I:88:ILE:HB    | 1:I:98:GLU:HB3   | 1.92                     | 0.52              |
| 1:K:88:ILE:HB    | 1:K:98:GLU:HB3   | 1.90                     | 0.52              |
| 1:C:172:PRO:CB   | 1:C:174:PHE:CE1  | 2.93                     | 0.51              |
| 1:E:141:PHE:HA   | 1:F:129:ARG:CG   | 2.40                     | 0.51              |
| 1:G:91:ILE:HG22  | 1:G:148:SER:O    | 2.10                     | 0.51              |
| 1:H:174:PHE:CE1  | 1:H:186:PHE:HB3  | 2.44                     | 0.51              |
| 1:I:49:TYR:HD2   | 1:I:125:GLN:HG3  | 1.75                     | 0.51              |
| 1:L:88:ILE:HG12  | 1:L:151:PHE:CE1  | 2.46                     | 0.51              |
| 1:G:172:PRO:CB   | 1:G:174:PHE:CE1  | 2.92                     | 0.51              |
| 1:J:19:ILE:CG2   | 1:J:20:VAL:N     | 2.73                     | 0.51              |
| 1:C:88:ILE:HB    | 1:C:98:GLU:HB3   | 1.92                     | 0.51              |
| 1:E:49:TYR:HD2   | 1:E:125:GLN:HG3  | 1.75                     | 0.51              |
| 1:G:24:PHE:O     | 1:G:28:ILE:HG13  | 2.10                     | 0.51              |
| 1:A:24:PHE:O     | 1:A:28:ILE:HG13  | 2.10                     | 0.51              |
| 1:B:122:LYS:HD3  | 1:G:41:GLU:HG3   | 1.93                     | 0.51              |
| 1:C:133:ARG:HD3  | 1:D:33:TYR:O     | 2.09                     | 0.51              |
| 1:J:91:ILE:CD1   | 1:J:150:SER:HB3  | 2.36                     | 0.51              |
| 1:L:197:VAL:HG11 | 1:L:199:TYR:OH   | 2.08                     | 0.51              |
| 1:C:49:TYR:HD2   | 1:C:125:GLN:HG3  | 1.75                     | 0.51              |
| 1:F:43:PHE:HD1   | 1:F:43:PHE:N     | 2.07                     | 0.51              |
| 1:G:43:PHE:CD1   | 1:G:43:PHE:N     | 2.78                     | 0.51              |
| 1:G:88:ILE:HB    | 1:G:98:GLU:HB3   | 1.93                     | 0.51              |
| 1:J:163:VAL:HG13 | 1:J:163:VAL:O    | 2.11                     | 0.51              |
| 1:A:49:TYR:HD2   | 1:A:125:GLN:HG3  | 1.75                     | 0.51              |
| 1:B:163:VAL:HG13 | 1:B:163:VAL:O    | 2.11                     | 0.51              |
| 1:E:141:PHE:O    | 1:F:129:ARG:HD3  | 2.10                     | 0.51              |
| 1:A:31:ILE:HD13  | 1:A:100:TRP:CD2  | 2.45                     | 0.51              |
| 1:D:32:LEU:HD13  | 1:D:61:LEU:HD21  | 1.93                     | 0.51              |
| 1:D:90:ASN:ND2   | 1:D:93:SER:HB2   | 2.25                     | 0.51              |
| 1:I:51:LEU:CD2   | 1:J:40:SER:OG    | 2.58                     | 0.51              |
| 1:I:139:VAL:HA   | 1:I:142:LEU:HD12 | 1.93                     | 0.51              |
| 1:A:88:ILE:HB    | 1:A:98:GLU:HB3   | 1.93                     | 0.51              |
| 1:C:78:LYS:O     | 1:C:79:CYS:HB2   | 2.09                     | 0.51              |
| 1:E:100:TRP:CD2  | 1:E:197:VAL:HG23 | 2.46                     | 0.51              |
| 1:K:49:TYR:HD2   | 1:K:125:GLN:HG3  | 1.76                     | 0.51              |
| 1:K:172:PRO:HB3  | 1:K:174:PHE:CZ   | 2.46                     | 0.51              |
| 1:C:188:THR:C    | 1:C:189:THR:HG23 | 2.37                     | 0.50              |
| 1:E:88:ILE:HB    | 1:E:98:GLU:HB3   | 1.93                     | 0.50              |
| 1:B:88:ILE:HG12  | 1:B:151:PHE:CE1  | 2.46                     | 0.50              |
| 1:C:24:PHE:CE2   | 1:C:84:LEU:HG    | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:91:ILE:HG22  | 1:C:148:SER:O    | 2.11                     | 0.50              |
| 1:E:178:SER:O    | 1:E:201:ILE:HD11 | 2.11                     | 0.50              |
| 1:F:90:ASN:CG    | 1:F:93:SER:HB2   | 2.37                     | 0.50              |
| 1:J:90:ASN:CG    | 1:J:93:SER:HB2   | 2.36                     | 0.50              |
| 1:K:51:LEU:HD21  | 1:K:129:ARG:CG   | 2.41                     | 0.50              |
| 1:C:24:PHE:O     | 1:C:28:ILE:HG13  | 2.12                     | 0.50              |
| 1:E:24:PHE:O     | 1:E:28:ILE:HG13  | 2.10                     | 0.50              |
| 1:H:136:THR:O    | 1:H:139:VAL:HG13 | 2.12                     | 0.50              |
| 1:L:75:TRP:CG    | 1:L:161:LEU:HD21 | 2.47                     | 0.50              |
| 1:L:135:ILE:O    | 1:L:139:VAL:HG12 | 2.11                     | 0.50              |
| 1:G:170:SER:O    | 1:J:198:ALA:CB   | 2.58                     | 0.50              |
| 1:H:8:HIS:CG     | 1:H:9:GLY:N      | 2.79                     | 0.50              |
| 1:I:35:ARG:NH2   | 1:I:98:GLU:OE1   | 2.44                     | 0.50              |
| 1:K:78:LYS:O     | 1:K:79:CYS:HB2   | 2.11                     | 0.50              |
| 1:L:19:ILE:HG23  | 1:L:20:VAL:N     | 2.26                     | 0.50              |
| 1:L:163:VAL:O    | 1:L:164:PRO:C    | 2.54                     | 0.50              |
| 1:E:43:PHE:CD1   | 1:E:43:PHE:N     | 2.77                     | 0.50              |
| 1:E:51:LEU:HD21  | 1:E:129:ARG:CG   | 2.42                     | 0.50              |
| 1:K:43:PHE:CD1   | 1:K:43:PHE:N     | 2.80                     | 0.50              |
| 1:L:197:VAL:CG1  | 1:L:199:TYR:CZ   | 2.94                     | 0.50              |
| 1:B:155:ILE:HB   | 1:B:190:ILE:HG12 | 1.93                     | 0.50              |
| 1:D:90:ASN:CG    | 1:D:93:SER:CB    | 2.85                     | 0.50              |
| 1:D:137:ALA:O    | 1:D:140:THR:HB   | 2.11                     | 0.50              |
| 1:H:91:ILE:CD1   | 1:H:150:SER:HB3  | 2.37                     | 0.50              |
| 1:L:75:TRP:CD1   | 1:L:161:LEU:HD11 | 2.46                     | 0.50              |
| 1:C:27:GLY:O     | 1:C:31:ILE:HG13  | 2.12                     | 0.50              |
| 1:D:90:ASN:CB    | 1:D:93:SER:HB3   | 2.35                     | 0.50              |
| 1:F:174:PHE:CE1  | 1:F:186:PHE:HB3  | 2.47                     | 0.50              |
| 1:I:164:PRO:HB2  | 1:I:167:TRP:HE1  | 1.76                     | 0.50              |
| 1:K:164:PRO:HB2  | 1:K:167:TRP:HE1  | 1.77                     | 0.50              |
| 1:G:78:LYS:O     | 1:G:79:CYS:HB2   | 2.12                     | 0.50              |
| 1:H:173:GLN:CB   | 1:H:187:THR:HG22 | 2.41                     | 0.50              |
| 1:K:32:LEU:HD22  | 1:K:37:ILE:CG2   | 2.36                     | 0.50              |
| 1:D:47:GLN:HB2   | 1:D:51:LEU:O     | 2.12                     | 0.50              |
| 1:F:16:SER:O     | 1:F:20:VAL:HG23  | 2.12                     | 0.50              |
| 1:G:33:TYR:CE2   | 1:G:54:LEU:HD13  | 2.47                     | 0.50              |
| 1:K:178:SER:O    | 1:K:201:ILE:HD11 | 2.12                     | 0.50              |
| 1:B:201:ILE:HD11 | 1:C:167:TRP:CZ3  | 2.47                     | 0.49              |
| 1:D:19:ILE:CG2   | 1:D:20:VAL:N     | 2.75                     | 0.49              |
| 1:D:161:LEU:C    | 1:D:163:VAL:H    | 2.19                     | 0.49              |
| 1:E:129:ARG:O    | 1:E:133:ARG:HB2  | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:164:PRO:HB2  | 1:E:167:TRP:HE1  | 1.76                     | 0.49              |
| 1:H:88:ILE:HG12  | 1:H:151:PHE:CE1  | 2.47                     | 0.49              |
| 1:I:34:GLN:HB3   | 1:I:139:VAL:HG11 | 1.93                     | 0.49              |
| 1:I:51:LEU:HD21  | 1:I:129:ARG:CG   | 2.41                     | 0.49              |
| 1:E:24:PHE:CE2   | 1:E:84:LEU:HG    | 2.48                     | 0.49              |
| 1:G:64:TYR:C     | 1:G:64:TYR:HD1   | 2.20                     | 0.49              |
| 1:I:91:ILE:HG22  | 1:I:148:SER:O    | 2.12                     | 0.49              |
| 1:J:88:ILE:HG12  | 1:J:151:PHE:CE1  | 2.46                     | 0.49              |
| 1:J:174:PHE:CE1  | 1:J:186:PHE:HB3  | 2.46                     | 0.49              |
| 1:C:51:LEU:HD21  | 1:C:129:ARG:HG2  | 1.93                     | 0.49              |
| 1:G:183:LEU:HB2  | 1:G:195:SER:O    | 2.12                     | 0.49              |
| 1:I:40:SER:O     | 1:I:43:PHE:N     | 2.45                     | 0.49              |
| 1:L:138:THR:C    | 1:L:140:THR:N    | 2.70                     | 0.49              |
| 1:A:24:PHE:CE2   | 1:A:84:LEU:HG    | 2.48                     | 0.49              |
| 1:A:51:LEU:HD21  | 1:A:129:ARG:CG   | 2.42                     | 0.49              |
| 1:B:174:PHE:CE1  | 1:B:186:PHE:HB3  | 2.48                     | 0.49              |
| 1:I:24:PHE:O     | 1:I:28:ILE:HG13  | 2.13                     | 0.49              |
| 1:C:32:LEU:HD22  | 1:C:37:ILE:CG2   | 2.38                     | 0.49              |
| 1:C:108:LYS:HD2  | 1:C:111:LYS:HZ1  | 1.78                     | 0.49              |
| 1:H:19:ILE:HG23  | 1:H:20:VAL:N     | 2.27                     | 0.49              |
| 1:B:16:SER:O     | 1:B:20:VAL:HG23  | 2.13                     | 0.49              |
| 1:D:174:PHE:CE1  | 1:D:186:PHE:HB3  | 2.47                     | 0.49              |
| 1:B:138:THR:C    | 1:B:140:THR:N    | 2.70                     | 0.49              |
| 1:C:24:PHE:CD2   | 1:C:84:LEU:HG    | 2.47                     | 0.49              |
| 1:D:16:SER:O     | 1:D:20:VAL:HG23  | 2.13                     | 0.49              |
| 1:F:33:TYR:CD2   | 1:F:54:LEU:HD23  | 2.47                     | 0.49              |
| 1:J:19:ILE:HG23  | 1:J:20:VAL:N     | 2.27                     | 0.49              |
| 1:A:178:SER:O    | 1:A:201:ILE:HD11 | 2.13                     | 0.49              |
| 1:E:91:ILE:HG22  | 1:E:148:SER:O    | 2.12                     | 0.49              |
| 1:K:131:VAL:HG12 | 1:K:132:ILE:N    | 2.28                     | 0.49              |
| 1:B:19:ILE:CG2   | 1:B:20:VAL:N     | 2.75                     | 0.49              |
| 1:D:122:LYS:CA   | 1:K:41:GLU:HB2   | 2.43                     | 0.49              |
| 1:A:170:SER:OG   | 1:D:200:LYS:HE3  | 2.13                     | 0.48              |
| 1:E:56:THR:CG2   | 1:E:61:LEU:HD23  | 2.42                     | 0.48              |
| 1:G:24:PHE:CE2   | 1:G:84:LEU:HG    | 2.48                     | 0.48              |
| 1:H:32:LEU:HD13  | 1:H:61:LEU:HD21  | 1.95                     | 0.48              |
| 1:H:201:ILE:HD11 | 1:I:167:TRP:HZ3  | 1.74                     | 0.48              |
| 1:K:64:TYR:C     | 1:K:64:TYR:HD1   | 2.21                     | 0.48              |
| 1:B:90:ASN:CB    | 1:B:93:SER:HB3   | 2.37                     | 0.48              |
| 1:C:38:TYR:CD1   | 1:C:61:LEU:HD22  | 2.48                     | 0.48              |
| 1:E:183:LEU:HB2  | 1:E:195:SER:O    | 2.12                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:F:155:ILE:HB  | 1:F:190:ILE:HG12 | 1.94                     | 0.48              |
| 1:H:163:VAL:O   | 1:H:164:PRO:C    | 2.55                     | 0.48              |
| 1:J:136:THR:O   | 1:J:139:VAL:HG13 | 2.13                     | 0.48              |
| 1:D:31:ILE:HD13 | 1:D:100:TRP:CD2  | 2.47                     | 0.48              |
| 1:E:129:ARG:NH1 | 2:E:206:SO4:O4   | 2.40                     | 0.48              |
| 1:F:49:TYR:CD2  | 1:F:124:ILE:HG21 | 2.48                     | 0.48              |
| 1:I:178:SER:O   | 1:I:201:ILE:HD11 | 2.13                     | 0.48              |
| 1:J:161:LEU:C   | 1:J:163:VAL:H    | 2.20                     | 0.48              |
| 1:K:56:THR:HG21 | 1:K:61:LEU:CD2   | 2.41                     | 0.48              |
| 1:A:164:PRO:HB2 | 1:A:167:TRP:HE1  | 1.78                     | 0.48              |
| 1:C:43:PHE:O    | 1:L:121:GLN:HB3  | 2.14                     | 0.48              |
| 1:F:47:GLN:NE2  | 1:I:38:TYR:CE2   | 2.76                     | 0.48              |
| 1:G:152:ASP:OD2 | 1:J:200:LYS:HD3  | 2.14                     | 0.48              |
| 1:H:90:ASN:CG   | 1:H:93:SER:HB2   | 2.38                     | 0.48              |
| 1:H:167:TRP:CH2 | 1:H:172:PRO:HD2  | 2.49                     | 0.48              |
| 1:A:24:PHE:CD2  | 1:A:84:LEU:HG    | 2.49                     | 0.48              |
| 1:F:14:ARG:HB3  | 1:F:105:GLU:HG2  | 1.94                     | 0.48              |
| 1:F:50:GLY:O    | 1:I:148:SER:HB3  | 2.14                     | 0.48              |
| 1:G:164:PRO:HB2 | 1:G:167:TRP:HE1  | 1.78                     | 0.48              |
| 1:H:135:ILE:O   | 1:H:139:VAL:HG12 | 2.12                     | 0.48              |
| 1:H:167:TRP:CZ3 | 1:H:171:GLY:HA2  | 2.48                     | 0.48              |
| 1:I:35:ARG:CZ   | 1:I:98:GLU:OE1   | 2.62                     | 0.48              |
| 1:K:28:ILE:HD13 | 1:K:153:LEU:HD21 | 1.95                     | 0.48              |
| 1:L:14:ARG:HB3  | 1:L:105:GLU:CB   | 2.44                     | 0.48              |
| 1:L:155:ILE:HB  | 1:L:190:ILE:HG12 | 1.96                     | 0.48              |
| 1:C:54:LEU:HD12 | 1:C:54:LEU:N     | 2.29                     | 0.48              |
| 1:F:135:ILE:O   | 1:F:139:VAL:HG12 | 2.13                     | 0.48              |
| 1:J:16:SER:O    | 1:J:19:ILE:HG22  | 2.14                     | 0.48              |
| 1:B:76:LEU:C    | 1:B:78:LYS:H     | 2.21                     | 0.48              |
| 1:F:14:ARG:HB3  | 1:F:105:GLU:CB   | 2.44                     | 0.48              |
| 1:J:76:LEU:C    | 1:J:78:LYS:H     | 2.21                     | 0.48              |
| 1:D:33:TYR:CD2  | 1:D:54:LEU:HD23  | 2.49                     | 0.48              |
| 1:E:78:LYS:O    | 1:E:79:CYS:HB2   | 2.13                     | 0.48              |
| 1:F:161:LEU:C   | 1:F:163:VAL:H    | 2.21                     | 0.48              |
| 1:G:129:ARG:O   | 1:G:133:ARG:HB2  | 2.13                     | 0.48              |
| 1:G:178:SER:O   | 1:G:201:ILE:HD11 | 2.14                     | 0.48              |
| 1:I:129:ARG:O   | 1:I:133:ARG:HB2  | 2.13                     | 0.48              |
| 1:I:138:THR:HA  | 1:I:141:PHE:HE1  | 1.75                     | 0.48              |
| 1:E:172:PRO:CB  | 1:E:174:PHE:CZ   | 2.97                     | 0.48              |
| 1:H:14:ARG:HB3  | 1:H:105:GLU:CB   | 2.44                     | 0.48              |
| 1:L:91:ILE:CD1  | 1:L:150:SER:HB3  | 2.39                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:164:PRO:HB2  | 1:C:167:TRP:HE1  | 1.79                     | 0.47              |
| 1:J:179:GLU:CG   | 1:J:180:GLU:N    | 2.77                     | 0.47              |
| 1:L:90:ASN:CG    | 1:L:93:SER:HB2   | 2.38                     | 0.47              |
| 1:D:14:ARG:HB3   | 1:D:105:GLU:CB   | 2.44                     | 0.47              |
| 1:D:179:GLU:CG   | 1:D:180:GLU:N    | 2.77                     | 0.47              |
| 1:E:56:THR:HG21  | 1:E:61:LEU:CD2   | 2.42                     | 0.47              |
| 1:G:38:TYR:CD1   | 1:G:61:LEU:HD22  | 2.49                     | 0.47              |
| 1:I:138:THR:HG22 | 1:J:136:THR:HG21 | 1.96                     | 0.47              |
| 1:J:33:TYR:CD2   | 1:J:54:LEU:HD23  | 2.49                     | 0.47              |
| 1:L:132:ILE:HD13 | 1:L:132:ILE:N    | 2.29                     | 0.47              |
| 1:B:14:ARG:HB3   | 1:B:105:GLU:CB   | 2.44                     | 0.47              |
| 1:C:51:LEU:HD21  | 1:C:129:ARG:CG   | 2.43                     | 0.47              |
| 1:D:16:SER:O     | 1:D:19:ILE:HG22  | 2.14                     | 0.47              |
| 1:G:42:THR:HB    | 1:G:43:PHE:CE1   | 2.49                     | 0.47              |
| 1:I:38:TYR:HB3   | 1:I:39:PRO:HD3   | 1.95                     | 0.47              |
| 1:J:135:ILE:O    | 1:J:139:VAL:HG12 | 2.14                     | 0.47              |
| 1:E:54:LEU:N     | 1:E:54:LEU:HD12  | 2.30                     | 0.47              |
| 1:F:120:SER:CB   | 1:I:58:ASP:CG    | 2.84                     | 0.47              |
| 1:F:163:VAL:O    | 1:F:163:VAL:HG13 | 2.14                     | 0.47              |
| 1:G:129:ARG:NH2  | 2:G:206:SO4:O1   | 2.47                     | 0.47              |
| 1:J:155:ILE:HB   | 1:J:190:ILE:HG12 | 1.96                     | 0.47              |
| 1:K:84:LEU:HD13  | 1:K:84:LEU:C     | 2.39                     | 0.47              |
| 1:K:84:LEU:HD13  | 1:K:85:VAL:N     | 2.29                     | 0.47              |
| 1:L:33:TYR:CD2   | 1:L:54:LEU:HD23  | 2.50                     | 0.47              |
| 1:B:135:ILE:O    | 1:B:139:VAL:HG12 | 2.15                     | 0.47              |
| 1:E:24:PHE:CD2   | 1:E:84:LEU:HG    | 2.49                     | 0.47              |
| 1:F:48:LYS:HG3   | 1:F:49:TYR:CE1   | 2.49                     | 0.47              |
| 1:F:138:THR:C    | 1:F:140:THR:N    | 2.72                     | 0.47              |
| 1:G:24:PHE:CD2   | 1:G:84:LEU:HG    | 2.49                     | 0.47              |
| 1:L:24:PHE:O     | 1:L:28:ILE:HG22  | 2.15                     | 0.47              |
| 1:L:76:LEU:C     | 1:L:78:LYS:N     | 2.73                     | 0.47              |
| 1:L:167:TRP:CZ3  | 1:L:171:GLY:HA2  | 2.49                     | 0.47              |
| 1:L:179:GLU:CG   | 1:L:180:GLU:N    | 2.78                     | 0.47              |
| 1:A:129:ARG:O    | 1:A:133:ARG:HB2  | 2.14                     | 0.47              |
| 1:E:42:THR:HB    | 1:E:43:PHE:CE1   | 2.50                     | 0.47              |
| 1:E:49:TYR:O     | 1:E:129:ARG:CD   | 2.59                     | 0.47              |
| 1:A:78:LYS:O     | 1:A:79:CYS:HB2   | 2.15                     | 0.47              |
| 1:A:153:LEU:O    | 1:A:154:LEU:HD23 | 2.14                     | 0.47              |
| 1:A:175:ILE:HB   | 1:A:178:SER:HB3  | 1.96                     | 0.47              |
| 1:B:90:ASN:CG    | 1:B:93:SER:CB    | 2.88                     | 0.47              |
| 1:B:196:MET:HE1  | 1:C:82:GLN:HB2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:76:LEU:C     | 1:D:78:LYS:H     | 2.21                     | 0.47              |
| 1:D:88:ILE:HG12  | 1:D:151:PHE:CE1  | 2.50                     | 0.47              |
| 1:D:163:VAL:O    | 1:D:163:VAL:HG13 | 2.15                     | 0.47              |
| 1:E:38:TYR:CD1   | 1:E:61:LEU:HD22  | 2.50                     | 0.47              |
| 1:E:64:TYR:C     | 1:E:64:TYR:HD1   | 2.22                     | 0.47              |
| 1:K:133:ARG:HD3  | 1:L:33:TYR:O     | 2.15                     | 0.47              |
| 1:A:42:THR:HB    | 1:A:43:PHE:CE1   | 2.50                     | 0.47              |
| 1:H:155:ILE:HB   | 1:H:190:ILE:HG12 | 1.96                     | 0.47              |
| 1:L:137:ALA:O    | 1:L:140:THR:HB   | 2.15                     | 0.47              |
| 1:A:56:THR:HG21  | 1:A:61:LEU:CD2   | 2.43                     | 0.47              |
| 1:A:154:LEU:HD22 | 1:D:199:TYR:O    | 2.15                     | 0.47              |
| 1:C:45:ARG:HD2   | 1:L:121:GLN:OE1  | 2.14                     | 0.47              |
| 1:D:155:ILE:HB   | 1:D:190:ILE:HG12 | 1.97                     | 0.47              |
| 1:E:20:VAL:O     | 1:E:24:PHE:HD1   | 1.98                     | 0.47              |
| 1:F:26:PHE:CE1   | 1:F:49:TYR:HE1   | 2.30                     | 0.47              |
| 1:H:76:LEU:C     | 1:H:78:LYS:H     | 2.23                     | 0.47              |
| 1:H:80:SER:HB2   | 1:H:161:LEU:HD22 | 1.97                     | 0.47              |
| 1:I:35:ARG:HH22  | 1:I:145:LEU:CD1  | 2.16                     | 0.47              |
| 1:I:78:LYS:O     | 1:I:79:CYS:HB2   | 2.13                     | 0.47              |
| 1:J:140:THR:HG22 | 1:J:141:PHE:CD1  | 2.50                     | 0.47              |
| 1:L:32:LEU:HD13  | 1:L:61:LEU:HD21  | 1.97                     | 0.47              |
| 1:B:76:LEU:C     | 1:B:78:LYS:N     | 2.73                     | 0.46              |
| 1:C:203:VAL:O    | 1:C:204:ASN:HB2  | 2.14                     | 0.46              |
| 1:D:180:GLU:OE1  | 1:D:180:GLU:HA   | 2.15                     | 0.46              |
| 1:H:39:PRO:HD3   | 1:H:181:VAL:HG22 | 1.98                     | 0.46              |
| 1:H:137:ALA:O    | 1:H:140:THR:HB   | 2.15                     | 0.46              |
| 1:I:27:GLY:O     | 1:I:31:ILE:HG13  | 2.15                     | 0.46              |
| 1:K:42:THR:HB    | 1:K:43:PHE:CE1   | 2.50                     | 0.46              |
| 1:B:161:LEU:C    | 1:B:163:VAL:H    | 2.22                     | 0.46              |
| 1:C:11:ILE:HD13  | 1:C:11:ILE:HA    | 1.75                     | 0.46              |
| 1:C:84:LEU:C     | 1:C:84:LEU:HD13  | 2.40                     | 0.46              |
| 1:D:33:TYR:HB2   | 1:D:43:PHE:CD2   | 2.51                     | 0.46              |
| 1:D:93:SER:OG    | 1:D:95:GLU:HG2   | 2.14                     | 0.46              |
| 1:G:167:TRP:CZ3  | 1:J:201:ILE:CD1  | 2.98                     | 0.46              |
| 1:K:175:ILE:HB   | 1:K:178:SER:HB3  | 1.97                     | 0.46              |
| 1:L:76:LEU:C     | 1:L:78:LYS:H     | 2.22                     | 0.46              |
| 1:D:76:LEU:C     | 1:D:78:LYS:N     | 2.72                     | 0.46              |
| 1:F:186:PHE:C    | 1:F:186:PHE:CD2  | 2.94                     | 0.46              |
| 1:J:16:SER:O     | 1:J:20:VAL:HG23  | 2.15                     | 0.46              |
| 1:K:24:PHE:CE2   | 1:K:84:LEU:HG    | 2.50                     | 0.46              |
| 1:C:131:VAL:HG12 | 1:C:132:ILE:N    | 2.29                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:138:THR:C    | 1:D:140:THR:N    | 2.71                     | 0.46              |
| 1:E:175:ILE:HB   | 1:E:178:SER:HB3  | 1.98                     | 0.46              |
| 1:F:179:GLU:CG   | 1:F:180:GLU:N    | 2.78                     | 0.46              |
| 1:G:175:ILE:HB   | 1:G:178:SER:HB3  | 1.98                     | 0.46              |
| 1:H:138:THR:C    | 1:H:140:THR:N    | 2.72                     | 0.46              |
| 1:I:153:LEU:O    | 1:I:154:LEU:HD23 | 2.16                     | 0.46              |
| 1:K:183:LEU:HB2  | 1:K:195:SER:O    | 2.16                     | 0.46              |
| 1:C:84:LEU:C     | 1:C:84:LEU:CD1   | 2.89                     | 0.46              |
| 1:G:28:ILE:HD13  | 1:G:153:LEU:HD21 | 1.96                     | 0.46              |
| 1:D:186:PHE:CD2  | 1:D:186:PHE:C    | 2.94                     | 0.46              |
| 1:H:80:SER:CB    | 1:H:161:LEU:HD22 | 2.46                     | 0.46              |
| 1:H:167:TRP:O    | 1:H:167:TRP:CE3  | 2.68                     | 0.46              |
| 1:I:133:ARG:NH1  | 1:J:33:TYR:O     | 2.47                     | 0.46              |
| 1:A:64:TYR:C     | 1:A:64:TYR:HD1   | 2.24                     | 0.46              |
| 1:B:32:LEU:HD13  | 1:B:61:LEU:HD21  | 1.98                     | 0.46              |
| 1:H:33:TYR:CD2   | 1:H:54:LEU:HD23  | 2.50                     | 0.46              |
| 1:A:48:LYS:O     | 1:A:49:TYR:HB2   | 2.16                     | 0.46              |
| 1:B:19:ILE:HG23  | 1:B:20:VAL:N     | 2.31                     | 0.46              |
| 1:B:196:MET:HE1  | 1:C:82:GLN:OE1   | 2.16                     | 0.46              |
| 1:H:21:ALA:HB1   | 1:H:69:VAL:HG13  | 1.98                     | 0.46              |
| 1:H:179:GLU:CG   | 1:H:180:GLU:N    | 2.79                     | 0.46              |
| 1:I:172:PRO:HB3  | 1:I:174:PHE:CZ   | 2.50                     | 0.46              |
| 1:J:75:TRP:CZ3   | 1:J:190:ILE:HD11 | 2.50                     | 0.46              |
| 1:L:136:THR:O    | 1:L:139:VAL:HG13 | 2.16                     | 0.46              |
| 1:A:129:ARG:HH12 | 1:A:133:ARG:HH22 | 1.64                     | 0.46              |
| 1:I:33:TYR:HD1   | 1:I:43:PHE:CD2   | 2.33                     | 0.46              |
| 1:J:76:LEU:C     | 1:J:78:LYS:N     | 2.73                     | 0.46              |
| 1:K:129:ARG:O    | 1:K:133:ARG:HB2  | 2.16                     | 0.46              |
| 1:L:58:ASP:O     | 1:L:62:ILE:HG13  | 2.16                     | 0.46              |
| 1:B:179:GLU:CG   | 1:B:180:GLU:N    | 2.79                     | 0.46              |
| 1:B:180:GLU:OE1  | 1:B:180:GLU:HA   | 2.16                     | 0.46              |
| 1:F:45:ARG:O     | 1:I:146:GLU:CD   | 2.59                     | 0.46              |
| 1:F:58:ASP:O     | 1:F:62:ILE:HG13  | 2.16                     | 0.46              |
| 1:H:64:TYR:CE1   | 1:H:172:PRO:O    | 2.68                     | 0.46              |
| 1:A:188:THR:C    | 1:A:189:THR:HG23 | 2.40                     | 0.45              |
| 1:C:42:THR:HB    | 1:C:43:PHE:CE1   | 2.52                     | 0.45              |
| 1:G:11:ILE:HD13  | 1:G:11:ILE:HA    | 1.77                     | 0.45              |
| 1:H:75:TRP:CD1   | 1:H:161:LEU:HD21 | 2.51                     | 0.45              |
| 1:I:131:VAL:HG12 | 1:I:132:ILE:N    | 2.31                     | 0.45              |
| 1:J:32:LEU:HD13  | 1:J:61:LEU:HD21  | 1.98                     | 0.45              |
| 1:K:84:LEU:C     | 1:K:84:LEU:CD1   | 2.89                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:153:LEU:O    | 1:K:154:LEU:HD23 | 2.17                     | 0.45              |
| 1:D:136:THR:O    | 1:D:139:VAL:HG13 | 2.15                     | 0.45              |
| 1:G:27:GLY:O     | 1:G:31:ILE:HG13  | 2.16                     | 0.45              |
| 1:G:56:THR:HG21  | 1:G:61:LEU:CD2   | 2.41                     | 0.45              |
| 1:I:34:GLN:HE22  | 1:I:136:THR:HA   | 1.81                     | 0.45              |
| 1:K:38:TYR:CD1   | 1:K:61:LEU:HD22  | 2.51                     | 0.45              |
| 1:J:14:ARG:HB3   | 1:J:105:GLU:CB   | 2.45                     | 0.45              |
| 1:L:64:TYR:HE1   | 1:L:172:PRO:O    | 1.98                     | 0.45              |
| 1:L:167:TRP:CH2  | 1:L:172:PRO:HD2  | 2.52                     | 0.45              |
| 1:A:108:LYS:HD2  | 1:A:111:LYS:HZ1  | 1.81                     | 0.45              |
| 1:B:33:TYR:CD2   | 1:B:54:LEU:HD23  | 2.51                     | 0.45              |
| 1:B:93:SER:OG    | 1:B:95:GLU:HG2   | 2.17                     | 0.45              |
| 1:C:129:ARG:O    | 1:C:133:ARG:HB2  | 2.17                     | 0.45              |
| 1:C:178:SER:O    | 1:C:201:ILE:HD11 | 2.16                     | 0.45              |
| 1:F:76:LEU:C     | 1:F:78:LYS:H     | 2.23                     | 0.45              |
| 1:G:34:GLN:OE1   | 1:G:136:THR:HA   | 2.16                     | 0.45              |
| 1:G:56:THR:CG2   | 1:G:61:LEU:HD23  | 2.42                     | 0.45              |
| 1:J:58:ASP:O     | 1:J:62:ILE:HG13  | 2.17                     | 0.45              |
| 1:L:59:LEU:HD12  | 1:L:59:LEU:HA    | 1.84                     | 0.45              |
| 1:L:75:TRP:CZ3   | 1:L:190:ILE:HD11 | 2.51                     | 0.45              |
| 1:B:160:ASP:O    | 1:B:161:LEU:HG   | 2.16                     | 0.45              |
| 1:E:34:GLN:OE1   | 1:E:136:THR:HA   | 2.16                     | 0.45              |
| 1:F:120:SER:HB3  | 1:I:58:ASP:OD1   | 2.16                     | 0.45              |
| 1:G:135:ILE:O    | 1:G:138:THR:HG22 | 2.17                     | 0.45              |
| 1:I:28:ILE:HD13  | 1:I:153:LEU:HD21 | 1.97                     | 0.45              |
| 1:K:56:THR:CG2   | 1:K:61:LEU:HD23  | 2.41                     | 0.45              |
| 1:L:78:LYS:HG3   | 1:L:80:SER:OG    | 2.17                     | 0.45              |
| 1:D:19:ILE:HG23  | 1:D:20:VAL:N     | 2.31                     | 0.45              |
| 1:F:186:PHE:C    | 1:F:186:PHE:HD2  | 2.24                     | 0.45              |
| 1:I:39:PRO:O     | 1:I:40:SER:C     | 2.60                     | 0.45              |
| 1:I:139:VAL:CG1  | 1:I:140:THR:N    | 2.80                     | 0.45              |
| 1:A:54:LEU:HD12  | 1:A:54:LEU:N     | 2.32                     | 0.45              |
| 1:F:72:LEU:HD21  | 1:F:84:LEU:HD11  | 1.99                     | 0.45              |
| 1:I:20:VAL:O     | 1:I:24:PHE:HD1   | 1.99                     | 0.45              |
| 1:K:24:PHE:CD2   | 1:K:84:LEU:HG    | 2.52                     | 0.45              |
| 1:E:175:ILE:O    | 1:E:176:THR:C    | 2.60                     | 0.45              |
| 1:G:131:VAL:HG12 | 1:G:132:ILE:N    | 2.31                     | 0.45              |
| 1:K:34:GLN:OE1   | 1:K:136:THR:HA   | 2.16                     | 0.45              |
| 1:K:54:LEU:HD12  | 1:K:54:LEU:N     | 2.31                     | 0.45              |
| 1:A:56:THR:CG2   | 1:A:61:LEU:HD23  | 2.42                     | 0.45              |
| 1:C:49:TYR:O     | 1:C:129:ARG:CD   | 2.61                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:64:TYR:C     | 1:C:64:TYR:HD1   | 2.24                     | 0.45              |
| 1:D:159:LYS:HA   | 1:D:192:LYS:HB3  | 1.99                     | 0.45              |
| 1:E:131:VAL:HG12 | 1:E:132:ILE:N    | 2.32                     | 0.45              |
| 1:F:137:ALA:O    | 1:F:140:THR:HB   | 2.17                     | 0.45              |
| 1:H:75:TRP:CZ3   | 1:H:190:ILE:HD11 | 2.51                     | 0.45              |
| 1:H:90:ASN:CB    | 1:H:93:SER:HB3   | 2.39                     | 0.45              |
| 1:I:142:LEU:O    | 1:I:143:PRO:O    | 2.34                     | 0.45              |
| 1:L:39:PRO:HD3   | 1:L:181:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:100:TRP:CE3  | 1:A:197:VAL:HG23 | 2.52                     | 0.45              |
| 1:B:47:GLN:HB2   | 1:B:51:LEU:O     | 2.17                     | 0.45              |
| 1:B:136:THR:O    | 1:B:139:VAL:HG13 | 2.16                     | 0.45              |
| 1:E:28:ILE:HD13  | 1:E:153:LEU:HD21 | 1.99                     | 0.45              |
| 1:F:90:ASN:CB    | 1:F:93:SER:HB3   | 2.39                     | 0.45              |
| 1:I:175:ILE:HB   | 1:I:178:SER:HB3  | 1.98                     | 0.45              |
| 1:L:167:TRP:O    | 1:L:167:TRP:CE3  | 2.70                     | 0.45              |
| 1:B:137:ALA:O    | 1:B:140:THR:HB   | 2.16                     | 0.44              |
| 1:D:17:ALA:C     | 1:D:19:ILE:N     | 2.72                     | 0.44              |
| 1:D:31:ILE:HD13  | 1:D:100:TRP:CE3  | 2.52                     | 0.44              |
| 1:L:93:SER:OG    | 1:L:95:GLU:HG2   | 2.17                     | 0.44              |
| 1:B:196:MET:HE1  | 1:C:82:GLN:CD    | 2.43                     | 0.44              |
| 1:C:175:ILE:HB   | 1:C:178:SER:HB3  | 1.97                     | 0.44              |
| 1:D:21:ALA:HB1   | 1:D:69:VAL:HG13  | 1.98                     | 0.44              |
| 1:F:76:LEU:C     | 1:F:78:LYS:N     | 2.74                     | 0.44              |
| 1:H:180:GLU:HA   | 1:H:180:GLU:OE1  | 2.17                     | 0.44              |
| 1:J:21:ALA:HB1   | 1:J:69:VAL:HG13  | 1.99                     | 0.44              |
| 1:B:76:LEU:O     | 1:B:78:LYS:N     | 2.51                     | 0.44              |
| 1:C:84:LEU:HD13  | 1:C:85:VAL:N     | 2.32                     | 0.44              |
| 1:D:48:LYS:O     | 1:D:49:TYR:HB2   | 2.17                     | 0.44              |
| 1:G:117:ARG:HA   | 1:G:117:ARG:HD2  | 1.45                     | 0.44              |
| 1:H:160:ASP:OD2  | 1:I:159:LYS:NZ   | 2.50                     | 0.44              |
| 1:I:35:ARG:HH11  | 1:I:35:ARG:CB    | 2.29                     | 0.44              |
| 1:A:32:LEU:HD22  | 1:A:37:ILE:CG2   | 2.39                     | 0.44              |
| 1:B:196:MET:CE   | 1:C:82:GLN:HB2   | 2.47                     | 0.44              |
| 1:D:184:ARG:HA   | 1:D:184:ARG:HD3  | 1.81                     | 0.44              |
| 1:D:186:PHE:C    | 1:D:186:PHE:HD2  | 2.25                     | 0.44              |
| 1:E:32:LEU:HD22  | 1:E:37:ILE:CG2   | 2.39                     | 0.44              |
| 1:L:72:LEU:HD21  | 1:L:84:LEU:HD11  | 1.99                     | 0.44              |
| 1:B:91:ILE:CD1   | 1:B:150:SER:HB3  | 2.43                     | 0.44              |
| 1:B:199:TYR:O    | 1:C:154:LEU:HD22 | 2.18                     | 0.44              |
| 1:C:56:THR:HG21  | 1:C:61:LEU:CD2   | 2.46                     | 0.44              |
| 1:F:48:LYS:HD2   | 1:F:48:LYS:HA    | 1.79                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:84:LEU:HD13  | 1:G:84:LEU:C     | 2.42                     | 0.44              |
| 1:I:64:TYR:C     | 1:I:64:TYR:HD1   | 2.23                     | 0.44              |
| 1:J:39:PRO:HD3   | 1:J:181:VAL:HG22 | 1.99                     | 0.44              |
| 1:J:90:ASN:ND2   | 1:J:93:SER:HB2   | 2.33                     | 0.44              |
| 1:B:59:LEU:HD12  | 1:B:59:LEU:HA    | 1.88                     | 0.44              |
| 1:D:76:LEU:O     | 1:D:78:LYS:N     | 2.50                     | 0.44              |
| 1:E:84:LEU:HD13  | 1:E:85:VAL:N     | 2.33                     | 0.44              |
| 1:F:75:TRP:CZ3   | 1:F:190:ILE:HD11 | 2.52                     | 0.44              |
| 1:G:188:THR:C    | 1:G:189:THR:HG23 | 2.43                     | 0.44              |
| 1:J:137:ALA:O    | 1:J:140:THR:HB   | 2.16                     | 0.44              |
| 1:K:129:ARG:NH2  | 2:K:206:SO4:O2   | 2.49                     | 0.44              |
| 1:L:28:ILE:O     | 1:L:32:LEU:HG    | 2.17                     | 0.44              |
| 1:L:138:THR:O    | 1:L:140:THR:N    | 2.51                     | 0.44              |
| 1:L:197:VAL:HG11 | 1:L:199:TYR:CZ   | 2.53                     | 0.44              |
| 1:B:16:SER:O     | 1:B:19:ILE:HG22  | 2.18                     | 0.44              |
| 1:G:175:ILE:O    | 1:G:176:THR:C    | 2.61                     | 0.44              |
| 1:B:90:ASN:ND2   | 1:B:93:SER:HB2   | 2.33                     | 0.44              |
| 1:D:135:ILE:O    | 1:D:139:VAL:HG12 | 2.17                     | 0.44              |
| 1:F:21:ALA:HB1   | 1:F:69:VAL:HG13  | 2.00                     | 0.44              |
| 1:G:84:LEU:HD13  | 1:G:85:VAL:N     | 2.33                     | 0.44              |
| 1:G:153:LEU:O    | 1:G:154:LEU:HD23 | 2.18                     | 0.44              |
| 1:G:172:PRO:HB3  | 1:G:174:PHE:CZ   | 2.53                     | 0.44              |
| 1:J:93:SER:OG    | 1:J:95:GLU:HG2   | 2.18                     | 0.44              |
| 1:K:133:ARG:NH2  | 2:K:206:SO4:O4   | 2.51                     | 0.44              |
| 1:A:135:ILE:O    | 1:A:138:THR:HG22 | 2.17                     | 0.43              |
| 1:C:34:GLN:OE1   | 1:C:136:THR:HA   | 2.18                     | 0.43              |
| 1:C:48:LYS:O     | 1:C:49:TYR:HB2   | 2.17                     | 0.43              |
| 1:J:186:PHE:C    | 1:J:186:PHE:CD2  | 2.96                     | 0.43              |
| 1:B:21:ALA:HB1   | 1:B:69:VAL:HG13  | 2.00                     | 0.43              |
| 1:B:65:LEU:HD23  | 1:B:65:LEU:HA    | 1.76                     | 0.43              |
| 1:B:72:LEU:HD21  | 1:B:84:LEU:HD11  | 2.00                     | 0.43              |
| 1:G:171:GLY:HA2  | 1:G:172:PRO:HD3  | 1.83                     | 0.43              |
| 1:H:72:LEU:HD21  | 1:H:84:LEU:HD11  | 2.00                     | 0.43              |
| 1:L:90:ASN:CG    | 1:L:93:SER:CB    | 2.92                     | 0.43              |
| 1:A:28:ILE:HD13  | 1:A:153:LEU:HD21 | 2.00                     | 0.43              |
| 1:D:160:ASP:O    | 1:D:161:LEU:HG   | 2.18                     | 0.43              |
| 1:H:90:ASN:ND2   | 1:H:93:SER:HB2   | 2.34                     | 0.43              |
| 1:J:72:LEU:HD21  | 1:J:84:LEU:HD11  | 1.99                     | 0.43              |
| 1:A:34:GLN:OE1   | 1:A:136:THR:HA   | 2.18                     | 0.43              |
| 1:A:38:TYR:CD1   | 1:A:61:LEU:HD22  | 2.53                     | 0.43              |
| 1:A:49:TYR:O     | 1:A:129:ARG:CD   | 2.63                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:129:ARG:NH2  | 2:A:207:SO4:O2   | 2.51                     | 0.43              |
| 1:B:58:ASP:O     | 1:B:62:ILE:HG13  | 2.19                     | 0.43              |
| 1:F:38:TYR:CZ    | 1:F:61:LEU:HD22  | 2.54                     | 0.43              |
| 1:G:32:LEU:HD22  | 1:G:37:ILE:CG2   | 2.40                     | 0.43              |
| 1:I:34:GLN:CD    | 1:I:139:VAL:HG11 | 2.43                     | 0.43              |
| 1:I:188:THR:C    | 1:I:189:THR:HG23 | 2.44                     | 0.43              |
| 1:J:160:ASP:O    | 1:J:161:LEU:HG   | 2.19                     | 0.43              |
| 1:K:71:GLN:HG2   | 1:K:167:TRP:CZ2  | 2.54                     | 0.43              |
| 1:L:140:THR:HG22 | 1:L:141:PHE:CD1  | 2.53                     | 0.43              |
| 1:E:153:LEU:O    | 1:E:154:LEU:HD23 | 2.17                     | 0.43              |
| 1:J:24:PHE:O     | 1:J:28:ILE:HG22  | 2.19                     | 0.43              |
| 1:J:90:ASN:CG    | 1:J:93:SER:CB    | 2.91                     | 0.43              |
| 1:K:24:PHE:O     | 1:K:28:ILE:HG13  | 2.18                     | 0.43              |
| 1:K:27:GLY:O     | 1:K:31:ILE:HG13  | 2.17                     | 0.43              |
| 1:L:160:ASP:O    | 1:L:161:LEU:C    | 2.62                     | 0.43              |
| 1:C:117:ARG:HD2  | 1:C:117:ARG:HA   | 1.48                     | 0.43              |
| 1:E:188:THR:C    | 1:E:189:THR:HG23 | 2.43                     | 0.43              |
| 1:H:28:ILE:O     | 1:H:32:LEU:HG    | 2.18                     | 0.43              |
| 1:H:140:THR:HG22 | 1:H:141:PHE:CD1  | 2.54                     | 0.43              |
| 1:J:121:GLN:HE21 | 1:J:125:GLN:HE21 | 1.66                     | 0.43              |
| 1:L:180:GLU:OE1  | 1:L:180:GLU:HA   | 2.19                     | 0.43              |
| 1:I:142:LEU:C    | 1:I:143:PRO:O    | 2.62                     | 0.43              |
| 1:D:175:ILE:CG2  | 1:D:176:THR:N    | 2.82                     | 0.43              |
| 1:F:180:GLU:HA   | 1:F:180:GLU:OE1  | 2.19                     | 0.43              |
| 1:H:90:ASN:CG    | 1:H:93:SER:CB    | 2.92                     | 0.43              |
| 1:I:133:ARG:HD2  | 1:J:34:GLN:HA    | 1.98                     | 0.43              |
| 1:J:138:THR:C    | 1:J:140:THR:N    | 2.73                     | 0.43              |
| 1:J:179:GLU:CG   | 1:J:180:GLU:H    | 2.32                     | 0.43              |
| 1:K:172:PRO:CB   | 1:K:174:PHE:CZ   | 3.02                     | 0.43              |
| 1:A:59:LEU:CD2   | 1:E:44:THR:CG2   | 2.97                     | 0.43              |
| 1:B:175:ILE:HD13 | 1:B:175:ILE:HA   | 1.67                     | 0.43              |
| 1:E:129:ARG:NH2  | 2:E:206:SO4:O3   | 2.49                     | 0.43              |
| 1:F:140:THR:HG22 | 1:F:141:PHE:CD1  | 2.54                     | 0.43              |
| 1:L:90:ASN:ND2   | 1:L:93:SER:HB2   | 2.34                     | 0.43              |
| 1:H:93:SER:OG    | 1:H:95:GLU:HG2   | 2.18                     | 0.43              |
| 1:J:33:TYR:HB2   | 1:J:43:PHE:CD2   | 2.54                     | 0.43              |
| 1:J:47:GLN:HB2   | 1:J:51:LEU:O     | 2.19                     | 0.43              |
| 1:J:159:LYS:HA   | 1:J:192:LYS:HB3  | 2.01                     | 0.43              |
| 1:J:186:PHE:C    | 1:J:186:PHE:HD2  | 2.27                     | 0.43              |
| 1:L:17:ALA:C     | 1:L:19:ILE:N     | 2.76                     | 0.43              |
| 1:L:179:GLU:CG   | 1:L:180:GLU:H    | 2.32                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:84:LEU:C     | 1:A:84:LEU:HD13  | 2.44                     | 0.42              |
| 1:B:186:PHE:C    | 1:B:186:PHE:CD2  | 2.97                     | 0.42              |
| 1:C:71:GLN:HG2   | 1:C:167:TRP:CZ2  | 2.54                     | 0.42              |
| 1:D:17:ALA:O     | 1:D:18:GLU:C     | 2.62                     | 0.42              |
| 1:I:34:GLN:CD    | 1:J:45:ARG:HH22  | 2.27                     | 0.42              |
| 1:I:171:GLY:HA2  | 1:I:172:PRO:HD3  | 1.84                     | 0.42              |
| 1:K:188:THR:C    | 1:K:189:THR:HG23 | 2.43                     | 0.42              |
| 1:L:31:ILE:HD13  | 1:L:100:TRP:CE3  | 2.54                     | 0.42              |
| 1:A:161:LEU:HG   | 1:A:162:VAL:N    | 2.33                     | 0.42              |
| 1:B:124:ILE:O    | 1:B:125:GLN:C    | 2.63                     | 0.42              |
| 1:F:179:GLU:CG   | 1:F:180:GLU:H    | 2.32                     | 0.42              |
| 1:G:84:LEU:C     | 1:G:84:LEU:CD1   | 2.92                     | 0.42              |
| 1:G:168:GLU:C    | 1:J:199:TYR:CD2  | 2.98                     | 0.42              |
| 1:H:16:SER:O     | 1:H:20:VAL:HG23  | 2.19                     | 0.42              |
| 1:H:31:ILE:HD13  | 1:H:100:TRP:CE3  | 2.54                     | 0.42              |
| 1:J:76:LEU:O     | 1:J:78:LYS:N     | 2.52                     | 0.42              |
| 1:L:71:GLN:HG2   | 1:L:167:TRP:CD1  | 2.54                     | 0.42              |
| 1:L:173:GLN:HB2  | 1:L:187:THR:HG22 | 2.00                     | 0.42              |
| 1:A:27:GLY:O     | 1:A:31:ILE:HG13  | 2.18                     | 0.42              |
| 1:C:56:THR:CG2   | 1:C:61:LEU:HD23  | 2.46                     | 0.42              |
| 1:D:179:GLU:CG   | 1:D:180:GLU:H    | 2.31                     | 0.42              |
| 1:E:84:LEU:HD13  | 1:E:84:LEU:C     | 2.44                     | 0.42              |
| 1:G:129:ARG:HH12 | 1:G:133:ARG:HH22 | 1.65                     | 0.42              |
| 1:I:84:LEU:HD13  | 1:I:84:LEU:C     | 2.43                     | 0.42              |
| 1:I:183:LEU:HB2  | 1:I:195:SER:O    | 2.18                     | 0.42              |
| 1:A:59:LEU:CD2   | 1:E:44:THR:HG21  | 2.49                     | 0.42              |
| 1:C:48:LYS:C     | 1:C:50:GLY:H     | 2.27                     | 0.42              |
| 1:C:153:LEU:O    | 1:C:154:LEU:HD23 | 2.20                     | 0.42              |
| 1:D:121:GLN:HE21 | 1:D:125:GLN:HE21 | 1.66                     | 0.42              |
| 1:E:134:GLN:HE21 | 1:F:139:VAL:HG13 | 1.83                     | 0.42              |
| 1:G:48:LYS:HD2   | 1:G:48:LYS:HA    | 1.90                     | 0.42              |
| 1:I:18:GLU:HG2   | 1:I:73:LYS:HD2   | 1.99                     | 0.42              |
| 1:J:28:ILE:O     | 1:J:32:LEU:HG    | 2.20                     | 0.42              |
| 1:K:10:SER:CA    | 1:K:117:ARG:O    | 2.64                     | 0.42              |
| 1:L:157:THR:HG21 | 1:L:161:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:172:PRO:HB3  | 1:A:174:PHE:CZ   | 2.54                     | 0.42              |
| 1:D:175:ILE:HG22 | 1:D:176:THR:N    | 2.33                     | 0.42              |
| 1:F:93:SER:OG    | 1:F:95:GLU:HG2   | 2.19                     | 0.42              |
| 1:F:179:GLU:HG3  | 1:F:180:GLU:N    | 2.35                     | 0.42              |
| 1:K:175:ILE:O    | 1:K:176:THR:C    | 2.61                     | 0.42              |
| 1:L:184:ARG:HD3  | 1:L:184:ARG:HA   | 1.85                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:84:LEU:C     | 1:A:84:LEU:CD1   | 2.92                     | 0.42              |
| 1:A:84:LEU:HD13  | 1:A:85:VAL:N     | 2.34                     | 0.42              |
| 1:B:27:GLY:O     | 1:B:31:ILE:HG13  | 2.19                     | 0.42              |
| 1:D:58:ASP:O     | 1:D:62:ILE:HG13  | 2.20                     | 0.42              |
| 1:D:63:LYS:HG3   | 1:L:59:LEU:CD2   | 2.46                     | 0.42              |
| 1:F:59:LEU:HD12  | 1:F:59:LEU:HA    | 1.88                     | 0.42              |
| 1:H:17:ALA:C     | 1:H:19:ILE:N     | 2.75                     | 0.42              |
| 1:H:76:LEU:C     | 1:H:78:LYS:N     | 2.74                     | 0.42              |
| 1:I:34:GLN:NE2   | 1:I:139:VAL:HB   | 2.35                     | 0.42              |
| 1:I:138:THR:O    | 1:I:139:VAL:C    | 2.61                     | 0.42              |
| 1:C:172:PRO:HB3  | 1:C:174:PHE:CZ   | 2.54                     | 0.42              |
| 1:D:77:TYR:HE2   | 1:D:78:LYS:HE2   | 1.85                     | 0.42              |
| 1:D:188:THR:HG22 | 1:D:189:THR:N    | 2.35                     | 0.42              |
| 1:F:32:LEU:HD13  | 1:F:61:LEU:HD21  | 2.01                     | 0.42              |
| 1:L:47:GLN:HB2   | 1:L:51:LEU:O     | 2.19                     | 0.42              |
| 1:L:48:LYS:O     | 1:L:49:TYR:HB2   | 2.20                     | 0.42              |
| 1:B:138:THR:O    | 1:B:140:THR:N    | 2.53                     | 0.42              |
| 1:B:203:VAL:HG12 | 1:B:203:VAL:O    | 2.20                     | 0.42              |
| 1:D:179:GLU:HG3  | 1:D:180:GLU:N    | 2.35                     | 0.42              |
| 1:E:84:LEU:C     | 1:E:84:LEU:CD1   | 2.93                     | 0.42              |
| 1:G:49:TYR:O     | 1:G:129:ARG:CD   | 2.62                     | 0.42              |
| 1:G:71:GLN:HG2   | 1:G:167:TRP:CZ2  | 2.55                     | 0.42              |
| 1:I:11:ILE:HD13  | 1:I:11:ILE:HA    | 1.78                     | 0.42              |
| 1:I:35:ARG:CZ    | 1:I:35:ARG:CB    | 2.87                     | 0.42              |
| 1:L:167:TRP:C    | 1:L:169:GLU:H    | 2.27                     | 0.42              |
| 1:B:28:ILE:O     | 1:B:32:LEU:HG    | 2.20                     | 0.42              |
| 1:B:31:ILE:HD13  | 1:B:100:TRP:CE3  | 2.55                     | 0.42              |
| 1:B:39:PRO:HD2   | 1:B:42:THR:OG1   | 2.19                     | 0.42              |
| 1:C:10:SER:CA    | 1:C:117:ARG:O    | 2.63                     | 0.42              |
| 1:E:11:ILE:HD13  | 1:E:11:ILE:HA    | 1.78                     | 0.42              |
| 1:E:26:PHE:HD1   | 1:E:49:TYR:CE1   | 2.38                     | 0.42              |
| 1:I:117:ARG:HA   | 1:I:117:ARG:HD2  | 1.44                     | 0.42              |
| 1:J:179:GLU:HG3  | 1:J:180:GLU:N    | 2.35                     | 0.42              |
| 1:L:16:SER:O     | 1:L:20:VAL:HG23  | 2.19                     | 0.42              |
| 1:L:186:PHE:C    | 1:L:186:PHE:CD2  | 2.98                     | 0.42              |
| 1:B:188:THR:HG22 | 1:B:189:THR:N    | 2.35                     | 0.42              |
| 1:E:71:GLN:HG2   | 1:E:167:TRP:CZ2  | 2.55                     | 0.42              |
| 1:I:49:TYR:O     | 1:I:129:ARG:CD   | 2.62                     | 0.42              |
| 1:I:84:LEU:HD13  | 1:I:85:VAL:N     | 2.35                     | 0.42              |
| 1:D:124:ILE:O    | 1:D:125:GLN:C    | 2.63                     | 0.41              |
| 1:D:203:VAL:O    | 1:D:203:VAL:HG12 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:78:LYS:HG3   | 1:F:80:SER:OG    | 2.19                     | 0.41              |
| 1:I:86:VAL:HB    | 1:I:100:TRP:HB2  | 2.01                     | 0.41              |
| 1:J:180:GLU:OE1  | 1:J:180:GLU:HA   | 2.19                     | 0.41              |
| 1:L:21:ALA:HB1   | 1:L:69:VAL:HG13  | 2.01                     | 0.41              |
| 1:D:38:TYR:CE1   | 1:D:61:LEU:HD22  | 2.55                     | 0.41              |
| 1:F:184:ARG:HA   | 1:F:184:ARG:HD3  | 1.84                     | 0.41              |
| 1:G:18:GLU:HG2   | 1:G:73:LYS:HD2   | 2.01                     | 0.41              |
| 1:J:31:ILE:HD13  | 1:J:100:TRP:CE3  | 2.55                     | 0.41              |
| 1:L:179:GLU:HG3  | 1:L:180:GLU:N    | 2.35                     | 0.41              |
| 1:A:48:LYS:HD2   | 1:A:48:LYS:HA    | 1.88                     | 0.41              |
| 1:B:140:THR:HG22 | 1:B:141:PHE:CD1  | 2.55                     | 0.41              |
| 1:F:45:ARG:O     | 1:I:146:GLU:OE2  | 2.38                     | 0.41              |
| 1:F:90:ASN:CG    | 1:F:93:SER:CB    | 2.93                     | 0.41              |
| 1:I:39:PRO:HD2   | 1:I:42:THR:OG1   | 2.19                     | 0.41              |
| 1:I:84:LEU:C     | 1:I:84:LEU:CD1   | 2.93                     | 0.41              |
| 1:J:132:ILE:N    | 1:J:132:ILE:HD13 | 2.35                     | 0.41              |
| 1:K:11:ILE:HA    | 1:K:11:ILE:HD13  | 1.75                     | 0.41              |
| 1:B:17:ALA:C     | 1:B:19:ILE:N     | 2.74                     | 0.41              |
| 1:D:14:ARG:HB3   | 1:D:105:GLU:HB3  | 2.02                     | 0.41              |
| 1:D:173:GLN:CB   | 1:D:187:THR:HG22 | 2.42                     | 0.41              |
| 1:F:17:ALA:C     | 1:F:19:ILE:N     | 2.76                     | 0.41              |
| 1:K:135:ILE:O    | 1:K:138:THR:HG22 | 2.20                     | 0.41              |
| 1:L:76:LEU:O     | 1:L:78:LYS:N     | 2.53                     | 0.41              |
| 1:B:77:TYR:HE2   | 1:B:78:LYS:HE2   | 1.86                     | 0.41              |
| 1:B:186:PHE:C    | 1:B:186:PHE:HD2  | 2.29                     | 0.41              |
| 1:F:186:PHE:HD2  | 1:F:187:THR:N    | 2.19                     | 0.41              |
| 1:H:14:ARG:HB3   | 1:H:105:GLU:HB3  | 2.01                     | 0.41              |
| 1:B:132:ILE:N    | 1:B:132:ILE:HD13 | 2.35                     | 0.41              |
| 1:B:179:GLU:CG   | 1:B:180:GLU:H    | 2.33                     | 0.41              |
| 1:F:121:GLN:HE21 | 1:F:125:GLN:HE21 | 1.68                     | 0.41              |
| 1:H:77:TYR:HE2   | 1:H:78:LYS:HE2   | 1.86                     | 0.41              |
| 1:I:175:ILE:O    | 1:I:176:THR:C    | 2.63                     | 0.41              |
| 1:L:14:ARG:HB3   | 1:L:105:GLU:CG   | 2.49                     | 0.41              |
| 1:B:163:VAL:HA   | 1:B:164:PRO:HD3  | 1.94                     | 0.41              |
| 1:F:14:ARG:HB3   | 1:F:105:GLU:HB3  | 2.03                     | 0.41              |
| 1:F:24:PHE:O     | 1:F:28:ILE:HG22  | 2.20                     | 0.41              |
| 1:H:184:ARG:HA   | 1:H:184:ARG:HD3  | 1.85                     | 0.41              |
| 1:J:16:SER:HB2   | 1:J:109:THR:CG2  | 2.36                     | 0.41              |
| 1:L:173:GLN:CB   | 1:L:187:THR:HG22 | 2.50                     | 0.41              |
| 1:L:186:PHE:C    | 1:L:186:PHE:HD2  | 2.29                     | 0.41              |
| 1:B:38:TYR:CZ    | 1:B:61:LEU:HD22  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:51:LEU:HB2   | 1:C:53:LEU:HD21  | 2.03                     | 0.41              |
| 1:D:39:PRO:HD2   | 1:D:42:THR:OG1   | 2.21                     | 0.41              |
| 1:F:159:LYS:HA   | 1:F:192:LYS:HB3  | 2.02                     | 0.41              |
| 1:H:168:GLU:C    | 1:H:170:SER:N    | 2.78                     | 0.41              |
| 1:H:179:GLU:CG   | 1:H:180:GLU:H    | 2.33                     | 0.41              |
| 1:I:37:ILE:HG13  | 1:I:37:ILE:O     | 2.20                     | 0.41              |
| 1:J:39:PRO:HD2   | 1:J:42:THR:OG1   | 2.20                     | 0.41              |
| 1:L:201:ILE:O    | 1:L:201:ILE:HG23 | 2.21                     | 0.41              |
| 1:A:12:THR:OG1   | 1:A:14:ARG:HB3   | 2.21                     | 0.41              |
| 1:B:200:LYS:HG3  | 1:C:170:SER:CB   | 2.51                     | 0.41              |
| 1:C:171:GLY:HA2  | 1:C:172:PRO:HD3  | 1.81                     | 0.41              |
| 1:D:175:ILE:HD13 | 1:D:175:ILE:HA   | 1.68                     | 0.41              |
| 1:E:140:THR:OG1  | 1:F:53:LEU:HD23  | 2.21                     | 0.41              |
| 1:F:28:ILE:O     | 1:F:32:LEU:HG    | 2.20                     | 0.41              |
| 1:F:48:LYS:HE3   | 1:I:37:ILE:O     | 2.21                     | 0.41              |
| 1:F:76:LEU:O     | 1:F:78:LYS:N     | 2.54                     | 0.41              |
| 1:F:197:VAL:HG12 | 1:F:199:TYR:CE2  | 2.56                     | 0.41              |
| 1:G:76:LEU:HD23  | 1:G:76:LEU:HA    | 1.89                     | 0.41              |
| 1:H:39:PRO:HD2   | 1:H:42:THR:OG1   | 2.21                     | 0.41              |
| 1:I:33:TYR:CE2   | 1:I:54:LEU:HD13  | 2.55                     | 0.41              |
| 1:I:141:PHE:O    | 1:J:129:ARG:CD   | 2.65                     | 0.41              |
| 1:K:49:TYR:O     | 1:K:129:ARG:CD   | 2.63                     | 0.41              |
| 1:K:95:GLU:HG2   | 1:K:96:VAL:N     | 2.34                     | 0.41              |
| 1:L:14:ARG:HB3   | 1:L:105:GLU:HB3  | 2.03                     | 0.41              |
| 1:L:138:THR:O    | 1:L:139:VAL:C    | 2.64                     | 0.41              |
| 1:B:104:ILE:HD13 | 1:B:104:ILE:HG21 | 1.83                     | 0.41              |
| 1:B:194:ASN:HB3  | 1:B:195:SER:H    | 1.77                     | 0.41              |
| 1:D:39:PRO:HD3   | 1:D:181:VAL:HG22 | 2.02                     | 0.41              |
| 1:F:138:THR:O    | 1:F:140:THR:N    | 2.54                     | 0.41              |
| 1:J:14:ARG:HB3   | 1:J:105:GLU:HB3  | 2.03                     | 0.41              |
| 1:K:48:LYS:O     | 1:K:49:TYR:HB2   | 2.21                     | 0.41              |
| 1:K:129:ARG:HH12 | 1:K:133:ARG:HH22 | 1.67                     | 0.41              |
| 1:E:18:GLU:HG2   | 1:E:73:LYS:HD2   | 2.01                     | 0.40              |
| 1:F:31:ILE:HD13  | 1:F:100:TRP:CE3  | 2.55                     | 0.40              |
| 1:H:167:TRP:C    | 1:H:169:GLU:H    | 2.28                     | 0.40              |
| 1:I:54:LEU:N     | 1:I:54:LEU:HD12  | 2.36                     | 0.40              |
| 1:I:188:THR:C    | 1:I:190:ILE:H    | 2.30                     | 0.40              |
| 1:K:18:GLU:HG2   | 1:K:73:LYS:HD2   | 2.03                     | 0.40              |
| 1:C:128:ILE:O    | 1:C:129:ARG:C    | 2.64                     | 0.40              |
| 1:D:72:LEU:HD21  | 1:D:84:LEU:HD11  | 2.02                     | 0.40              |
| 1:A:48:LYS:C     | 1:A:50:GLY:H     | 2.29                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:76:LEU:HD23  | 1:C:76:LEU:HA    | 1.92                     | 0.40              |
| 1:H:199:TYR:O    | 1:I:154:LEU:HA   | 2.22                     | 0.40              |
| 1:K:64:TYR:HE1   | 1:K:68:VAL:HG21  | 1.86                     | 0.40              |
| 1:L:168:GLU:C    | 1:L:170:SER:N    | 2.79                     | 0.40              |
| 1:A:18:GLU:HG2   | 1:A:73:LYS:HD2   | 2.02                     | 0.40              |
| 1:A:131:VAL:HG12 | 1:A:132:ILE:N    | 2.34                     | 0.40              |
| 1:C:103:ASP:HB2  | 1:C:194:ASN:HB2  | 2.04                     | 0.40              |
| 1:D:121:GLN:HB3  | 1:K:43:PHE:O     | 2.21                     | 0.40              |
| 1:E:95:GLU:HG2   | 1:E:96:VAL:N     | 2.35                     | 0.40              |
| 1:H:138:THR:O    | 1:H:140:THR:N    | 2.53                     | 0.40              |
| 1:H:186:PHE:C    | 1:H:186:PHE:CD2  | 2.99                     | 0.40              |
| 1:I:43:PHE:HB3   | 1:I:54:LEU:HB3   | 2.02                     | 0.40              |
| 1:J:161:LEU:HD23 | 1:J:161:LEU:HA   | 1.90                     | 0.40              |
| 1:J:203:VAL:O    | 1:J:203:VAL:HG12 | 2.22                     | 0.40              |
| 1:K:117:ARG:HA   | 1:K:117:ARG:HD2  | 1.44                     | 0.40              |
| 1:K:161:LEU:HG   | 1:K:162:VAL:N    | 2.36                     | 0.40              |
| 1:K:171:GLY:HA2  | 1:K:172:PRO:HD3  | 1.84                     | 0.40              |
| 1:C:175:ILE:O    | 1:C:176:THR:C    | 2.64                     | 0.40              |
| 1:F:42:THR:HB    | 1:F:43:PHE:CE1   | 2.57                     | 0.40              |
| 1:G:49:TYR:CD2   | 1:G:125:GLN:HG3  | 2.56                     | 0.40              |
| 1:H:33:TYR:HB2   | 1:H:43:PHE:CD2   | 2.56                     | 0.40              |
| 1:H:58:ASP:O     | 1:H:62:ILE:HG13  | 2.21                     | 0.40              |
| 1:H:132:ILE:N    | 1:H:132:ILE:HD13 | 2.35                     | 0.40              |
| 1:H:179:GLU:HG3  | 1:H:180:GLU:N    | 2.36                     | 0.40              |
| 1:K:76:LEU:HD23  | 1:K:76:LEU:HA    | 1.91                     | 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     | 191/207 (92%) | 173 (91%) | 18 (9%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | B     | 181/207 (87%)   | 156 (86%)  | 25 (14%)  | 0        | 100         | 100 |
| 1   | C     | 193/207 (93%)   | 174 (90%)  | 18 (9%)   | 1 (0%)   | 24          | 60  |
| 1   | D     | 183/207 (88%)   | 158 (86%)  | 25 (14%)  | 0        | 100         | 100 |
| 1   | E     | 184/207 (89%)   | 167 (91%)  | 16 (9%)   | 1 (0%)   | 24          | 60  |
| 1   | F     | 181/207 (87%)   | 159 (88%)  | 21 (12%)  | 1 (1%)   | 21          | 56  |
| 1   | G     | 183/207 (88%)   | 169 (92%)  | 13 (7%)   | 1 (0%)   | 24          | 60  |
| 1   | H     | 182/207 (88%)   | 154 (85%)  | 28 (15%)  | 0        | 100         | 100 |
| 1   | I     | 184/207 (89%)   | 165 (90%)  | 16 (9%)   | 3 (2%)   | 7           | 37  |
| 1   | J     | 181/207 (87%)   | 158 (87%)  | 22 (12%)  | 1 (1%)   | 21          | 56  |
| 1   | K     | 184/207 (89%)   | 167 (91%)  | 16 (9%)   | 1 (0%)   | 24          | 60  |
| 1   | L     | 183/207 (88%)   | 157 (86%)  | 26 (14%)  | 0        | 100         | 100 |
| All | All   | 2210/2484 (89%) | 1957 (89%) | 244 (11%) | 9 (0%)   | 30          | 65  |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 176 | THR  |
| 1   | G     | 176 | THR  |
| 1   | I     | 176 | THR  |
| 1   | J     | 169 | GLU  |
| 1   | K     | 176 | THR  |
| 1   | C     | 176 | THR  |
| 1   | F     | 169 | GLU  |
| 1   | I     | 143 | PRO  |
| 1   | I     | 37  | ILE  |

### 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     | 180/192 (94%) | 165 (92%) | 15 (8%)  | 10          | 34 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | B     | 173/192 (90%)   | 156 (90%)  | 17 (10%) | 7           | 27 |
| 1   | C     | 182/192 (95%)   | 167 (92%)  | 15 (8%)  | 10          | 34 |
| 1   | D     | 175/192 (91%)   | 157 (90%)  | 18 (10%) | 7           | 25 |
| 1   | E     | 176/192 (92%)   | 164 (93%)  | 12 (7%)  | 14          | 40 |
| 1   | F     | 173/192 (90%)   | 153 (88%)  | 20 (12%) | 5           | 21 |
| 1   | G     | 175/192 (91%)   | 160 (91%)  | 15 (9%)  | 10          | 33 |
| 1   | H     | 174/192 (91%)   | 158 (91%)  | 16 (9%)  | 8           | 30 |
| 1   | I     | 176/192 (92%)   | 162 (92%)  | 14 (8%)  | 11          | 35 |
| 1   | J     | 173/192 (90%)   | 157 (91%)  | 16 (9%)  | 8           | 30 |
| 1   | K     | 176/192 (92%)   | 161 (92%)  | 15 (8%)  | 10          | 33 |
| 1   | L     | 174/192 (91%)   | 156 (90%)  | 18 (10%) | 7           | 25 |
| All | All   | 2107/2304 (91%) | 1916 (91%) | 191 (9%) | 9           | 31 |

All (191) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 11  | ILE  |
| 1   | A     | 31  | ILE  |
| 1   | A     | 37  | ILE  |
| 1   | A     | 40  | SER  |
| 1   | A     | 46  | VAL  |
| 1   | A     | 53  | LEU  |
| 1   | A     | 64  | TYR  |
| 1   | A     | 68  | VAL  |
| 1   | A     | 84  | LEU  |
| 1   | A     | 88  | ILE  |
| 1   | A     | 117 | ARG  |
| 1   | A     | 131 | VAL  |
| 1   | A     | 138 | THR  |
| 1   | A     | 139 | VAL  |
| 1   | A     | 144 | LEU  |
| 1   | B     | 31  | ILE  |
| 1   | B     | 43  | PHE  |
| 1   | B     | 46  | VAL  |
| 1   | B     | 65  | LEU  |
| 1   | B     | 66  | ASN  |
| 1   | B     | 69  | VAL  |
| 1   | B     | 86  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 105 | GLU  |
| 1   | B     | 128 | ILE  |
| 1   | B     | 139 | VAL  |
| 1   | B     | 140 | THR  |
| 1   | B     | 147 | VAL  |
| 1   | B     | 153 | LEU  |
| 1   | B     | 165 | GLU  |
| 1   | B     | 166 | LYS  |
| 1   | B     | 175 | ILE  |
| 1   | B     | 192 | LYS  |
| 1   | C     | 11  | ILE  |
| 1   | C     | 31  | ILE  |
| 1   | C     | 40  | SER  |
| 1   | C     | 45  | ARG  |
| 1   | C     | 46  | VAL  |
| 1   | C     | 53  | LEU  |
| 1   | C     | 64  | TYR  |
| 1   | C     | 68  | VAL  |
| 1   | C     | 84  | LEU  |
| 1   | C     | 88  | ILE  |
| 1   | C     | 117 | ARG  |
| 1   | C     | 131 | VAL  |
| 1   | C     | 138 | THR  |
| 1   | C     | 139 | VAL  |
| 1   | C     | 144 | LEU  |
| 1   | D     | 31  | ILE  |
| 1   | D     | 43  | PHE  |
| 1   | D     | 46  | VAL  |
| 1   | D     | 62  | ILE  |
| 1   | D     | 65  | LEU  |
| 1   | D     | 66  | ASN  |
| 1   | D     | 69  | VAL  |
| 1   | D     | 86  | VAL  |
| 1   | D     | 105 | GLU  |
| 1   | D     | 128 | ILE  |
| 1   | D     | 139 | VAL  |
| 1   | D     | 140 | THR  |
| 1   | D     | 147 | VAL  |
| 1   | D     | 153 | LEU  |
| 1   | D     | 166 | LYS  |
| 1   | D     | 175 | ILE  |
| 1   | D     | 190 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 192 | LYS  |
| 1   | E     | 11  | ILE  |
| 1   | E     | 31  | ILE  |
| 1   | E     | 40  | SER  |
| 1   | E     | 46  | VAL  |
| 1   | E     | 53  | LEU  |
| 1   | E     | 64  | TYR  |
| 1   | E     | 84  | LEU  |
| 1   | E     | 88  | ILE  |
| 1   | E     | 131 | VAL  |
| 1   | E     | 138 | THR  |
| 1   | E     | 139 | VAL  |
| 1   | E     | 144 | LEU  |
| 1   | F     | 31  | ILE  |
| 1   | F     | 43  | PHE  |
| 1   | F     | 46  | VAL  |
| 1   | F     | 47  | GLN  |
| 1   | F     | 48  | LYS  |
| 1   | F     | 49  | TYR  |
| 1   | F     | 62  | ILE  |
| 1   | F     | 65  | LEU  |
| 1   | F     | 66  | ASN  |
| 1   | F     | 69  | VAL  |
| 1   | F     | 86  | VAL  |
| 1   | F     | 105 | GLU  |
| 1   | F     | 128 | ILE  |
| 1   | F     | 139 | VAL  |
| 1   | F     | 140 | THR  |
| 1   | F     | 147 | VAL  |
| 1   | F     | 153 | LEU  |
| 1   | F     | 166 | LYS  |
| 1   | F     | 192 | LYS  |
| 1   | F     | 201 | ILE  |
| 1   | G     | 11  | ILE  |
| 1   | G     | 31  | ILE  |
| 1   | G     | 37  | ILE  |
| 1   | G     | 40  | SER  |
| 1   | G     | 46  | VAL  |
| 1   | G     | 53  | LEU  |
| 1   | G     | 64  | TYR  |
| 1   | G     | 68  | VAL  |
| 1   | G     | 84  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 88  | ILE  |
| 1   | G     | 117 | ARG  |
| 1   | G     | 131 | VAL  |
| 1   | G     | 138 | THR  |
| 1   | G     | 139 | VAL  |
| 1   | G     | 144 | LEU  |
| 1   | H     | 14  | ARG  |
| 1   | H     | 31  | ILE  |
| 1   | H     | 43  | PHE  |
| 1   | H     | 46  | VAL  |
| 1   | H     | 62  | ILE  |
| 1   | H     | 65  | LEU  |
| 1   | H     | 66  | ASN  |
| 1   | H     | 69  | VAL  |
| 1   | H     | 86  | VAL  |
| 1   | H     | 105 | GLU  |
| 1   | H     | 128 | ILE  |
| 1   | H     | 139 | VAL  |
| 1   | H     | 140 | THR  |
| 1   | H     | 153 | LEU  |
| 1   | H     | 166 | LYS  |
| 1   | H     | 192 | LYS  |
| 1   | I     | 11  | ILE  |
| 1   | I     | 31  | ILE  |
| 1   | I     | 35  | ARG  |
| 1   | I     | 46  | VAL  |
| 1   | I     | 53  | LEU  |
| 1   | I     | 64  | TYR  |
| 1   | I     | 68  | VAL  |
| 1   | I     | 84  | LEU  |
| 1   | I     | 88  | ILE  |
| 1   | I     | 117 | ARG  |
| 1   | I     | 131 | VAL  |
| 1   | I     | 144 | LEU  |
| 1   | I     | 155 | ILE  |
| 1   | I     | 167 | TRP  |
| 1   | J     | 31  | ILE  |
| 1   | J     | 43  | PHE  |
| 1   | J     | 46  | VAL  |
| 1   | J     | 62  | ILE  |
| 1   | J     | 65  | LEU  |
| 1   | J     | 66  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 69  | VAL  |
| 1   | J     | 86  | VAL  |
| 1   | J     | 105 | GLU  |
| 1   | J     | 128 | ILE  |
| 1   | J     | 139 | VAL  |
| 1   | J     | 140 | THR  |
| 1   | J     | 153 | LEU  |
| 1   | J     | 165 | GLU  |
| 1   | J     | 166 | LYS  |
| 1   | J     | 192 | LYS  |
| 1   | K     | 11  | ILE  |
| 1   | K     | 31  | ILE  |
| 1   | K     | 37  | ILE  |
| 1   | K     | 40  | SER  |
| 1   | K     | 46  | VAL  |
| 1   | K     | 53  | LEU  |
| 1   | K     | 64  | TYR  |
| 1   | K     | 68  | VAL  |
| 1   | K     | 84  | LEU  |
| 1   | K     | 88  | ILE  |
| 1   | K     | 117 | ARG  |
| 1   | K     | 131 | VAL  |
| 1   | K     | 138 | THR  |
| 1   | K     | 139 | VAL  |
| 1   | K     | 144 | LEU  |
| 1   | L     | 14  | ARG  |
| 1   | L     | 28  | ILE  |
| 1   | L     | 31  | ILE  |
| 1   | L     | 43  | PHE  |
| 1   | L     | 46  | VAL  |
| 1   | L     | 62  | ILE  |
| 1   | L     | 65  | LEU  |
| 1   | L     | 66  | ASN  |
| 1   | L     | 69  | VAL  |
| 1   | L     | 86  | VAL  |
| 1   | L     | 105 | GLU  |
| 1   | L     | 128 | ILE  |
| 1   | L     | 139 | VAL  |
| 1   | L     | 140 | THR  |
| 1   | L     | 147 | VAL  |
| 1   | L     | 153 | LEU  |
| 1   | L     | 166 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 192 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | ASN  |
| 1   | A     | 194 | ASN  |
| 1   | C     | 66  | ASN  |
| 1   | C     | 194 | ASN  |
| 1   | D     | 121 | GLN  |
| 1   | E     | 66  | ASN  |
| 1   | E     | 194 | ASN  |
| 1   | F     | 121 | GLN  |
| 1   | G     | 194 | ASN  |
| 1   | I     | 66  | ASN  |
| 1   | I     | 194 | ASN  |
| 1   | J     | 34  | GLN  |
| 1   | J     | 121 | GLN  |
| 1   | K     | 66  | ASN  |
| 1   | K     | 194 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | SO4  | B     | 206 | -    | 4,4,4        | 0.22 | 0           | 6,6,6       | 0.32 | 0           |
| 2   | SO4  | L     | 206 | -    | 4,4,4        | 0.32 | 0           | 6,6,6       | 0.45 | 0           |
| 2   | SO4  | E     | 206 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.23 | 0           |
| 2   | SO4  | C     | 206 | -    | 4,4,4        | 0.19 | 0           | 6,6,6       | 0.50 | 0           |
| 2   | SO4  | D     | 206 | -    | 4,4,4        | 0.21 | 0           | 6,6,6       | 0.44 | 0           |
| 2   | SO4  | A     | 207 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.46 | 0           |
| 2   | SO4  | A     | 206 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.20 | 0           |
| 2   | SO4  | K     | 206 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.23 | 0           |
| 2   | SO4  | H     | 206 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.26 | 0           |
| 2   | SO4  | G     | 206 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.26 | 0           |
| 2   | SO4  | I     | 206 | -    | 4,4,4        | 0.26 | 0           | 6,6,6       | 0.18 | 0           |
| 2   | SO4  | C     | 207 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 0.18 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | E     | 206 | SO4  | 2       | 0            |
| 2   | C     | 206 | SO4  | 2       | 0            |
| 2   | A     | 207 | SO4  | 3       | 0            |
| 2   | K     | 206 | SO4  | 2       | 0            |
| 2   | G     | 206 | SO4  | 1       | 0            |

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 193/207 (93%)   | -0.22  | 0 100 100     | 71, 120, 205, 262     | 0     |
| 1   | B     | 185/207 (89%)   | -0.13  | 5 (2%) 56 39  | 69, 104, 175, 238     | 0     |
| 1   | C     | 195/207 (94%)   | -0.26  | 0 100 100     | 69, 129, 220, 348     | 0     |
| 1   | D     | 187/207 (90%)   | -0.10  | 3 (1%) 70 50  | 67, 101, 187, 271     | 0     |
| 1   | E     | 188/207 (90%)   | 0.11   | 4 (2%) 63 45  | 104, 186, 265, 315    | 0     |
| 1   | F     | 185/207 (89%)   | -0.04  | 2 (1%) 78 58  | 96, 149, 241, 315     | 0     |
| 1   | G     | 187/207 (90%)   | -0.05  | 4 (2%) 63 45  | 104, 175, 247, 312    | 0     |
| 1   | H     | 186/207 (89%)   | -0.05  | 1 (0%) 87 72  | 92, 159, 236, 277     | 0     |
| 1   | I     | 188/207 (90%)   | 0.12   | 3 (1%) 70 50  | 111, 180, 273, 324    | 0     |
| 1   | J     | 185/207 (89%)   | -0.06  | 4 (2%) 62 44  | 108, 169, 246, 283    | 0     |
| 1   | K     | 188/207 (90%)   | -0.07  | 0 100 100     | 94, 176, 250, 315     | 0     |
| 1   | L     | 187/207 (90%)   | 0.07   | 3 (1%) 70 50  | 81, 146, 241, 396     | 0     |
| All | All   | 2254/2484 (90%) | -0.06  | 29 (1%) 75 55 | 67, 151, 245, 396     | 0     |

All (29) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 203 | VAL  | 3.0  |
| 1   | L     | 105 | GLU  | 3.0  |
| 1   | B     | 177 | ASN  | 2.9  |
| 1   | E     | 44  | THR  | 2.8  |
| 1   | D     | 162 | VAL  | 2.8  |
| 1   | B     | 9   | GLY  | 2.7  |
| 1   | E     | 162 | VAL  | 2.6  |
| 1   | H     | 82  | GLN  | 2.4  |
| 1   | F     | 203 | VAL  | 2.4  |
| 1   | B     | 92  | GLU  | 2.4  |
| 1   | J     | 98  | GLU  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 166 | LYS  | 2.4  |
| 1   | G     | 110 | ALA  | 2.3  |
| 1   | G     | 105 | GLU  | 2.3  |
| 1   | G     | 202 | PRO  | 2.2  |
| 1   | F     | 166 | LYS  | 2.2  |
| 1   | I     | 49  | TYR  | 2.2  |
| 1   | D     | 180 | GLU  | 2.1  |
| 1   | L     | 203 | VAL  | 2.1  |
| 1   | B     | 162 | VAL  | 2.1  |
| 1   | B     | 193 | VAL  | 2.1  |
| 1   | J     | 94  | GLY  | 2.0  |
| 1   | E     | 176 | THR  | 2.0  |
| 1   | L     | 201 | ILE  | 2.0  |
| 1   | J     | 169 | GLU  | 2.0  |
| 1   | E     | 203 | VAL  | 2.0  |
| 1   | D     | 77  | TYR  | 2.0  |
| 1   | G     | 146 | GLU  | 2.0  |
| 1   | I     | 147 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | SO4  | E     | 206 | 5/5   | 0.76 | 0.09 | 188,188,188,188            | 0     |
| 2   | SO4  | G     | 206 | 5/5   | 0.81 | 0.11 | 184,184,184,184            | 0     |
| 2   | SO4  | I     | 206 | 5/5   | 0.85 | 0.06 | 192,192,192,192            | 0     |
| 2   | SO4  | K     | 206 | 5/5   | 0.85 | 0.07 | 196,196,196,196            | 0     |
| 2   | SO4  | A     | 206 | 5/5   | 0.89 | 0.08 | 185,185,185,185            | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | SO4  | B     | 206 | 5/5   | 0.90 | 0.07 | 138,138,138,138             | 0     |
| 2   | SO4  | D     | 206 | 5/5   | 0.90 | 0.07 | 138,138,138,138             | 0     |
| 2   | SO4  | C     | 207 | 5/5   | 0.92 | 0.06 | 191,191,191,191             | 0     |
| 2   | SO4  | A     | 207 | 5/5   | 0.92 | 0.09 | 128,128,128,128             | 0     |
| 2   | SO4  | C     | 206 | 5/5   | 0.93 | 0.08 | 120,120,120,120             | 0     |
| 2   | SO4  | L     | 206 | 5/5   | 0.93 | 0.08 | 121,121,121,121             | 0     |
| 2   | SO4  | H     | 206 | 5/5   | 0.94 | 0.06 | 133,133,133,133             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.