



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 AM UTC

PDB ID : 1QGH / pdb\_00001qgh  
Title : THE X-RAY STRUCTURE OF THE UNUSUAL DODECAMERIC FER-  
RITIN FROM LISTERIA INNOCUA, REVEALS A NOVEL INTERSUB-  
UNIT IRON BINDING SITE.  
Authors : Ilari, A.; Stefanini, S.; Chiancone, E.; Tsernoglou, D.  
Deposited on : 1999-04-27  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

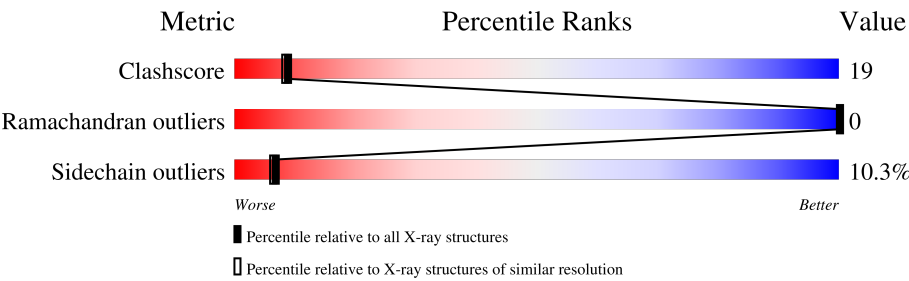
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1663 (2.36-2.36)                                      |
| Ramachandran outliers | 187476                      | 1646 (2.36-2.36)                                      |
| Sidechain outliers    | 187428                      | 1646 (2.36-2.36)                                      |

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  $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain                   |
|-----|-------|--------|------------------------------------|
| 1   | A     | 156    | <div><div>65%24%6% . .</div></div> |
| 1   | B     | 156    | <div><div>64%24%8% .</div></div>   |
| 1   | C     | 156    | <div><div>64%27%5% .</div></div>   |
| 1   | D     | 156    | <div><div>63%26%7% .</div></div>   |
| 1   | E     | 156    | <div><div>64%28%. .</div></div>    |
| 1   | F     | 156    | <div><div>60%28%8% .</div></div>   |
| 1   | G     | 156    | <div><div>67%21%7% . .</div></div> |
| 1   | H     | 156    | <div><div>60%31%. . .</div></div>  |

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| Mol | Chain | Length | Quality of chain                              |
|-----|-------|--------|-----------------------------------------------|
| 1   | I     | 156    | <div><div></div><div>56%31%8% . .</div></div> |
| 1   | J     | 156    | <div><div></div><div>62%31% . . .</div></div> |
| 1   | K     | 156    | <div><div></div><div>59%28%8% . .</div></div> |
| 1   | L     | 156    | <div><div></div><div>60%31% . . .</div></div> |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15155 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 NON-HEME IRON-CONTAINING FERRITIN.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 150      | Total | C   | N   | O   | S | 32      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | B     | 150      | Total | C   | N   | O   | S | 57      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | C     | 150      | Total | C   | N   | O   | S | 44      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | D     | 150      | Total | C   | N   | O   | S | 47      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | E     | 150      | Total | C   | N   | O   | S | 46      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | F     | 150      | Total | C   | N   | O   | S | 42      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | G     | 150      | Total | C   | N   | O   | S | 41      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | H     | 150      | Total | C   | N   | O   | S | 34      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | I     | 150      | Total | C   | N   | O   | S | 45      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | J     | 150      | Total | C   | N   | O   | S | 44      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | K     | 150      | Total | C   | N   | O   | S | 43      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |
| 1   | L     | 150      | Total | C   | N   | O   | S | 50      | 0       | 0     |
|     |       |          | 1222  | 784 | 196 | 235 | 7 |         |         |       |

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Fe | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | C     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | D     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | E     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | F     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | G     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | H     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | I     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | K     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |
| 2   | L     | 1        | Total<br>1 | Fe<br>1 | 0       | 0       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | A     | 38       | Total<br>38 | O<br>38 | 0       | 0       |
| 3   | B     | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 3   | C     | 36       | Total<br>36 | O<br>36 | 0       | 0       |
| 3   | D     | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 3   | E     | 50       | Total<br>50 | O<br>50 | 0       | 0       |
| 3   | F     | 42       | Total<br>42 | O<br>42 | 0       | 0       |
| 3   | G     | 54       | Total<br>54 | O<br>54 | 0       | 0       |
| 3   | H     | 44       | Total<br>44 | O<br>44 | 0       | 0       |
| 3   | I     | 33       | Total<br>33 | O<br>33 | 0       | 0       |

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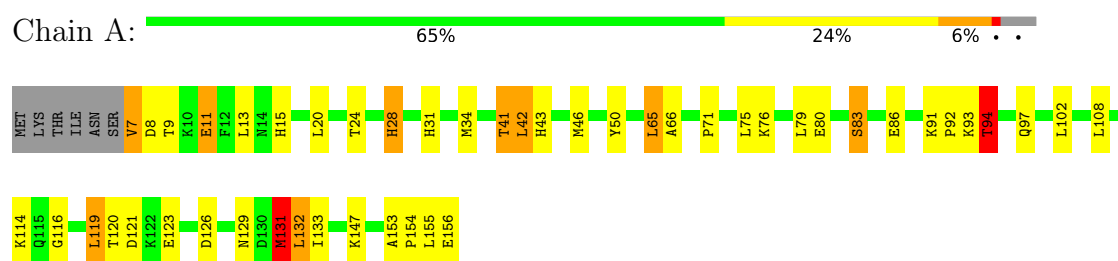
| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | J     | 46       | Total | O  | 0       | 0       |
|     |       |          | 46    | 46 |         |         |
| 3   | K     | 41       | Total | O  | 0       | 0       |
|     |       |          | 41    | 41 |         |         |
| 3   | L     | 45       | Total | O  | 0       | 0       |
|     |       |          | 45    | 45 |         |         |

### 3 Residue-property plots

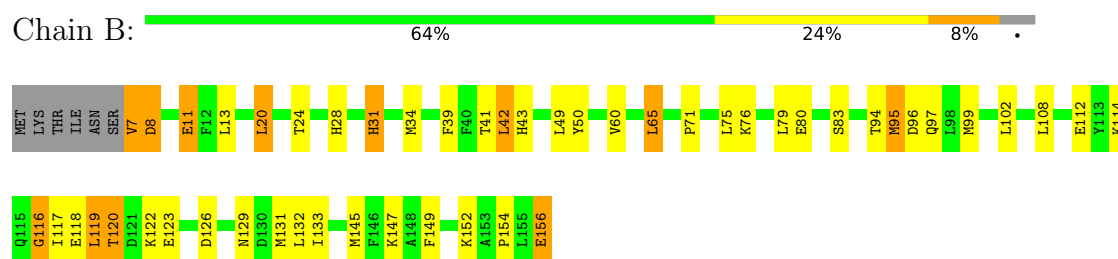
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

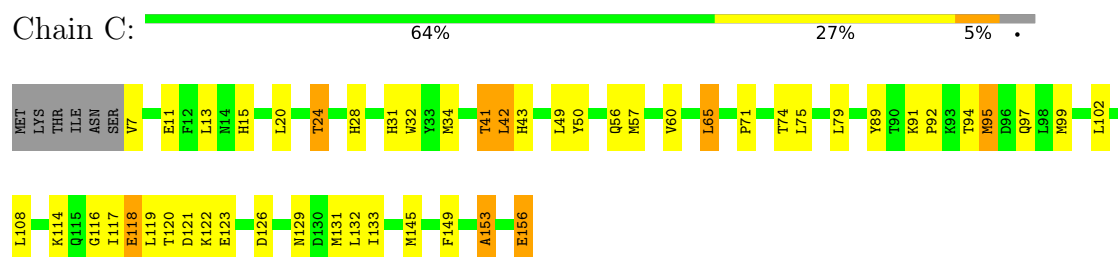
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



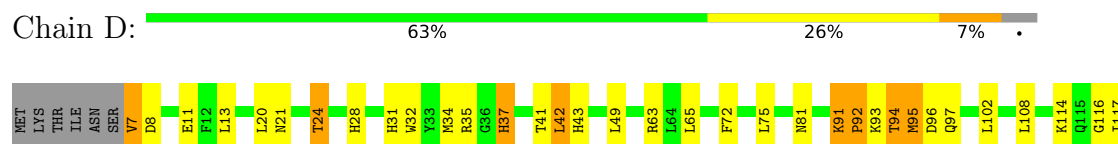
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN



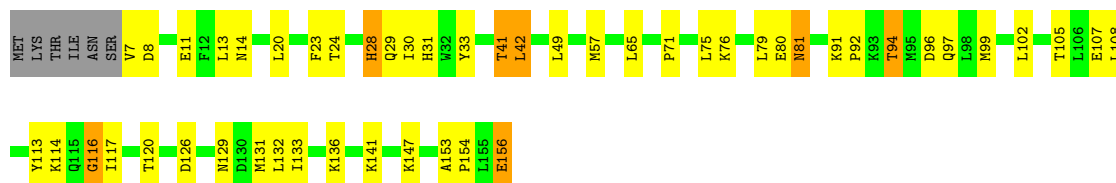
#### • Molecule 1: NON-HEME IRON-CONTAINING FERRITIN





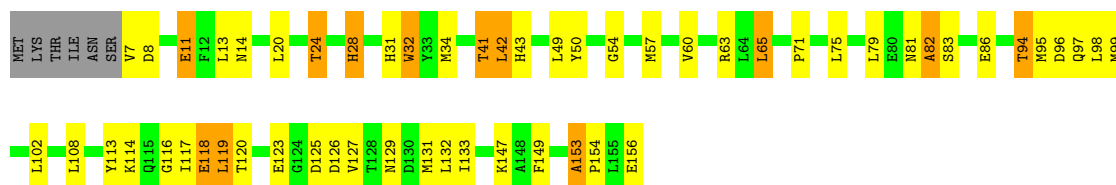
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain E: 64% 28%



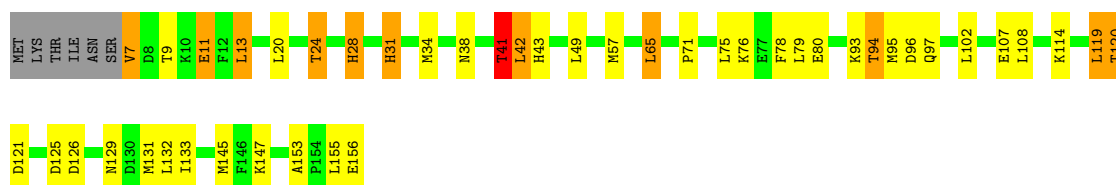
• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain F: 60% 28% 8%



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain G: 67% 21% 7%



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain H: 60% 31% 8%



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

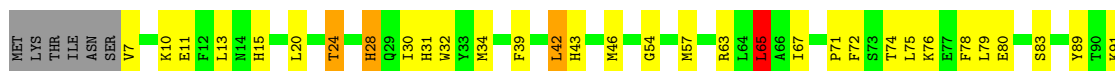
Chain I: 56% 31% 8%





• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain J: 62% 31% . . .



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain K: 59% 28% 8% . . .



• Molecule 1: NON-HEME IRON-CONTAINING FERRITIN

Chain L: 60% 31% . . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                          | Source    |
|----------------------------------------------------------|------------------------------------------------|-----------|
| Space group                                              | P 21 21 21                                     | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 87.54Å 137.50Å 173.36Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 10.00 – 2.35                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 91.0 (10.00-2.35)                              | Depositor |
| $R_{merge}$                                              | (Not available)                                | Depositor |
| $R_{sym}$                                                | 0.08                                           | Depositor |
| Refinement program                                       | TNT 5E                                         | Depositor |
| R, $R_{free}$                                            | 0.219 , (Not available)                        | Depositor |
| Estimated twinning fraction                              | No twinning to report.                         | Xtriage   |
| Total number of atoms                                    | 15155                                          | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 17.0                                           | wwPDB-VP  |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.88         | 1/1249 (0.1%)   | 1.49        | 12/1684 (0.7%)   |
| 1   | B     | 0.83         | 1/1249 (0.1%)   | 1.53        | 11/1684 (0.7%)   |
| 1   | C     | 0.88         | 2/1249 (0.2%)   | 1.42        | 9/1684 (0.5%)    |
| 1   | D     | 0.84         | 1/1249 (0.1%)   | 1.54        | 12/1684 (0.7%)   |
| 1   | E     | 0.92         | 1/1249 (0.1%)   | 1.47        | 8/1684 (0.5%)    |
| 1   | F     | 0.84         | 1/1249 (0.1%)   | 1.53        | 12/1684 (0.7%)   |
| 1   | G     | 0.86         | 0/1249          | 1.41        | 6/1684 (0.4%)    |
| 1   | H     | 0.90         | 2/1249 (0.2%)   | 1.43        | 9/1684 (0.5%)    |
| 1   | I     | 0.86         | 1/1249 (0.1%)   | 1.55        | 20/1684 (1.2%)   |
| 1   | J     | 0.86         | 3/1249 (0.2%)   | 1.48        | 9/1684 (0.5%)    |
| 1   | K     | 0.84         | 1/1249 (0.1%)   | 1.48        | 11/1684 (0.7%)   |
| 1   | L     | 0.92         | 2/1249 (0.2%)   | 1.52        | 15/1684 (0.9%)   |
| All | All   | 0.87         | 16/14988 (0.1%) | 1.49        | 134/20208 (0.7%) |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 99  | MET  | SD-CE   | -6.32 | 1.63        | 1.79     |
| 1   | L     | 118 | GLU  | C-N     | -6.28 | 1.25        | 1.33     |
| 1   | A     | 8   | ASP  | N-CA    | 6.16  | 1.53        | 1.45     |
| 1   | H     | 8   | ASP  | N-CA    | 5.72  | 1.52        | 1.46     |
| 1   | C     | 32  | TRP  | NE1-CE2 | -5.46 | 1.31        | 1.37     |
| 1   | D     | 32  | TRP  | NE1-CE2 | -5.45 | 1.31        | 1.37     |
| 1   | F     | 32  | TRP  | NE1-CE2 | -5.42 | 1.31        | 1.37     |
| 1   | H     | 32  | TRP  | NE1-CE2 | -5.42 | 1.31        | 1.37     |
| 1   | J     | 95  | MET  | SD-CE   | 5.38  | 1.93        | 1.79     |
| 1   | J     | 32  | TRP  | NE1-CE2 | -5.33 | 1.31        | 1.37     |
| 1   | C     | 95  | MET  | SD-CE   | 5.30  | 1.92        | 1.79     |
| 1   | J     | 156 | GLU  | C-O     | 5.28  | 1.34        | 1.23     |
| 1   | I     | 32  | TRP  | NE1-CE2 | -5.26 | 1.31        | 1.37     |
| 1   | L     | 32  | TRP  | NE1-CE2 | -5.23 | 1.31        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 32  | TRP  | NE1-CE2 | -5.10 | 1.31        | 1.37     |
| 1   | B     | 7   | VAL  | N-CA    | 5.04  | 1.55        | 1.46     |

All (134) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1   | D     | 156 | GLU  | CA-C-O   | 11.68  | 140.65      | 120.80   |
| 1   | E     | 30  | ILE  | CA-C-O   | 11.21  | 133.05      | 121.17   |
| 1   | A     | 91  | LYS  | N-CA-C   | -10.67 | 95.36       | 110.08   |
| 1   | L     | 7   | VAL  | O-C-N    | -9.02  | 108.56      | 123.00   |
| 1   | L     | 156 | GLU  | CB-CG-CD | 8.69   | 127.38      | 112.60   |
| 1   | G     | 131 | MET  | CB-CA-C  | -8.17  | 98.05       | 110.88   |
| 1   | C     | 131 | MET  | CB-CA-C  | -7.61  | 98.94       | 110.88   |
| 1   | A     | 92  | PRO  | N-CA-C   | -7.34  | 100.40      | 111.41   |
| 1   | K     | 122 | LYS  | O-C-N    | 7.28   | 129.87      | 122.08   |
| 1   | E     | 31  | HIS  | N-CA-CB  | -7.28  | 99.00       | 110.28   |
| 1   | B     | 65  | LEU  | N-CA-CB  | -7.21  | 99.53       | 110.12   |
| 1   | H     | 83  | SER  | N-CA-C   | -7.11  | 104.76      | 113.50   |
| 1   | G     | 65  | LEU  | N-CA-CB  | -7.07  | 99.76       | 110.01   |
| 1   | A     | 131 | MET  | CB-CA-C  | -7.03  | 99.85       | 110.88   |
| 1   | I     | 131 | MET  | CB-CA-C  | -6.96  | 99.95       | 110.88   |
| 1   | E     | 131 | MET  | CB-CA-C  | -6.95  | 100.26      | 110.96   |
| 1   | I     | 65  | LEU  | N-CA-CB  | -6.93  | 99.93       | 110.12   |
| 1   | C     | 15  | HIS  | N-CA-C   | -6.92  | 103.81      | 111.36   |
| 1   | K     | 131 | MET  | CB-CA-C  | -6.85  | 99.86       | 110.81   |
| 1   | D     | 81  | ASN  | N-CA-C   | 6.84   | 121.92      | 113.50   |
| 1   | J     | 116 | GLY  | N-CA-C   | -6.83  | 104.53      | 112.73   |
| 1   | B     | 145 | MET  | N-CA-C   | 6.77   | 118.66      | 111.28   |
| 1   | F     | 131 | MET  | CB-CA-C  | -6.71  | 100.34      | 110.88   |
| 1   | F     | 153 | ALA  | N-CA-C   | -6.69  | 100.35      | 110.39   |
| 1   | I     | 92  | PRO  | N-CA-C   | -6.68  | 98.71       | 112.47   |
| 1   | D     | 156 | GLU  | CB-CA-C  | 6.58   | 122.59      | 110.10   |
| 1   | I     | 120 | THR  | N-CA-CB  | -6.57  | 100.10      | 110.22   |
| 1   | L     | 131 | MET  | CB-CA-C  | -6.54  | 100.61      | 110.88   |
| 1   | L     | 72  | PHE  | N-CA-C   | -6.53  | 101.29      | 110.50   |
| 1   | K     | 63  | ARG  | N-CA-C   | -6.43  | 104.35      | 111.36   |
| 1   | J     | 131 | MET  | CB-CA-C  | -6.38  | 100.86      | 110.88   |
| 1   | B     | 131 | MET  | CB-CA-C  | -6.35  | 100.91      | 110.88   |
| 1   | D     | 116 | GLY  | N-CA-C   | -6.25  | 105.05      | 113.24   |
| 1   | F     | 60  | VAL  | N-CA-C   | -6.25  | 104.42      | 110.42   |
| 1   | C     | 56  | GLN  | N-CA-C   | -6.23  | 104.49      | 111.28   |
| 1   | B     | 83  | SER  | N-CA-C   | -6.18  | 105.90      | 113.50   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | L     | 78  | PHE  | N-CA-C   | -6.18 | 104.46      | 111.07   |
| 1   | E     | 81  | ASN  | N-CA-C   | 6.17  | 121.08      | 113.50   |
| 1   | D     | 72  | PHE  | N-CA-C   | -6.15 | 101.98      | 110.35   |
| 1   | K     | 116 | GLY  | N-CA-C   | -6.15 | 105.35      | 112.73   |
| 1   | J     | 72  | PHE  | N-CA-C   | -6.14 | 102.38      | 110.43   |
| 1   | H     | 131 | MET  | CB-CA-C  | -6.10 | 101.30      | 110.88   |
| 1   | D     | 153 | ALA  | N-CA-C   | -6.10 | 101.34      | 110.24   |
| 1   | G     | 31  | HIS  | N-CA-CB  | -6.04 | 100.99      | 110.30   |
| 1   | D     | 95  | MET  | N-CA-C   | -6.03 | 104.62      | 111.07   |
| 1   | C     | 116 | GLY  | N-CA-C   | -6.01 | 105.52      | 112.73   |
| 1   | K     | 65  | LEU  | N-CA-CB  | -5.92 | 101.42      | 110.12   |
| 1   | A     | 94  | THR  | N-CA-C   | 5.89  | 118.50      | 110.55   |
| 1   | C     | 95  | MET  | N-CA-C   | -5.87 | 104.96      | 111.36   |
| 1   | B     | 116 | GLY  | N-CA-C   | -5.86 | 105.70      | 112.73   |
| 1   | D     | 65  | LEU  | N-CA-CB  | -5.84 | 101.54      | 110.12   |
| 1   | K     | 54  | GLY  | N-CA-C   | -5.81 | 105.62      | 113.24   |
| 1   | I     | 73  | SER  | N-CA-C   | 5.78  | 117.23      | 110.41   |
| 1   | B     | 120 | THR  | N-CA-CB  | -5.75 | 101.37      | 110.22   |
| 1   | B     | 119 | LEU  | N-CA-CB  | -5.72 | 101.72      | 110.01   |
| 1   | B     | 95  | MET  | N-CA-C   | -5.71 | 104.96      | 111.07   |
| 1   | D     | 41  | THR  | CB-CA-C  | 5.70  | 119.82      | 110.88   |
| 1   | B     | 60  | VAL  | N-CA-C   | -5.69 | 104.96      | 110.42   |
| 1   | A     | 65  | LEU  | N-CA-C   | -5.69 | 105.08      | 111.28   |
| 1   | I     | 23  | PHE  | CA-C-O   | 5.66  | 126.55      | 120.55   |
| 1   | F     | 118 | GLU  | CA-C-O   | 5.66  | 126.55      | 120.55   |
| 1   | F     | 83  | SER  | N-CA-C   | -5.65 | 106.55      | 113.50   |
| 1   | I     | 123 | GLU  | N-CA-C   | 5.64  | 119.91      | 113.19   |
| 1   | A     | 91  | LYS  | CA-C-N   | 5.62  | 125.60      | 120.03   |
| 1   | A     | 91  | LYS  | C-N-CA   | 5.62  | 125.60      | 120.03   |
| 1   | A     | 83  | SER  | N-CA-C   | -5.61 | 106.60      | 113.50   |
| 1   | F     | 54  | GLY  | N-CA-C   | -5.58 | 105.63      | 112.77   |
| 1   | I     | 131 | MET  | CA-CB-CG | 5.58  | 125.25      | 114.10   |
| 1   | G     | 78  | PHE  | N-CA-C   | -5.57 | 105.11      | 111.07   |
| 1   | J     | 78  | PHE  | N-CA-C   | -5.56 | 105.12      | 111.07   |
| 1   | K     | 56  | GLN  | N-CA-C   | -5.55 | 105.23      | 111.28   |
| 1   | L     | 119 | LEU  | N-CA-CB  | -5.54 | 101.97      | 110.01   |
| 1   | I     | 72  | PHE  | N-CA-C   | -5.54 | 102.81      | 110.35   |
| 1   | I     | 31  | HIS  | N-CA-CB  | -5.54 | 101.98      | 110.12   |
| 1   | L     | 120 | THR  | N-CA-C   | -5.53 | 105.63      | 112.38   |
| 1   | A     | 116 | GLY  | N-CA-C   | -5.51 | 106.02      | 113.24   |
| 1   | E     | 7   | VAL  | CB-CA-C  | -5.51 | 100.93      | 111.40   |
| 1   | F     | 65  | LEU  | N-CA-CB  | -5.50 | 102.04      | 110.12   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | K     | 80  | GLU  | CA-C-N  | -5.48 | 113.55      | 122.26   |
| 1   | K     | 80  | GLU  | C-N-CA  | -5.48 | 113.55      | 122.26   |
| 1   | A     | 41  | THR  | CB-CA-C | 5.47  | 119.47      | 110.88   |
| 1   | D     | 37  | HIS  | N-CA-C  | 5.46  | 119.44      | 112.34   |
| 1   | F     | 116 | GLY  | N-CA-C  | -5.45 | 106.11      | 113.24   |
| 1   | L     | 119 | LEU  | CA-C-O  | 5.45  | 126.54      | 120.82   |
| 1   | K     | 72  | PHE  | N-CA-C  | -5.44 | 103.34      | 110.53   |
| 1   | I     | 67  | ILE  | N-CA-C  | -5.43 | 107.07      | 111.91   |
| 1   | I     | 118 | GLU  | CB-CA-C | 5.41  | 119.88      | 110.68   |
| 1   | J     | 67  | ILE  | N-CA-C  | -5.39 | 107.22      | 112.29   |
| 1   | K     | 153 | ALA  | N-CA-C  | -5.37 | 102.33      | 110.39   |
| 1   | A     | 121 | ASP  | N-CA-C  | -5.35 | 105.14      | 110.97   |
| 1   | J     | 30  | ILE  | O-C-N   | 5.35  | 127.15      | 121.91   |
| 1   | I     | 40  | PHE  | N-CA-C  | 5.33  | 116.78      | 111.07   |
| 1   | I     | 91  | LYS  | CA-C-N  | 5.32  | 126.49      | 119.84   |
| 1   | I     | 91  | LYS  | C-N-CA  | 5.32  | 126.49      | 119.84   |
| 1   | L     | 63  | ARG  | N-CA-C  | -5.31 | 105.57      | 111.36   |
| 1   | J     | 63  | ARG  | N-CA-C  | -5.31 | 105.58      | 111.36   |
| 1   | I     | 91  | LYS  | N-CA-C  | -5.29 | 102.51      | 110.24   |
| 1   | E     | 65  | LEU  | N-CA-CB | -5.27 | 102.09      | 109.94   |
| 1   | C     | 65  | LEU  | N-CA-CB | -5.26 | 102.39      | 110.12   |
| 1   | C     | 60  | VAL  | N-CA-C  | -5.25 | 105.38      | 110.42   |
| 1   | B     | 122 | LYS  | N-CA-C  | -5.24 | 105.46      | 111.07   |
| 1   | H     | 41  | THR  | CB-CA-C | 5.23  | 119.09      | 110.88   |
| 1   | L     | 145 | MET  | N-CA-C  | 5.23  | 116.67      | 111.07   |
| 1   | J     | 54  | GLY  | N-CA-C  | -5.21 | 106.38      | 113.37   |
| 1   | J     | 65  | LEU  | N-CA-CB | -5.21 | 102.17      | 109.94   |
| 1   | E     | 136 | LYS  | N-CA-CB | 5.20  | 117.77      | 110.12   |
| 1   | H     | 95  | MET  | N-CA-C  | -5.20 | 105.62      | 111.28   |
| 1   | L     | 65  | LEU  | N-CA-CB | -5.18 | 102.29      | 110.06   |
| 1   | L     | 82  | ALA  | N-CA-C  | 5.18  | 117.73      | 110.23   |
| 1   | F     | 63  | ARG  | N-CA-C  | -5.16 | 105.73      | 111.36   |
| 1   | H     | 56  | GLN  | N-CA-C  | -5.16 | 105.65      | 111.28   |
| 1   | F     | 41  | THR  | CB-CA-C | 5.16  | 118.98      | 110.88   |
| 1   | I     | 118 | GLU  | CA-C-N  | 5.14  | 127.43      | 120.65   |
| 1   | I     | 118 | GLU  | C-N-CA  | 5.14  | 127.43      | 120.65   |
| 1   | G     | 145 | MET  | N-CA-C  | 5.10  | 116.65      | 111.14   |
| 1   | H     | 124 | GLY  | CA-C-N  | -5.10 | 115.22      | 122.41   |
| 1   | H     | 124 | GLY  | C-N-CA  | -5.10 | 115.22      | 122.41   |
| 1   | L     | 7   | VAL  | N-CA-C  | -5.10 | 96.72       | 111.00   |
| 1   | E     | 116 | GLY  | N-CA-C  | -5.10 | 106.61      | 112.73   |
| 1   | C     | 153 | ALA  | N-CA-C  | -5.09 | 102.75      | 110.39   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | I     | 106 | LEU  | N-CA-C  | -5.09 | 105.81      | 111.36   |
| 1   | H     | 81  | ASN  | N-CA-C  | 5.06  | 119.73      | 113.50   |
| 1   | I     | 153 | ALA  | N-CA-C  | -5.06 | 102.80      | 110.39   |
| 1   | L     | 67  | ILE  | N-CA-C  | -5.05 | 107.41      | 111.91   |
| 1   | B     | 31  | HIS  | N-CA-CB | -5.05 | 102.70      | 110.12   |
| 1   | F     | 82  | ALA  | N-CA-C  | 5.05  | 117.62      | 110.50   |
| 1   | H     | 72  | PHE  | N-CA-C  | -5.05 | 103.49      | 110.35   |
| 1   | L     | 56  | GLN  | N-CA-C  | -5.04 | 105.79      | 111.28   |
| 1   | A     | 66  | ALA  | N-CA-C  | 5.02  | 117.48      | 111.71   |
| 1   | F     | 127 | VAL  | N-CA-C  | 5.01  | 115.23      | 110.42   |
| 1   | G     | 41  | THR  | CB-CA-C | 5.01  | 118.75      | 110.88   |
| 1   | C     | 145 | MET  | N-CA-C  | 5.01  | 116.55      | 111.14   |
| 1   | D     | 93  | LYS  | CA-C-N  | 5.00  | 128.79      | 120.94   |
| 1   | D     | 93  | LYS  | C-N-CA  | 5.00  | 128.79      | 120.94   |

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     | 1222  | 0        | 1186     | 35      | 0            |
| 1   | B     | 1222  | 0        | 1186     | 37      | 0            |
| 1   | C     | 1222  | 0        | 1186     | 37      | 0            |
| 1   | D     | 1222  | 0        | 1186     | 45      | 0            |
| 1   | E     | 1222  | 0        | 1186     | 41      | 0            |
| 1   | F     | 1222  | 0        | 1186     | 60      | 0            |
| 1   | G     | 1222  | 0        | 1186     | 49      | 0            |
| 1   | H     | 1222  | 0        | 1186     | 41      | 0            |
| 1   | I     | 1222  | 0        | 1186     | 51      | 0            |
| 1   | J     | 1222  | 0        | 1186     | 37      | 0            |
| 1   | K     | 1222  | 0        | 1186     | 72      | 0            |
| 1   | L     | 1222  | 0        | 1186     | 43      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 38    | 0        | 0        | 3       | 0            |
| 3   | B     | 22    | 0        | 0        | 0       | 0            |
| 3   | C     | 36    | 0        | 0        | 3       | 0            |
| 3   | D     | 28    | 0        | 0        | 5       | 0            |
| 3   | E     | 50    | 0        | 0        | 7       | 0            |
| 3   | F     | 42    | 0        | 0        | 7       | 0            |
| 3   | G     | 54    | 0        | 0        | 7       | 0            |
| 3   | H     | 44    | 0        | 0        | 3       | 0            |
| 3   | I     | 33    | 0        | 0        | 3       | 0            |
| 3   | J     | 46    | 0        | 0        | 6       | 0            |
| 3   | K     | 41    | 0        | 0        | 10      | 0            |
| 3   | L     | 45    | 0        | 0        | 4       | 0            |
| All | All   | 15155 | 0        | 14232    | 521     | 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 19.

All (521) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:G:94:THR:HG22 | 1:G:97:GLN:H    | 1.11                     | 1.12              |
| 1:F:94:THR:HB   | 1:F:97:GLN:HG3  | 1.20                     | 1.12              |
| 1:F:94:THR:HG22 | 1:F:96:ASP:N    | 1.69                     | 1.08              |
| 1:F:7:VAL:HG12  | 1:F:8:ASP:H     | 1.22                     | 1.04              |
| 1:I:94:THR:HB   | 1:I:97:GLN:HG3  | 1.40                     | 1.03              |
| 1:D:94:THR:HB   | 1:D:97:GLN:HG3  | 1.37                     | 1.03              |
| 1:K:94:THR:HB   | 1:K:97:GLN:HG3  | 1.41                     | 1.03              |
| 1:D:147:LYS:HZ2 | 1:D:156:GLU:HG2 | 1.29                     | 0.97              |
| 1:K:114:LYS:HA  | 3:K:164:HOH:O   | 1.64                     | 0.96              |
| 1:E:91:LYS:HG2  | 1:E:92:PRO:HD2  | 1.46                     | 0.95              |
| 1:F:11:GLU:HG2  | 3:F:172:HOH:O   | 1.67                     | 0.93              |
| 1:D:147:LYS:NZ  | 1:D:156:GLU:HG2 | 1.83                     | 0.91              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:117:ILE:HD13 | 1:K:133:ILE:HG12 | 1.52                     | 0.91              |
| 1:F:120:THR:HG22 | 1:F:129:ASN:HB2  | 1.51                     | 0.90              |
| 1:F:34:MET:HG2   | 3:F:178:HOH:O    | 1.71                     | 0.90              |
| 1:G:120:THR:HG22 | 1:G:129:ASN:HB2  | 1.53                     | 0.90              |
| 1:F:94:THR:HG22  | 1:F:96:ASP:H     | 1.29                     | 0.88              |
| 1:H:100:GLU:HG2  | 3:H:160:HOH:O    | 1.71                     | 0.88              |
| 1:B:156:GLU:HA   | 1:B:156:GLU:OE1  | 1.75                     | 0.86              |
| 1:G:94:THR:HG23  | 3:G:193:HOH:O    | 1.74                     | 0.86              |
| 1:G:120:THR:HG21 | 1:G:129:ASN:CA   | 2.05                     | 0.86              |
| 1:F:94:THR:CG2   | 1:F:96:ASP:H     | 1.89                     | 0.85              |
| 1:H:94:THR:HB    | 1:H:97:GLN:HG3   | 1.59                     | 0.85              |
| 1:G:94:THR:HG22  | 1:G:97:GLN:N     | 1.93                     | 0.84              |
| 1:K:94:THR:HG22  | 1:K:96:ASP:N     | 1.93                     | 0.84              |
| 1:F:113:TYR:O    | 1:F:117:ILE:HG13 | 1.77                     | 0.83              |
| 1:F:82:ALA:HA    | 3:F:179:HOH:O    | 1.78                     | 0.83              |
| 1:E:91:LYS:CG    | 1:E:92:PRO:HD2   | 2.08                     | 0.82              |
| 1:F:120:THR:HG21 | 1:F:129:ASN:N    | 1.96                     | 0.81              |
| 1:I:120:THR:CG2  | 1:I:129:ASN:HB2  | 2.11                     | 0.80              |
| 1:G:120:THR:CG2  | 1:G:129:ASN:HB2  | 2.11                     | 0.80              |
| 1:I:120:THR:HG21 | 1:I:129:ASN:HA   | 1.62                     | 0.80              |
| 1:H:94:THR:HG22  | 1:H:97:GLN:H     | 1.47                     | 0.79              |
| 1:I:153:ALA:O    | 1:I:156:GLU:HB2  | 1.83                     | 0.78              |
| 1:E:94:THR:HB    | 1:E:97:GLN:HG3   | 1.63                     | 0.78              |
| 1:F:94:THR:HB    | 1:F:97:GLN:CG    | 2.07                     | 0.78              |
| 1:B:94:THR:HG22  | 1:B:96:ASP:H     | 1.49                     | 0.77              |
| 1:A:7:VAL:HG12   | 1:A:11:GLU:CB    | 2.14                     | 0.77              |
| 1:H:116:GLY:O    | 1:H:120:THR:HG22 | 1.85                     | 0.77              |
| 1:L:155:LEU:O    | 1:L:156:GLU:HB2  | 1.84                     | 0.77              |
| 1:K:34:MET:HB2   | 1:K:95:MET:HE1   | 1.65                     | 0.77              |
| 1:A:7:VAL:HG12   | 1:A:11:GLU:HB2   | 1.66                     | 0.76              |
| 1:K:120:THR:HG21 | 1:K:129:ASN:HA   | 1.67                     | 0.76              |
| 1:L:24:THR:HG23  | 3:L:199:HOH:O    | 1.85                     | 0.75              |
| 1:G:41:THR:HG21  | 3:G:180:HOH:O    | 1.85                     | 0.75              |
| 1:L:120:THR:HG21 | 1:L:129:ASN:HA   | 1.69                     | 0.75              |
| 1:E:94:THR:HG22  | 1:E:97:GLN:H     | 1.53                     | 0.74              |
| 1:C:120:THR:CG2  | 1:C:129:ASN:HD22 | 1.99                     | 0.74              |
| 1:K:94:THR:HG22  | 1:K:96:ASP:H     | 1.51                     | 0.74              |
| 1:G:120:THR:HG21 | 1:G:129:ASN:N    | 2.03                     | 0.74              |
| 1:K:94:THR:CG2   | 1:K:96:ASP:H     | 2.02                     | 0.73              |
| 1:I:120:THR:HG21 | 1:I:129:ASN:CA   | 2.16                     | 0.73              |
| 1:K:120:THR:HG21 | 1:K:129:ASN:CA   | 2.18                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:29:GLN:NE2   | 3:E:207:HOH:O    | 2.13                     | 0.72              |
| 1:K:116:GLY:O    | 1:K:120:THR:HB   | 1.89                     | 0.72              |
| 1:F:7:VAL:HG12   | 1:F:8:ASP:N      | 2.01                     | 0.71              |
| 1:E:117:ILE:HD13 | 1:E:133:ILE:HG12 | 1.70                     | 0.71              |
| 1:C:120:THR:HG21 | 1:C:129:ASN:HA   | 1.73                     | 0.71              |
| 1:A:119:LEU:HD23 | 1:A:120:THR:HG23 | 1.71                     | 0.71              |
| 1:F:94:THR:HG21  | 1:F:96:ASP:HB2   | 1.72                     | 0.70              |
| 1:D:31:HIS:CE1   | 1:D:43:HIS:CE1   | 2.80                     | 0.70              |
| 1:L:117:ILE:O    | 1:L:120:THR:HG22 | 1.91                     | 0.70              |
| 1:D:145:MET:HE3  | 3:D:165:HOH:O    | 1.91                     | 0.70              |
| 1:L:120:THR:CG2  | 1:L:129:ASN:HD22 | 2.04                     | 0.70              |
| 1:E:141:LYS:HD3  | 3:E:203:HOH:O    | 1.92                     | 0.69              |
| 1:F:114:LYS:O    | 1:F:118:GLU:HG3  | 1.92                     | 0.69              |
| 1:K:94:THR:CG2   | 1:K:96:ASP:HB2   | 2.22                     | 0.69              |
| 1:A:7:VAL:CG1    | 1:A:11:GLU:HB3   | 2.23                     | 0.69              |
| 1:B:117:ILE:O    | 1:B:120:THR:HG22 | 1.93                     | 0.69              |
| 1:J:94:THR:HG22  | 1:J:95:MET:N     | 2.08                     | 0.68              |
| 1:B:114:LYS:HE3  | 1:B:118:GLU:OE2  | 1.93                     | 0.68              |
| 1:D:129:ASN:O    | 1:D:133:ILE:HG13 | 1.92                     | 0.68              |
| 1:K:42:LEU:HD23  | 1:K:95:MET:SD    | 2.33                     | 0.68              |
| 1:F:120:THR:CG2  | 1:F:129:ASN:HB2  | 2.21                     | 0.68              |
| 1:I:89:TYR:OH    | 1:I:92:PRO:HA    | 1.93                     | 0.68              |
| 1:D:94:THR:CB    | 1:D:97:GLN:HG3   | 2.19                     | 0.68              |
| 1:G:120:THR:HG21 | 1:G:129:ASN:HA   | 1.76                     | 0.68              |
| 3:J:188:HOH:O    | 1:L:28:HIS:HD2   | 1.77                     | 0.68              |
| 1:D:120:THR:HG21 | 1:D:129:ASN:HA   | 1.75                     | 0.68              |
| 1:G:76:LYS:HG3   | 3:G:169:HOH:O    | 1.94                     | 0.68              |
| 1:F:120:THR:HG21 | 1:F:129:ASN:CA   | 2.25                     | 0.67              |
| 1:G:153:ALA:HB3  | 1:G:156:GLU:HB2  | 1.75                     | 0.67              |
| 1:J:24:THR:HG23  | 3:J:202:HOH:O    | 1.95                     | 0.67              |
| 1:J:28:HIS:HD2   | 3:L:188:HOH:O    | 1.77                     | 0.67              |
| 1:E:28:HIS:HD2   | 3:G:189:HOH:O    | 1.78                     | 0.67              |
| 1:D:94:THR:HB    | 1:D:97:GLN:CG    | 2.18                     | 0.67              |
| 1:D:155:LEU:HB2  | 3:D:159:HOH:O    | 1.94                     | 0.66              |
| 3:J:158:HOH:O    | 1:L:88:PRO:HD3   | 1.95                     | 0.66              |
| 1:L:120:THR:HG23 | 1:L:129:ASN:HB2  | 1.76                     | 0.66              |
| 1:D:119:LEU:HD11 | 1:D:123:GLU:OE2  | 1.95                     | 0.66              |
| 1:I:120:THR:HG23 | 1:I:129:ASN:HB2  | 1.76                     | 0.66              |
| 3:A:176:HOH:O    | 1:C:28:HIS:HD2   | 1.79                     | 0.66              |
| 1:F:94:THR:HG22  | 1:F:97:GLN:H     | 1.61                     | 0.65              |
| 1:I:31:HIS:CE1   | 1:I:43:HIS:CE1   | 2.84                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:120:THR:HG23 | 1:C:129:ASN:HD22 | 1.61                     | 0.65              |
| 1:I:94:THR:HG22  | 1:I:96:ASP:H     | 1.61                     | 0.65              |
| 1:B:94:THR:HB    | 1:B:97:GLN:HG3   | 1.77                     | 0.65              |
| 1:B:119:LEU:O    | 1:B:123:GLU:HG3  | 1.95                     | 0.65              |
| 1:F:34:MET:N     | 3:F:178:HOH:O    | 2.30                     | 0.65              |
| 1:K:94:THR:HG22  | 1:K:97:GLN:H     | 1.62                     | 0.64              |
| 1:L:119:LEU:HD11 | 1:L:123:GLU:OE2  | 1.97                     | 0.64              |
| 1:F:81:ASN:HB3   | 3:F:159:HOH:O    | 1.97                     | 0.64              |
| 1:J:119:LEU:O    | 1:J:123:GLU:HG3  | 1.97                     | 0.64              |
| 1:L:75:LEU:N     | 1:L:75:LEU:HD12  | 2.12                     | 0.64              |
| 1:E:94:THR:HG23  | 3:E:196:HOH:O    | 1.97                     | 0.64              |
| 1:K:117:ILE:HD12 | 3:K:164:HOH:O    | 1.97                     | 0.64              |
| 1:E:91:LYS:HG2   | 1:E:92:PRO:CD    | 2.23                     | 0.63              |
| 1:H:119:LEU:C    | 1:H:119:LEU:HD23 | 2.22                     | 0.63              |
| 1:A:7:VAL:HG11   | 1:A:11:GLU:HB3   | 1.81                     | 0.63              |
| 1:D:95:MET:N     | 3:D:167:HOH:O    | 2.25                     | 0.63              |
| 1:C:117:ILE:O    | 1:C:121:ASP:HB2  | 1.99                     | 0.63              |
| 1:B:94:THR:HG22  | 1:B:95:MET:N     | 2.12                     | 0.63              |
| 1:B:94:THR:HG22  | 1:B:96:ASP:N     | 2.13                     | 0.63              |
| 1:J:120:THR:HG21 | 1:J:129:ASN:HA   | 1.80                     | 0.63              |
| 1:E:41:THR:HG21  | 3:E:161:HOH:O    | 1.99                     | 0.62              |
| 1:L:94:THR:HG22  | 1:L:96:ASP:H     | 1.63                     | 0.62              |
| 1:K:31:HIS:CE1   | 1:K:43:HIS:CE1   | 2.87                     | 0.62              |
| 1:A:7:VAL:CG1    | 1:A:11:GLU:CB    | 2.77                     | 0.62              |
| 1:H:120:THR:HG23 | 1:H:129:ASN:HD22 | 1.65                     | 0.62              |
| 1:F:119:LEU:HD12 | 1:F:119:LEU:O    | 1.99                     | 0.62              |
| 1:I:120:THR:CG2  | 1:I:129:ASN:CB   | 2.77                     | 0.62              |
| 1:F:94:THR:CG2   | 1:F:96:ASP:HB2   | 2.30                     | 0.62              |
| 1:H:94:THR:HG22  | 1:H:96:ASP:N     | 2.14                     | 0.61              |
| 1:I:120:THR:HG22 | 1:I:129:ASN:HD22 | 1.64                     | 0.61              |
| 1:G:24:THR:HG23  | 3:G:166:HOH:O    | 1.99                     | 0.61              |
| 1:L:94:THR:HB    | 1:L:97:GLN:HG3   | 1.81                     | 0.61              |
| 1:A:28:HIS:HD2   | 3:C:161:HOH:O    | 1.83                     | 0.61              |
| 1:I:75:LEU:HD12  | 1:I:75:LEU:H     | 1.65                     | 0.61              |
| 1:L:42:LEU:HD23  | 1:L:95:MET:SD    | 2.40                     | 0.61              |
| 1:A:129:ASN:O    | 1:A:133:ILE:HG13 | 2.01                     | 0.61              |
| 1:H:31:HIS:CE1   | 1:H:43:HIS:CE1   | 2.89                     | 0.61              |
| 1:K:155:LEU:O    | 1:K:156:GLU:HB3  | 1.99                     | 0.61              |
| 1:F:153:ALA:O    | 1:F:156:GLU:HB2  | 2.00                     | 0.61              |
| 1:G:94:THR:HB    | 1:G:97:GLN:HG3   | 1.81                     | 0.61              |
| 1:I:45:LYS:NZ    | 3:I:161:HOH:O    | 2.29                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:153:ALA:O    | 1:C:156:GLU:HB2  | 2.01                     | 0.61              |
| 1:B:152:LYS:HB3  | 1:B:156:GLU:OE1  | 2.01                     | 0.61              |
| 1:B:65:LEU:HD13  | 1:B:71:PRO:HD3   | 1.83                     | 0.60              |
| 1:F:24:THR:HG23  | 3:F:186:HOH:O    | 2.00                     | 0.60              |
| 1:G:7:VAL:CG1    | 1:G:11:GLU:HB3   | 2.31                     | 0.60              |
| 1:D:126:ASP:HB3  | 1:F:133:ILE:HD13 | 1.84                     | 0.60              |
| 1:K:94:THR:HG21  | 1:K:96:ASP:HB2   | 1.82                     | 0.60              |
| 1:K:120:THR:CG2  | 1:K:129:ASN:HB2  | 2.31                     | 0.60              |
| 1:K:24:THR:HG23  | 3:K:190:HOH:O    | 2.00                     | 0.60              |
| 1:K:34:MET:HB2   | 1:K:95:MET:CE    | 2.30                     | 0.60              |
| 1:F:119:LEU:HD12 | 1:F:119:LEU:C    | 2.26                     | 0.60              |
| 1:J:94:THR:HB    | 1:J:97:GLN:HG3   | 1.84                     | 0.59              |
| 1:E:75:LEU:N     | 1:E:75:LEU:HD12  | 2.17                     | 0.59              |
| 1:H:129:ASN:O    | 1:H:133:ILE:HG13 | 2.01                     | 0.59              |
| 1:D:8:ASP:C      | 1:D:119:LEU:HD21 | 2.28                     | 0.59              |
| 1:I:75:LEU:HD12  | 1:I:75:LEU:N     | 2.15                     | 0.59              |
| 1:G:7:VAL:HG12   | 1:G:11:GLU:CB    | 2.32                     | 0.59              |
| 1:L:31:HIS:CE1   | 1:L:43:HIS:CE1   | 2.91                     | 0.59              |
| 1:I:120:THR:CG2  | 1:I:129:ASN:HD22 | 2.16                     | 0.59              |
| 1:I:145:MET:HE3  | 3:I:161:HOH:O    | 2.02                     | 0.59              |
| 1:D:8:ASP:HA     | 1:D:123:GLU:OE2  | 2.03                     | 0.58              |
| 1:G:94:THR:CG2   | 1:G:97:GLN:HG3   | 2.32                     | 0.58              |
| 1:I:44:GLU:HG2   | 3:I:187:HOH:O    | 2.03                     | 0.58              |
| 1:H:34:MET:HE1   | 1:H:42:LEU:HB3   | 1.86                     | 0.58              |
| 1:I:120:THR:HG22 | 1:I:121:ASP:N    | 2.18                     | 0.58              |
| 1:A:94:THR:HG22  | 1:A:97:GLN:H     | 1.68                     | 0.57              |
| 1:C:117:ILE:HD13 | 1:C:133:ILE:HG12 | 1.86                     | 0.57              |
| 3:E:171:HOH:O    | 1:G:28:HIS:HD2   | 1.87                     | 0.57              |
| 1:K:117:ILE:CD1  | 1:K:133:ILE:HG12 | 2.28                     | 0.57              |
| 1:B:116:GLY:O    | 1:B:120:THR:HG22 | 2.03                     | 0.57              |
| 1:F:31:HIS:CE1   | 1:F:43:HIS:CE1   | 2.93                     | 0.57              |
| 1:D:147:LYS:HZ2  | 1:D:156:GLU:CG   | 2.10                     | 0.57              |
| 1:G:120:THR:CG2  | 1:G:129:ASN:CB   | 2.82                     | 0.57              |
| 1:A:9:THR:HA     | 1:A:119:LEU:HD21 | 1.86                     | 0.57              |
| 1:I:42:LEU:HD23  | 1:I:95:MET:SD    | 2.45                     | 0.57              |
| 1:J:120:THR:HG23 | 1:J:129:ASN:HB2  | 1.86                     | 0.57              |
| 1:B:108:LEU:HD23 | 1:B:108:LEU:C    | 2.29                     | 0.57              |
| 1:A:31:HIS:CE1   | 1:A:43:HIS:CE1   | 2.92                     | 0.57              |
| 1:D:7:VAL:HG12   | 1:D:8:ASP:H      | 1.68                     | 0.57              |
| 1:C:24:THR:HG23  | 3:C:193:HOH:O    | 2.04                     | 0.56              |
| 1:I:34:MET:HE1   | 1:I:42:LEU:HB3   | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:108:LEU:C    | 1:I:108:LEU:HD23 | 2.29                     | 0.56              |
| 1:C:117:ILE:O    | 1:C:120:THR:HG22 | 2.06                     | 0.56              |
| 1:D:133:ILE:HD13 | 1:K:126:ASP:HB3  | 1.87                     | 0.56              |
| 1:H:118:GLU:O    | 1:H:122:LYS:HG3  | 2.05                     | 0.56              |
| 1:C:108:LEU:C    | 1:C:108:LEU:HD23 | 2.31                     | 0.56              |
| 1:H:153:ALA:HB3  | 1:H:156:GLU:HB2  | 1.87                     | 0.56              |
| 1:B:7:VAL:HG12   | 1:B:8:ASP:N      | 2.20                     | 0.55              |
| 1:D:34:MET:HE1   | 1:D:42:LEU:HB3   | 1.89                     | 0.55              |
| 1:A:108:LEU:C    | 1:A:108:LEU:HD23 | 2.31                     | 0.55              |
| 1:D:155:LEU:C    | 1:D:156:GLU:HG3  | 2.32                     | 0.55              |
| 1:E:81:ASN:HB3   | 3:E:173:HOH:O    | 2.06                     | 0.55              |
| 1:E:120:THR:HG21 | 1:E:129:ASN:HA   | 1.88                     | 0.55              |
| 1:I:120:THR:HG21 | 1:I:129:ASN:CB   | 2.37                     | 0.55              |
| 1:B:31:HIS:CE1   | 1:B:43:HIS:CE1   | 2.95                     | 0.54              |
| 1:G:31:HIS:CE1   | 1:G:43:HIS:CE1   | 2.95                     | 0.54              |
| 1:I:116:GLY:O    | 1:I:120:THR:HB   | 2.06                     | 0.54              |
| 1:F:7:VAL:HG12   | 1:F:11:GLU:HB2   | 1.90                     | 0.54              |
| 1:F:94:THR:CG2   | 1:F:95:MET:N     | 2.70                     | 0.54              |
| 1:A:75:LEU:HD12  | 1:A:75:LEU:N     | 2.23                     | 0.54              |
| 1:I:94:THR:HG22  | 1:I:96:ASP:N     | 2.23                     | 0.54              |
| 1:L:108:LEU:HD23 | 1:L:108:LEU:C    | 2.32                     | 0.54              |
| 1:F:94:THR:HG22  | 1:F:96:ASP:CA    | 2.38                     | 0.54              |
| 1:I:28:HIS:HD2   | 3:K:189:HOH:O    | 1.90                     | 0.54              |
| 1:B:94:THR:CG2   | 1:B:95:MET:N     | 2.70                     | 0.54              |
| 1:K:108:LEU:C    | 1:K:108:LEU:HD23 | 2.33                     | 0.54              |
| 1:F:94:THR:O     | 1:F:98:LEU:HG    | 2.07                     | 0.53              |
| 1:L:7:VAL:HG12   | 1:L:11:GLU:CB    | 2.38                     | 0.53              |
| 1:G:93:LYS:HD2   | 3:G:207:HOH:O    | 2.09                     | 0.53              |
| 1:G:120:THR:CG2  | 1:G:129:ASN:CA   | 2.85                     | 0.53              |
| 1:K:95:MET:O     | 1:K:99:MET:HG2   | 2.08                     | 0.53              |
| 1:K:7:VAL:HG11   | 1:K:11:GLU:HB3   | 1.89                     | 0.53              |
| 1:K:75:LEU:HD12  | 1:K:75:LEU:N     | 2.23                     | 0.53              |
| 1:C:94:THR:HB    | 1:C:97:GLN:HG3   | 1.90                     | 0.53              |
| 1:L:129:ASN:O    | 1:L:133:ILE:HG13 | 2.09                     | 0.53              |
| 1:J:34:MET:HE1   | 1:J:42:LEU:HB3   | 1.91                     | 0.52              |
| 1:C:94:THR:HG22  | 1:C:95:MET:N     | 2.25                     | 0.52              |
| 1:F:94:THR:CG2   | 1:F:97:GLN:H     | 2.22                     | 0.52              |
| 1:G:7:VAL:HG12   | 1:G:11:GLU:HB3   | 1.90                     | 0.52              |
| 1:L:34:MET:HE1   | 1:L:42:LEU:HB3   | 1.91                     | 0.52              |
| 1:L:75:LEU:HD12  | 1:L:75:LEU:H     | 1.74                     | 0.52              |
| 1:C:94:THR:HG22  | 1:C:95:MET:H     | 1.75                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:89:TYR:CE2   | 1:I:93:LYS:HD3   | 2.45                     | 0.52              |
| 1:J:31:HIS:CE1   | 1:J:43:HIS:CE1   | 2.98                     | 0.52              |
| 1:L:155:LEU:O    | 1:L:156:GLU:CB   | 2.57                     | 0.52              |
| 1:H:119:LEU:HD23 | 1:H:120:THR:N    | 2.25                     | 0.52              |
| 1:J:42:LEU:HD23  | 1:J:95:MET:SD    | 2.49                     | 0.52              |
| 1:J:117:ILE:O    | 1:J:120:THR:HG22 | 2.09                     | 0.52              |
| 1:E:153:ALA:HB3  | 1:E:156:GLU:HB2  | 1.90                     | 0.52              |
| 1:B:75:LEU:N     | 1:B:75:LEU:HD12  | 2.25                     | 0.52              |
| 1:F:75:LEU:HD12  | 1:F:75:LEU:N     | 2.25                     | 0.52              |
| 1:A:75:LEU:HD12  | 1:A:75:LEU:H     | 1.75                     | 0.52              |
| 1:G:76:LYS:O     | 1:G:80:GLU:HG3   | 2.10                     | 0.52              |
| 1:A:86:GLU:CD    | 1:C:74:THR:HB    | 2.35                     | 0.51              |
| 1:C:31:HIS:CE1   | 1:C:43:HIS:CE1   | 2.97                     | 0.51              |
| 1:J:112:GLU:HA   | 1:J:115:GLN:HG2  | 1.92                     | 0.51              |
| 1:H:94:THR:HB    | 1:H:97:GLN:CG    | 2.36                     | 0.51              |
| 1:H:99:MET:HA    | 1:H:99:MET:HE2   | 1.93                     | 0.51              |
| 1:L:141:LYS:HD3  | 3:L:193:HOH:O    | 2.09                     | 0.51              |
| 1:B:117:ILE:HD13 | 1:B:133:ILE:HG12 | 1.93                     | 0.51              |
| 1:L:119:LEU:C    | 1:L:119:LEU:HD12 | 2.35                     | 0.51              |
| 1:E:120:THR:HG23 | 1:E:129:ASN:HD22 | 1.76                     | 0.51              |
| 1:D:63:ARG:NH2   | 1:D:127:VAL:HB   | 2.26                     | 0.51              |
| 1:E:75:LEU:HD12  | 1:E:75:LEU:H     | 1.75                     | 0.51              |
| 1:H:117:ILE:O    | 1:H:120:THR:HG22 | 2.10                     | 0.51              |
| 1:H:120:THR:HG21 | 1:H:129:ASN:HA   | 1.92                     | 0.50              |
| 1:H:147:LYS:HD2  | 1:H:154:PRO:O    | 2.11                     | 0.50              |
| 1:L:94:THR:HG22  | 1:L:95:MET:N     | 2.26                     | 0.50              |
| 1:L:75:LEU:H     | 1:L:75:LEU:CD1   | 2.25                     | 0.50              |
| 1:C:28:HIS:CD2   | 1:C:50:TYR:CE2   | 2.99                     | 0.50              |
| 1:K:7:VAL:HG11   | 1:K:11:GLU:CB    | 2.42                     | 0.50              |
| 1:D:147:LYS:HD2  | 1:D:154:PRO:O    | 2.10                     | 0.50              |
| 1:I:89:TYR:CZ    | 1:I:92:PRO:HA    | 2.47                     | 0.50              |
| 1:E:126:ASP:OD2  | 1:I:114:LYS:NZ   | 2.42                     | 0.50              |
| 1:J:146:PHE:O    | 1:J:149:PHE:HB3  | 2.12                     | 0.50              |
| 1:D:147:LYS:HZ1  | 1:D:156:GLU:HG2  | 1.73                     | 0.50              |
| 1:B:116:GLY:O    | 1:B:120:THR:CG2  | 2.60                     | 0.49              |
| 1:F:99:MET:HG3   | 1:F:149:PHE:CE2  | 2.46                     | 0.49              |
| 1:F:120:THR:CG2  | 1:F:125:ASP:O    | 2.59                     | 0.49              |
| 1:H:108:LEU:C    | 1:H:108:LEU:HD23 | 2.37                     | 0.49              |
| 1:F:108:LEU:C    | 1:F:108:LEU:HD23 | 2.37                     | 0.49              |
| 1:J:24:THR:HG21  | 3:J:165:HOH:O    | 2.11                     | 0.49              |
| 1:G:34:MET:HE1   | 1:G:42:LEU:HB3   | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:41:THR:HG22  | 3:H:180:HOH:O    | 2.13                     | 0.49              |
| 1:K:94:THR:H     | 1:K:97:GLN:CD    | 2.20                     | 0.49              |
| 1:K:117:ILE:HB   | 3:K:164:HOH:O    | 2.12                     | 0.49              |
| 1:E:108:LEU:HD23 | 1:E:108:LEU:C    | 2.38                     | 0.49              |
| 1:G:94:THR:HG23  | 1:G:96:ASP:H     | 1.78                     | 0.49              |
| 1:E:147:LYS:HD2  | 1:E:154:PRO:O    | 2.13                     | 0.49              |
| 1:G:94:THR:CB    | 1:G:97:GLN:HG3   | 2.43                     | 0.49              |
| 1:J:114:LYS:HD2  | 1:J:114:LYS:O    | 2.13                     | 0.49              |
| 1:J:120:THR:CG2  | 1:J:129:ASN:HD22 | 2.25                     | 0.49              |
| 1:L:99:MET:HE2   | 1:L:99:MET:HA    | 1.95                     | 0.49              |
| 1:B:7:VAL:HG12   | 1:B:8:ASP:H      | 1.78                     | 0.48              |
| 1:G:42:LEU:HD23  | 1:G:95:MET:SD    | 2.53                     | 0.48              |
| 1:J:10:LYS:HG3   | 3:J:179:HOH:O    | 2.13                     | 0.48              |
| 1:C:94:THR:HB    | 1:C:97:GLN:H     | 1.78                     | 0.48              |
| 1:C:119:LEU:O    | 1:C:123:GLU:HG3  | 2.14                     | 0.48              |
| 1:E:28:HIS:CD2   | 1:G:57:MET:HE1   | 2.47                     | 0.48              |
| 1:F:94:THR:HG22  | 1:F:97:GLN:N     | 2.28                     | 0.48              |
| 1:I:94:THR:HB    | 1:I:97:GLN:CG    | 2.28                     | 0.48              |
| 1:D:114:LYS:HD2  | 1:D:114:LYS:O    | 2.13                     | 0.48              |
| 1:G:120:THR:HG23 | 1:G:125:ASP:O    | 2.13                     | 0.48              |
| 1:B:99:MET:HE2   | 1:B:99:MET:HA    | 1.93                     | 0.48              |
| 1:F:7:VAL:CG1    | 1:F:11:GLU:HB2   | 2.44                     | 0.48              |
| 1:G:108:LEU:HD23 | 1:G:108:LEU:C    | 2.39                     | 0.48              |
| 1:C:75:LEU:HD12  | 1:C:75:LEU:N     | 2.29                     | 0.48              |
| 1:F:94:THR:H     | 1:F:97:GLN:HB2   | 1.78                     | 0.48              |
| 1:A:34:MET:HE1   | 1:A:42:LEU:HB3   | 1.96                     | 0.48              |
| 1:C:41:THR:HG21  | 3:C:189:HOH:O    | 2.13                     | 0.48              |
| 1:D:75:LEU:N     | 1:D:75:LEU:HD12  | 2.29                     | 0.48              |
| 1:G:147:LYS:NZ   | 1:G:156:GLU:O    | 2.45                     | 0.48              |
| 1:B:42:LEU:HD21  | 1:B:149:PHE:CZ   | 2.49                     | 0.48              |
| 1:F:7:VAL:CG1    | 1:F:8:ASP:H      | 2.05                     | 0.48              |
| 1:F:126:ASP:OD2  | 1:K:114:LYS:NZ   | 2.42                     | 0.48              |
| 1:J:74:THR:HB    | 1:L:86:GLU:CD    | 2.39                     | 0.48              |
| 1:E:113:TYR:O    | 1:E:117:ILE:HG13 | 2.14                     | 0.48              |
| 1:K:114:LYS:O    | 1:K:118:GLU:HG3  | 2.14                     | 0.48              |
| 1:L:76:LYS:O     | 1:L:80:GLU:HG3   | 2.14                     | 0.48              |
| 1:H:114:LYS:HD2  | 1:H:114:LYS:O    | 2.14                     | 0.47              |
| 1:I:91:LYS:HA    | 1:I:92:PRO:HD3   | 1.61                     | 0.47              |
| 1:C:94:THR:OG1   | 1:C:97:GLN:HG3   | 2.14                     | 0.47              |
| 1:E:94:THR:HG22  | 1:E:96:ASP:N     | 2.28                     | 0.47              |
| 1:K:34:MET:HE1   | 1:K:42:LEU:HB3   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:126:ASP:O    | 1:K:129:ASN:HB3  | 2.14                     | 0.47              |
| 1:C:114:LYS:HD2  | 1:C:114:LYS:O    | 2.15                     | 0.47              |
| 1:B:99:MET:HG3   | 1:B:149:PHE:CE2  | 2.49                     | 0.47              |
| 1:K:117:ILE:CG1  | 3:K:164:HOH:O    | 2.62                     | 0.47              |
| 1:L:65:LEU:HD13  | 1:L:71:PRO:HD3   | 1.95                     | 0.47              |
| 1:B:7:VAL:HG11   | 1:B:11:GLU:HG2   | 1.97                     | 0.47              |
| 1:C:89:TYR:OH    | 1:C:92:PRO:HA    | 2.15                     | 0.47              |
| 1:D:147:LYS:HZ2  | 1:D:156:GLU:HA   | 1.79                     | 0.47              |
| 1:E:116:GLY:O    | 1:E:120:THR:HG22 | 2.14                     | 0.47              |
| 1:G:7:VAL:HG11   | 1:G:11:GLU:HB3   | 1.95                     | 0.47              |
| 1:H:65:LEU:HD13  | 1:H:71:PRO:HD3   | 1.97                     | 0.47              |
| 1:H:94:THR:CG2   | 1:H:96:ASP:H     | 2.27                     | 0.47              |
| 1:L:120:THR:HG22 | 1:L:129:ASN:HD22 | 1.77                     | 0.47              |
| 1:G:79:LEU:HA    | 1:G:79:LEU:HD23  | 1.59                     | 0.47              |
| 1:I:79:LEU:HA    | 1:I:79:LEU:HD23  | 1.54                     | 0.47              |
| 1:L:8:ASP:H      | 1:L:11:GLU:HB2   | 1.80                     | 0.47              |
| 1:B:79:LEU:HA    | 1:B:79:LEU:HD23  | 1.55                     | 0.47              |
| 1:L:75:LEU:N     | 1:L:75:LEU:CD1   | 2.77                     | 0.47              |
| 1:L:116:GLY:O    | 1:L:120:THR:HB   | 2.14                     | 0.47              |
| 1:H:94:THR:HG22  | 1:H:97:GLN:N     | 2.23                     | 0.46              |
| 1:I:75:LEU:H     | 1:I:75:LEU:CD1   | 2.27                     | 0.46              |
| 1:C:94:THR:CB    | 1:C:97:GLN:HG3   | 2.45                     | 0.46              |
| 1:G:126:ASP:OD2  | 1:L:114:LYS:NZ   | 2.42                     | 0.46              |
| 1:K:94:THR:HG22  | 1:K:96:ASP:CA    | 2.44                     | 0.46              |
| 1:F:57:MET:HE1   | 1:H:28:HIS:CD2   | 2.51                     | 0.46              |
| 1:L:28:HIS:CD2   | 1:L:50:TYR:CE2   | 3.03                     | 0.46              |
| 1:I:28:HIS:CD2   | 1:I:50:TYR:CE2   | 3.04                     | 0.46              |
| 1:G:94:THR:HG22  | 1:G:97:GLN:HG3   | 1.97                     | 0.46              |
| 1:J:76:LYS:O     | 1:J:80:GLU:HG3   | 2.16                     | 0.46              |
| 1:C:126:ASP:HB3  | 1:H:133:ILE:HD13 | 1.96                     | 0.46              |
| 1:E:120:THR:CG2  | 1:E:129:ASN:HD22 | 2.29                     | 0.46              |
| 1:A:147:LYS:HD2  | 1:A:154:PRO:O    | 2.16                     | 0.46              |
| 1:C:79:LEU:HA    | 1:C:79:LEU:HD23  | 1.67                     | 0.46              |
| 1:E:94:THR:H     | 1:E:97:GLN:CD    | 2.24                     | 0.46              |
| 1:G:119:LEU:HG   | 1:G:120:THR:N    | 2.31                     | 0.46              |
| 1:H:37:HIS:CD2   | 3:K:178:HOH:O    | 2.69                     | 0.46              |
| 1:H:75:LEU:HD12  | 1:H:75:LEU:N     | 2.31                     | 0.46              |
| 1:A:28:HIS:CD2   | 1:C:57:MET:HE1   | 2.51                     | 0.45              |
| 1:K:94:THR:HG22  | 1:K:96:ASP:HB2   | 1.97                     | 0.45              |
| 1:D:154:PRO:C    | 1:D:156:GLU:H    | 2.23                     | 0.45              |
| 1:F:114:LYS:O    | 1:F:114:LYS:HD2  | 2.14                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:75:LEU:N     | 1:G:75:LEU:HD12  | 2.31                     | 0.45              |
| 1:G:155:LEU:O    | 1:G:156:GLU:C    | 2.58                     | 0.45              |
| 1:J:75:LEU:N     | 1:J:75:LEU:HD12  | 2.32                     | 0.45              |
| 1:A:28:HIS:CD2   | 1:A:50:TYR:CE1   | 3.05                     | 0.45              |
| 1:C:99:MET:HE2   | 1:C:99:MET:HA    | 1.99                     | 0.45              |
| 1:K:79:LEU:HD23  | 1:K:79:LEU:HA    | 1.65                     | 0.45              |
| 1:L:79:LEU:HD23  | 1:L:79:LEU:HA    | 1.68                     | 0.45              |
| 1:E:42:LEU:HD12  | 1:E:42:LEU:HA    | 1.73                     | 0.45              |
| 1:F:129:ASN:O    | 1:F:133:ILE:HG13 | 2.17                     | 0.45              |
| 1:J:79:LEU:HD23  | 1:J:79:LEU:HA    | 1.70                     | 0.45              |
| 1:G:129:ASN:O    | 1:G:133:ILE:HG13 | 2.17                     | 0.45              |
| 1:K:24:THR:CG2   | 3:K:190:HOH:O    | 2.61                     | 0.45              |
| 1:K:76:LYS:O     | 1:K:80:GLU:HG3   | 2.17                     | 0.45              |
| 1:E:94:THR:HG22  | 1:E:97:GLN:N     | 2.27                     | 0.45              |
| 1:I:117:ILE:HD13 | 1:I:133:ILE:HG12 | 1.98                     | 0.45              |
| 1:K:117:ILE:HD11 | 1:K:133:ILE:HA   | 1.98                     | 0.45              |
| 1:L:7:VAL:HG12   | 1:L:11:GLU:HB3   | 1.98                     | 0.45              |
| 1:A:94:THR:HB    | 1:A:97:GLN:HG3   | 1.98                     | 0.45              |
| 1:A:114:LYS:HD2  | 1:A:114:LYS:O    | 2.16                     | 0.45              |
| 1:B:28:HIS:CD2   | 1:B:50:TYR:CE2   | 3.04                     | 0.45              |
| 1:D:114:LYS:NZ   | 1:K:126:ASP:OD2  | 2.45                     | 0.45              |
| 1:H:10:LYS:HG3   | 3:H:168:HOH:O    | 2.17                     | 0.45              |
| 1:H:75:LEU:HD12  | 1:H:75:LEU:H     | 1.82                     | 0.45              |
| 1:A:153:ALA:HB3  | 1:A:156:GLU:CB   | 2.47                     | 0.44              |
| 1:B:117:ILE:C    | 1:B:120:THR:HG22 | 2.41                     | 0.44              |
| 1:E:57:MET:HE1   | 1:G:28:HIS:CD2   | 2.52                     | 0.44              |
| 1:F:42:LEU:HD21  | 1:F:149:PHE:CZ   | 2.52                     | 0.44              |
| 1:K:94:THR:HG22  | 1:K:97:GLN:N     | 2.31                     | 0.44              |
| 1:B:39:PHE:O     | 1:B:43:HIS:HB2   | 2.17                     | 0.44              |
| 1:I:147:LYS:NZ   | 1:I:156:GLU:HB3  | 2.32                     | 0.44              |
| 1:K:8:ASP:HA     | 1:K:123:GLU:OE2  | 2.17                     | 0.44              |
| 1:G:107:GLU:OE2  | 3:G:202:HOH:O    | 2.21                     | 0.44              |
| 1:I:8:ASP:OD1    | 1:I:8:ASP:C      | 2.59                     | 0.44              |
| 1:I:76:LYS:O     | 1:I:80:GLU:HG3   | 2.18                     | 0.44              |
| 1:B:117:ILE:CD1  | 1:B:133:ILE:HG12 | 2.46                     | 0.44              |
| 1:D:126:ASP:HB3  | 1:F:133:ILE:CD1  | 2.45                     | 0.44              |
| 1:F:95:MET:O     | 1:F:99:MET:HG2   | 2.17                     | 0.44              |
| 1:B:114:LYS:HD2  | 1:B:114:LYS:O    | 2.17                     | 0.44              |
| 1:K:131:MET:HE3  | 1:K:132:LEU:HD13 | 1.99                     | 0.44              |
| 1:I:42:LEU:HD12  | 1:I:42:LEU:HA    | 1.81                     | 0.44              |
| 1:B:76:LYS:O     | 1:B:80:GLU:HG3   | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:28:HIS:NE2   | 1:C:50:TYR:CE2   | 2.86                     | 0.44              |
| 1:H:94:THR:CG2   | 1:H:96:ASP:N     | 2.80                     | 0.44              |
| 1:J:108:LEU:C    | 1:J:108:LEU:HD23 | 2.43                     | 0.44              |
| 1:L:42:LEU:O     | 1:L:46:MET:HG2   | 2.18                     | 0.44              |
| 1:A:79:LEU:HA    | 1:A:79:LEU:HD23  | 1.61                     | 0.44              |
| 1:J:28:HIS:CD2   | 3:L:188:HOH:O    | 2.62                     | 0.44              |
| 1:A:126:ASP:OD2  | 1:E:114:LYS:NZ   | 2.48                     | 0.44              |
| 1:D:117:ILE:O    | 1:D:120:THR:HG22 | 2.18                     | 0.44              |
| 1:C:34:MET:HE1   | 1:C:42:LEU:HB3   | 1.99                     | 0.43              |
| 1:C:42:LEU:HD21  | 1:C:149:PHE:CZ   | 2.53                     | 0.43              |
| 1:D:21:ASN:O     | 1:D:24:THR:HG22  | 2.18                     | 0.43              |
| 1:K:75:LEU:HD12  | 1:K:75:LEU:H     | 1.83                     | 0.43              |
| 1:L:89:TYR:OH    | 1:L:92:PRO:HA    | 2.17                     | 0.43              |
| 1:D:96:ASP:OD1   | 1:I:37:HIS:CE1   | 2.71                     | 0.43              |
| 1:K:7:VAL:CG1    | 1:K:11:GLU:CB    | 2.96                     | 0.43              |
| 1:A:65:LEU:HD13  | 1:A:71:PRO:HD3   | 2.01                     | 0.43              |
| 1:G:153:ALA:O    | 1:G:156:GLU:HB3  | 2.18                     | 0.43              |
| 1:H:79:LEU:HA    | 1:H:79:LEU:HD23  | 1.57                     | 0.43              |
| 1:C:65:LEU:HD13  | 1:C:71:PRO:HD3   | 2.00                     | 0.43              |
| 1:D:108:LEU:C    | 1:D:108:LEU:HD23 | 2.43                     | 0.43              |
| 1:D:126:ASP:O    | 3:D:173:HOH:O    | 2.21                     | 0.43              |
| 1:F:114:LYS:HD2  | 1:F:114:LYS:C    | 2.43                     | 0.43              |
| 1:I:42:LEU:HD21  | 1:I:149:PHE:CZ   | 2.53                     | 0.43              |
| 1:K:23:PHE:CD1   | 1:K:105:THR:HG21 | 2.53                     | 0.43              |
| 1:A:153:ALA:HB3  | 1:A:156:GLU:HB2  | 2.00                     | 0.43              |
| 1:J:94:THR:CG2   | 1:J:95:MET:N     | 2.77                     | 0.43              |
| 1:G:38:ASN:HB3   | 1:G:42:LEU:HD22  | 2.00                     | 0.43              |
| 1:F:28:HIS:CD2   | 1:H:57:MET:HE1   | 2.54                     | 0.43              |
| 1:B:147:LYS:HD2  | 1:B:154:PRO:O    | 2.19                     | 0.43              |
| 1:H:114:LYS:HD2  | 1:H:114:LYS:C    | 2.43                     | 0.43              |
| 1:K:120:THR:CG2  | 1:K:129:ASN:CB   | 2.97                     | 0.43              |
| 1:L:112:GLU:HA   | 1:L:115:GLN:HG2  | 2.01                     | 0.43              |
| 1:B:34:MET:HE1   | 1:B:42:LEU:HB3   | 2.00                     | 0.43              |
| 1:D:120:THR:HG21 | 1:D:129:ASN:CA   | 2.47                     | 0.43              |
| 1:D:120:THR:OG1  | 1:D:125:ASP:HB3  | 2.19                     | 0.43              |
| 1:F:7:VAL:CG1    | 1:F:8:ASP:N      | 2.72                     | 0.43              |
| 1:H:90:THR:OG1   | 1:H:91:LYS:N     | 2.52                     | 0.43              |
| 1:K:147:LYS:HD2  | 1:K:154:PRO:O    | 2.19                     | 0.43              |
| 1:B:20:LEU:HD12  | 1:B:20:LEU:HA    | 1.91                     | 0.43              |
| 1:C:118:GLU:O    | 1:C:122:LYS:HG3  | 2.19                     | 0.43              |
| 1:A:42:LEU:HD12  | 1:A:42:LEU:HA    | 1.86                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:112:GLU:HA   | 1:I:115:GLN:HG2  | 2.01                     | 0.42              |
| 1:J:57:MET:HE1   | 1:L:28:HIS:CD2   | 2.54                     | 0.42              |
| 1:K:94:THR:O     | 1:K:97:GLN:N     | 2.52                     | 0.42              |
| 1:D:91:LYS:HA    | 1:D:92:PRO:HD3   | 1.80                     | 0.42              |
| 1:K:65:LEU:HD13  | 1:K:71:PRO:CD    | 2.50                     | 0.42              |
| 1:F:32:TRP:C     | 3:F:178:HOH:O    | 2.62                     | 0.42              |
| 1:J:114:LYS:HD2  | 1:J:114:LYS:C    | 2.44                     | 0.42              |
| 1:K:75:LEU:H     | 1:K:75:LEU:CD1   | 2.33                     | 0.42              |
| 1:G:9:THR:HG22   | 1:G:13:LEU:HD22  | 2.01                     | 0.42              |
| 1:G:94:THR:HB    | 1:G:97:GLN:OE1   | 2.19                     | 0.42              |
| 1:K:7:VAL:CG1    | 1:K:11:GLU:HB2   | 2.50                     | 0.42              |
| 1:A:15:HIS:HE1   | 1:A:83:SER:OG    | 2.03                     | 0.42              |
| 1:A:75:LEU:H     | 1:A:75:LEU:CD1   | 2.32                     | 0.42              |
| 1:A:155:LEU:HB2  | 3:A:178:HOH:O    | 2.19                     | 0.42              |
| 1:D:114:LYS:HD2  | 1:D:114:LYS:C    | 2.44                     | 0.42              |
| 1:E:33:TYR:OH    | 1:G:71:PRO:O     | 2.35                     | 0.42              |
| 1:F:28:HIS:CD2   | 1:F:50:TYR:CE1   | 3.08                     | 0.42              |
| 1:I:33:TYR:OH    | 1:K:71:PRO:O     | 2.36                     | 0.42              |
| 1:I:74:THR:HB    | 1:K:86:GLU:CD    | 2.45                     | 0.42              |
| 1:J:42:LEU:O     | 1:J:46:MET:HG2   | 2.20                     | 0.42              |
| 1:K:20:LEU:HD12  | 1:K:20:LEU:HA    | 1.94                     | 0.42              |
| 1:K:114:LYS:O    | 1:K:114:LYS:HD2  | 2.19                     | 0.42              |
| 1:E:79:LEU:HD23  | 1:E:79:LEU:HA    | 1.59                     | 0.42              |
| 1:F:34:MET:HB2   | 1:F:95:MET:HE1   | 2.01                     | 0.42              |
| 1:J:34:MET:HG3   | 1:J:39:PHE:CD1   | 2.55                     | 0.42              |
| 1:D:120:THR:HG23 | 1:D:129:ASN:HB2  | 2.02                     | 0.42              |
| 1:F:14:ASN:OD1   | 1:F:71:PRO:HA    | 2.19                     | 0.42              |
| 1:J:65:LEU:HD13  | 1:J:71:PRO:CD    | 2.49                     | 0.42              |
| 1:D:37:HIS:CE1   | 1:G:96:ASP:OD1   | 2.72                     | 0.41              |
| 1:D:131:MET:HE3  | 1:D:131:MET:HB3  | 1.96                     | 0.41              |
| 1:I:75:LEU:N     | 1:I:75:LEU:CD1   | 2.83                     | 0.41              |
| 1:B:108:LEU:O    | 1:B:112:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:76:LYS:O     | 1:E:80:GLU:HG3   | 2.20                     | 0.41              |
| 1:K:28:HIS:CD2   | 1:K:50:TYR:CE2   | 3.08                     | 0.41              |
| 1:K:65:LEU:HD13  | 1:K:71:PRO:HD3   | 2.02                     | 0.41              |
| 1:B:129:ASN:O    | 1:B:133:ILE:HG13 | 2.20                     | 0.41              |
| 1:C:120:THR:HG23 | 1:C:129:ASN:HB2  | 2.02                     | 0.41              |
| 1:D:75:LEU:HD12  | 1:D:75:LEU:H     | 1.85                     | 0.41              |
| 1:E:23:PHE:CD1   | 1:E:105:THR:HG21 | 2.56                     | 0.41              |
| 1:E:114:LYS:HD2  | 1:E:114:LYS:O    | 2.21                     | 0.41              |
| 1:J:65:LEU:HD13  | 1:J:71:PRO:HD3   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:154:PRO:C    | 1:K:156:GLU:H    | 2.28                     | 0.41              |
| 1:B:65:LEU:HD13  | 1:B:71:PRO:CD    | 2.48                     | 0.41              |
| 1:C:42:LEU:HD12  | 1:C:42:LEU:HA    | 1.96                     | 0.41              |
| 1:H:8:ASP:O      | 1:H:9:THR:C      | 2.61                     | 0.41              |
| 1:J:94:THR:HG22  | 1:J:95:MET:H     | 1.85                     | 0.41              |
| 1:K:7:VAL:HG12   | 1:K:11:GLU:HB2   | 2.01                     | 0.41              |
| 1:L:65:LEU:HD13  | 1:L:71:PRO:CD    | 2.50                     | 0.41              |
| 1:L:116:GLY:O    | 1:L:117:ILE:C    | 2.61                     | 0.41              |
| 1:A:42:LEU:O     | 1:A:46:MET:HG2   | 2.21                     | 0.41              |
| 1:D:128:THR:HG22 | 1:D:132:LEU:HD22 | 2.02                     | 0.41              |
| 1:K:128:THR:HG22 | 1:K:132:LEU:HD22 | 2.02                     | 0.41              |
| 1:K:130:ASP:O    | 1:K:131:MET:C    | 2.63                     | 0.41              |
| 1:E:129:ASN:O    | 1:E:133:ILE:HG13 | 2.20                     | 0.41              |
| 1:G:65:LEU:HD13  | 1:G:71:PRO:HD3   | 2.02                     | 0.41              |
| 1:J:89:TYR:OH    | 1:J:92:PRO:HA    | 2.20                     | 0.41              |
| 1:K:147:LYS:O    | 1:K:148:ALA:C    | 2.61                     | 0.41              |
| 1:A:119:LEU:O    | 1:A:123:GLU:HG3  | 2.20                     | 0.41              |
| 1:E:75:LEU:N     | 1:E:75:LEU:CD1   | 2.84                     | 0.41              |
| 1:E:75:LEU:H     | 1:E:75:LEU:CD1   | 2.32                     | 0.41              |
| 1:I:154:PRO:C    | 1:I:156:GLU:H    | 2.27                     | 0.41              |
| 1:K:94:THR:O     | 1:K:97:GLN:HB2   | 2.20                     | 0.41              |
| 1:A:76:LYS:O     | 1:A:80:GLU:HG3   | 2.21                     | 0.41              |
| 1:A:154:PRO:HD3  | 3:A:185:HOH:O    | 2.20                     | 0.41              |
| 1:H:89:TYR:CZ    | 1:H:92:PRO:HA    | 2.55                     | 0.41              |
| 1:J:93:LYS:HB3   | 1:J:93:LYS:HE2   | 1.68                     | 0.41              |
| 1:K:117:ILE:CD1  | 3:K:164:HOH:O    | 2.64                     | 0.41              |
| 1:B:126:ASP:OD2  | 1:G:114:LYS:NZ   | 2.46                     | 0.41              |
| 1:D:35:ARG:NE    | 3:D:166:HOH:O    | 2.38                     | 0.41              |
| 1:E:107:GLU:OE2  | 3:E:182:HOH:O    | 2.21                     | 0.41              |
| 1:F:7:VAL:CG1    | 1:F:11:GLU:CB    | 2.99                     | 0.41              |
| 1:H:152:LYS:HA   | 1:H:152:LYS:HD3  | 1.91                     | 0.41              |
| 1:I:21:ASN:O     | 1:I:24:THR:HG22  | 2.21                     | 0.41              |
| 1:I:120:THR:HG22 | 1:I:129:ASN:ND2  | 2.32                     | 0.41              |
| 1:J:94:THR:CG2   | 3:J:189:HOH:O    | 2.69                     | 0.41              |
| 1:K:42:LEU:HD12  | 1:K:42:LEU:HA    | 1.81                     | 0.41              |
| 1:F:79:LEU:HD23  | 1:F:79:LEU:HA    | 1.47                     | 0.41              |
| 1:H:21:ASN:O     | 1:H:24:THR:HG22  | 2.20                     | 0.41              |
| 1:A:131:MET:HE3  | 1:A:132:LEU:HD13 | 2.02                     | 0.40              |
| 1:F:147:LYS:HD2  | 1:F:154:PRO:O    | 2.22                     | 0.40              |
| 1:J:113:TYR:O    | 1:J:117:ILE:N    | 2.48                     | 0.40              |
| 1:F:34:MET:HE1   | 1:F:42:LEU:HB3   | 2.04                     | 0.40              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:I:118:GLU:O   | 1:I:121:ASP:HB3 | 2.21                     | 0.40              |
| 1:J:28:HIS:CD2  | 1:L:57:MET:HE1  | 2.57                     | 0.40              |
| 1:K:94:THR:HG23 | 1:K:96:ASP:H    | 1.84                     | 0.40              |
| 1:C:89:TYR:CZ   | 1:C:92:PRO:HA   | 2.57                     | 0.40              |
| 1:C:114:LYS:HD2 | 1:C:114:LYS:C   | 2.46                     | 0.40              |
| 1:D:7:VAL:CG1   | 1:D:8:ASP:H     | 2.30                     | 0.40              |
| 1:E:14:ASN:OD1  | 1:E:71:PRO:HA   | 2.21                     | 0.40              |
| 1:F:86:GLU:CD   | 1:H:74:THR:HB   | 2.46                     | 0.40              |
| 1:K:114:LYS:CA  | 3:K:164:HOH:O   | 2.42                     | 0.40              |
| 1:H:99:MET:HE2  | 1:H:99:MET:CA   | 2.52                     | 0.40              |
| 1:I:86:GLU:CD   | 1:K:74:THR:HB   | 2.47                     | 0.40              |
| 1:E:94:THR:CG2  | 1:E:96:ASP:HB2  | 2.51                     | 0.40              |
| 1:F:126:ASP:O   | 1:F:129:ASN:HB3 | 2.22                     | 0.40              |
| 1:I:8:ASP:OD1   | 1:I:11:GLU:HB2  | 2.21                     | 0.40              |
| 1:I:28:HIS:CD2  | 1:K:57:MET:HE1  | 2.56                     | 0.40              |
| 1:J:15:HIS:HE1  | 1:J:83:SER:OG   | 2.05                     | 0.40              |
| 1:K:92:PRO:O    | 1:K:92:PRO:HG2  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 148/156 (95%) | 145 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | B     | 148/156 (95%) | 146 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | C     | 148/156 (95%) | 146 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | D     | 148/156 (95%) | 142 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | E     | 148/156 (95%) | 145 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | F     | 148/156 (95%) | 143 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | G     | 148/156 (95%) | 146 (99%) | 2 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | H     | 148/156 (95%)   | 146 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | I     | 148/156 (95%)   | 145 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | J     | 148/156 (95%)   | 145 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | K     | 148/156 (95%)   | 144 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 1   | L     | 148/156 (95%)   | 143 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| All | All   | 1776/1872 (95%) | 1736 (98%) | 40 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 133/139 (96%)   | 119 (90%)  | 14 (10%)  | 6           | 6  |
| 1   | B     | 133/139 (96%)   | 122 (92%)  | 11 (8%)   | 10          | 11 |
| 1   | C     | 133/139 (96%)   | 120 (90%)  | 13 (10%)  | 7           | 7  |
| 1   | D     | 133/139 (96%)   | 119 (90%)  | 14 (10%)  | 6           | 6  |
| 1   | E     | 133/139 (96%)   | 120 (90%)  | 13 (10%)  | 7           | 7  |
| 1   | F     | 133/139 (96%)   | 119 (90%)  | 14 (10%)  | 6           | 6  |
| 1   | G     | 133/139 (96%)   | 118 (89%)  | 15 (11%)  | 5           | 5  |
| 1   | H     | 133/139 (96%)   | 118 (89%)  | 15 (11%)  | 5           | 5  |
| 1   | I     | 133/139 (96%)   | 118 (89%)  | 15 (11%)  | 5           | 5  |
| 1   | J     | 133/139 (96%)   | 121 (91%)  | 12 (9%)   | 9           | 9  |
| 1   | K     | 133/139 (96%)   | 118 (89%)  | 15 (11%)  | 5           | 5  |
| 1   | L     | 133/139 (96%)   | 119 (90%)  | 14 (10%)  | 6           | 6  |
| All | All   | 1596/1668 (96%) | 1431 (90%) | 165 (10%) | 7           | 6  |

All (165) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 7   | VAL  |
| 1   | A     | 11  | GLU  |
| 1   | A     | 13  | LEU  |
| 1   | A     | 20  | LEU  |
| 1   | A     | 24  | THR  |
| 1   | A     | 28  | HIS  |
| 1   | A     | 41  | THR  |
| 1   | A     | 42  | LEU  |
| 1   | A     | 93  | LYS  |
| 1   | A     | 94  | THR  |
| 1   | A     | 102 | LEU  |
| 1   | A     | 119 | LEU  |
| 1   | A     | 131 | MET  |
| 1   | A     | 132 | LEU  |
| 1   | B     | 8   | ASP  |
| 1   | B     | 11  | GLU  |
| 1   | B     | 13  | LEU  |
| 1   | B     | 20  | LEU  |
| 1   | B     | 24  | THR  |
| 1   | B     | 41  | THR  |
| 1   | B     | 42  | LEU  |
| 1   | B     | 49  | LEU  |
| 1   | B     | 102 | LEU  |
| 1   | B     | 132 | LEU  |
| 1   | B     | 156 | GLU  |
| 1   | C     | 7   | VAL  |
| 1   | C     | 11  | GLU  |
| 1   | C     | 13  | LEU  |
| 1   | C     | 20  | LEU  |
| 1   | C     | 24  | THR  |
| 1   | C     | 41  | THR  |
| 1   | C     | 42  | LEU  |
| 1   | C     | 49  | LEU  |
| 1   | C     | 91  | LYS  |
| 1   | C     | 102 | LEU  |
| 1   | C     | 118 | GLU  |
| 1   | C     | 132 | LEU  |
| 1   | C     | 156 | GLU  |
| 1   | D     | 7   | VAL  |
| 1   | D     | 11  | GLU  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 20  | LEU  |
| 1   | D     | 24  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 28  | HIS  |
| 1   | D     | 42  | LEU  |
| 1   | D     | 49  | LEU  |
| 1   | D     | 91  | LYS  |
| 1   | D     | 92  | PRO  |
| 1   | D     | 94  | THR  |
| 1   | D     | 102 | LEU  |
| 1   | D     | 131 | MET  |
| 1   | D     | 132 | LEU  |
| 1   | E     | 8   | ASP  |
| 1   | E     | 11  | GLU  |
| 1   | E     | 13  | LEU  |
| 1   | E     | 20  | LEU  |
| 1   | E     | 24  | THR  |
| 1   | E     | 28  | HIS  |
| 1   | E     | 41  | THR  |
| 1   | E     | 42  | LEU  |
| 1   | E     | 49  | LEU  |
| 1   | E     | 94  | THR  |
| 1   | E     | 102 | LEU  |
| 1   | E     | 132 | LEU  |
| 1   | E     | 156 | GLU  |
| 1   | F     | 11  | GLU  |
| 1   | F     | 13  | LEU  |
| 1   | F     | 20  | LEU  |
| 1   | F     | 24  | THR  |
| 1   | F     | 28  | HIS  |
| 1   | F     | 41  | THR  |
| 1   | F     | 42  | LEU  |
| 1   | F     | 49  | LEU  |
| 1   | F     | 65  | LEU  |
| 1   | F     | 94  | THR  |
| 1   | F     | 102 | LEU  |
| 1   | F     | 119 | LEU  |
| 1   | F     | 123 | GLU  |
| 1   | F     | 132 | LEU  |
| 1   | G     | 7   | VAL  |
| 1   | G     | 11  | GLU  |
| 1   | G     | 13  | LEU  |
| 1   | G     | 20  | LEU  |
| 1   | G     | 24  | THR  |
| 1   | G     | 28  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 41  | THR  |
| 1   | G     | 42  | LEU  |
| 1   | G     | 49  | LEU  |
| 1   | G     | 94  | THR  |
| 1   | G     | 102 | LEU  |
| 1   | G     | 119 | LEU  |
| 1   | G     | 120 | THR  |
| 1   | G     | 121 | ASP  |
| 1   | G     | 132 | LEU  |
| 1   | H     | 7   | VAL  |
| 1   | H     | 8   | ASP  |
| 1   | H     | 11  | GLU  |
| 1   | H     | 13  | LEU  |
| 1   | H     | 20  | LEU  |
| 1   | H     | 24  | THR  |
| 1   | H     | 41  | THR  |
| 1   | H     | 42  | LEU  |
| 1   | H     | 49  | LEU  |
| 1   | H     | 65  | LEU  |
| 1   | H     | 94  | THR  |
| 1   | H     | 102 | LEU  |
| 1   | H     | 119 | LEU  |
| 1   | H     | 132 | LEU  |
| 1   | H     | 156 | GLU  |
| 1   | I     | 7   | VAL  |
| 1   | I     | 8   | ASP  |
| 1   | I     | 11  | GLU  |
| 1   | I     | 13  | LEU  |
| 1   | I     | 20  | LEU  |
| 1   | I     | 24  | THR  |
| 1   | I     | 28  | HIS  |
| 1   | I     | 41  | THR  |
| 1   | I     | 42  | LEU  |
| 1   | I     | 49  | LEU  |
| 1   | I     | 65  | LEU  |
| 1   | I     | 102 | LEU  |
| 1   | I     | 120 | THR  |
| 1   | I     | 132 | LEU  |
| 1   | I     | 156 | GLU  |
| 1   | J     | 7   | VAL  |
| 1   | J     | 11  | GLU  |
| 1   | J     | 13  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 20  | LEU  |
| 1   | J     | 24  | THR  |
| 1   | J     | 28  | HIS  |
| 1   | J     | 42  | LEU  |
| 1   | J     | 65  | LEU  |
| 1   | J     | 91  | LYS  |
| 1   | J     | 102 | LEU  |
| 1   | J     | 132 | LEU  |
| 1   | J     | 156 | GLU  |
| 1   | K     | 7   | VAL  |
| 1   | K     | 11  | GLU  |
| 1   | K     | 13  | LEU  |
| 1   | K     | 20  | LEU  |
| 1   | K     | 24  | THR  |
| 1   | K     | 28  | HIS  |
| 1   | K     | 41  | THR  |
| 1   | K     | 42  | LEU  |
| 1   | K     | 49  | LEU  |
| 1   | K     | 65  | LEU  |
| 1   | K     | 94  | THR  |
| 1   | K     | 102 | LEU  |
| 1   | K     | 120 | THR  |
| 1   | K     | 132 | LEU  |
| 1   | K     | 156 | GLU  |
| 1   | L     | 7   | VAL  |
| 1   | L     | 11  | GLU  |
| 1   | L     | 13  | LEU  |
| 1   | L     | 20  | LEU  |
| 1   | L     | 24  | THR  |
| 1   | L     | 28  | HIS  |
| 1   | L     | 41  | THR  |
| 1   | L     | 42  | LEU  |
| 1   | L     | 49  | LEU  |
| 1   | L     | 65  | LEU  |
| 1   | L     | 102 | LEU  |
| 1   | L     | 120 | THR  |
| 1   | L     | 132 | LEU  |
| 1   | L     | 156 | GLU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 15  | HIS  |
| 1   | A     | 28  | HIS  |
| 1   | A     | 29  | GLN  |
| 1   | A     | 37  | HIS  |
| 1   | B     | 15  | HIS  |
| 1   | B     | 29  | GLN  |
| 1   | B     | 37  | HIS  |
| 1   | B     | 43  | HIS  |
| 1   | B     | 129 | ASN  |
| 1   | C     | 15  | HIS  |
| 1   | C     | 28  | HIS  |
| 1   | C     | 29  | GLN  |
| 1   | C     | 37  | HIS  |
| 1   | C     | 43  | HIS  |
| 1   | C     | 129 | ASN  |
| 1   | D     | 15  | HIS  |
| 1   | D     | 37  | HIS  |
| 1   | E     | 15  | HIS  |
| 1   | E     | 28  | HIS  |
| 1   | E     | 81  | ASN  |
| 1   | E     | 129 | ASN  |
| 1   | F     | 15  | HIS  |
| 1   | F     | 29  | GLN  |
| 1   | F     | 37  | HIS  |
| 1   | F     | 81  | ASN  |
| 1   | F     | 97  | GLN  |
| 1   | G     | 15  | HIS  |
| 1   | G     | 28  | HIS  |
| 1   | G     | 29  | GLN  |
| 1   | G     | 43  | HIS  |
| 1   | G     | 81  | ASN  |
| 1   | H     | 15  | HIS  |
| 1   | H     | 29  | GLN  |
| 1   | H     | 37  | HIS  |
| 1   | H     | 81  | ASN  |
| 1   | H     | 129 | ASN  |
| 1   | I     | 15  | HIS  |
| 1   | I     | 28  | HIS  |
| 1   | I     | 29  | GLN  |
| 1   | I     | 31  | HIS  |
| 1   | I     | 37  | HIS  |
| 1   | I     | 81  | ASN  |
| 1   | I     | 129 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 15  | HIS  |
| 1   | J     | 28  | HIS  |
| 1   | J     | 29  | GLN  |
| 1   | J     | 37  | HIS  |
| 1   | J     | 43  | HIS  |
| 1   | J     | 81  | ASN  |
| 1   | J     | 129 | ASN  |
| 1   | K     | 15  | HIS  |
| 1   | K     | 28  | HIS  |
| 1   | K     | 43  | HIS  |
| 1   | K     | 81  | ASN  |
| 1   | L     | 15  | HIS  |
| 1   | L     | 28  | HIS  |
| 1   | L     | 43  | HIS  |
| 1   | L     | 129 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.