



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:51 am GMT

PDB ID : 2ED6  
Title : Crystal Structure of Envelope Protein VP28 from White Spot Syndrome Virus (WSSV)  
Authors : Hew, C.L.; Sivaraman, J.; Tang, X.H.  
Deposited on : 2007-02-14  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

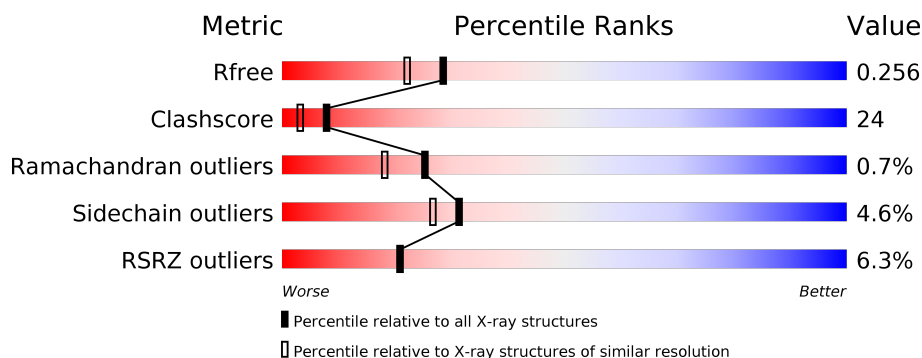
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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






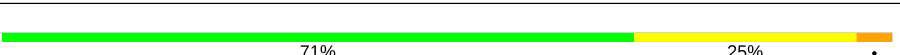
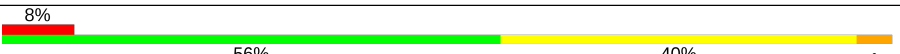
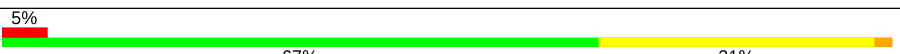
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 6609 (2.00-2.00)                                      |
| Clashscore            | 112137                      | 7775 (2.00-2.00)                                      |
| Ramachandran outliers | 110173                      | 7679 (2.00-2.00)                                      |
| Sidechain outliers    | 110143                      | 7678 (2.00-2.00)                                      |
| RSRZ outliers         | 101464                      | 6696 (2.00-2.00)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 170    | <div> <div>5%</div> <div> <div>68%</div> <div>28%</div> <div>•</div> </div> </div>  |
| 1   | B     | 170    | <div> <div>6%</div> <div> <div>68%</div> <div>28%</div> <div>•</div> </div> </div>  |
| 1   | C     | 170    | <div> <div>4%</div> <div> <div>67%</div> <div>29%</div> <div>•</div> </div> </div>  |
| 1   | D     | 170    | <div> <div>6%</div> <div> <div>66%</div> <div>29%</div> <div>5%</div> </div> </div> |
| 1   | E     | 170    | <div> <div>7%</div> <div> <div>65%</div> <div>31%</div> <div>•</div> </div> </div>  |
| 1   | F     | 170    | <div> <div>10%</div> <div> <div>65%</div> <div>31%</div> <div>•</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | G     | 170    |  |
| 1   | H     | 170    |  |
| 1   | I     | 170    |  |
| 1   | J     | 170    |  |
| 1   | K     | 170    |  |
| 1   | L     | 170    |  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16843 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 25kDa structural protein VP25.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | B     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | C     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | D     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | E     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | F     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | G     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | H     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | I     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | J     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | K     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |
| 1   | L     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1288  | 803 | 211 | 267 | 7 |         |         |       |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 2   | A     | 107      | Total | O   | 0       | 0       |
|     |       |          | 107   | 107 |         |         |
| 2   | B     | 133      | Total | O   | 0       | 0       |
|     |       |          | 133   | 133 |         |         |

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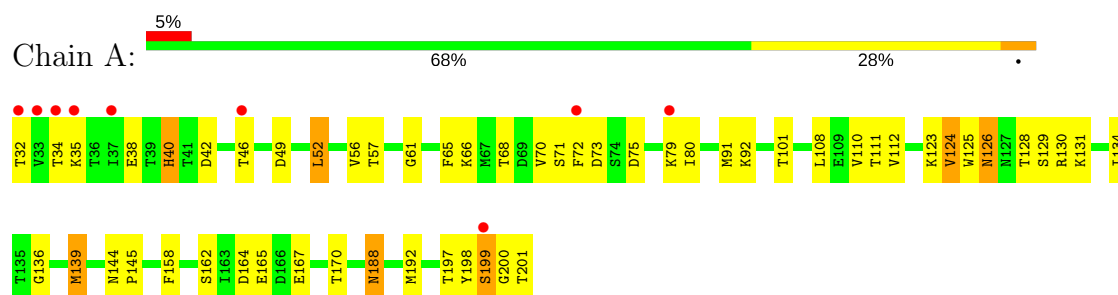
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 2   | C     | 124      | Total<br>124 | O<br>124 | 0       | 0       |
| 2   | D     | 112      | Total<br>112 | O<br>112 | 0       | 0       |
| 2   | E     | 138      | Total<br>138 | O<br>138 | 0       | 0       |
| 2   | F     | 154      | Total<br>154 | O<br>154 | 0       | 0       |
| 2   | G     | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 2   | H     | 122      | Total<br>122 | O<br>122 | 0       | 0       |
| 2   | I     | 125      | Total<br>125 | O<br>125 | 0       | 0       |
| 2   | J     | 102      | Total<br>102 | O<br>102 | 0       | 0       |
| 2   | K     | 53       | Total<br>53  | O<br>53  | 0       | 0       |
| 2   | L     | 81       | Total<br>81  | O<br>81  | 0       | 0       |

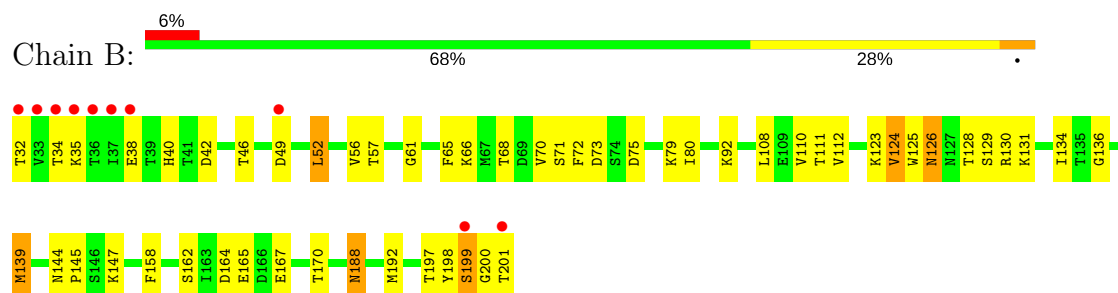
### 3 Residue-property plots [i](#)

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

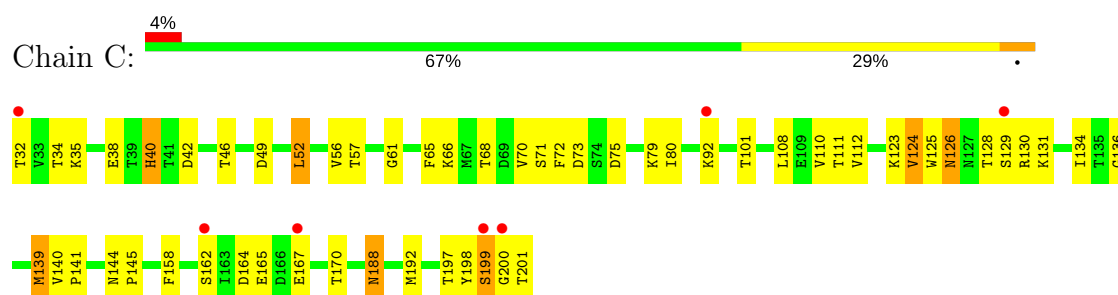
#### • Molecule 1: 25kDa structural protein VP25



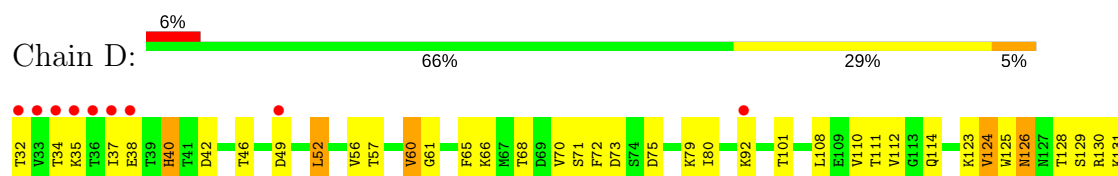
#### • Molecule 1: 25kDa structural protein VP25



#### • Molecule 1: 25kDa structural protein VP25

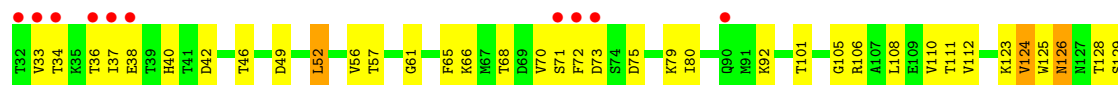


#### • Molecule 1: 25kDa structural protein VP25

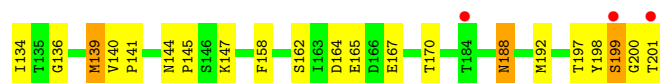




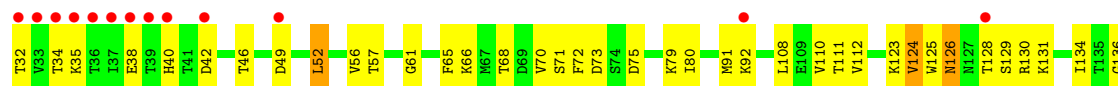
- Molecule 1: 25kDa structural protein VP25



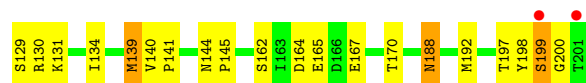
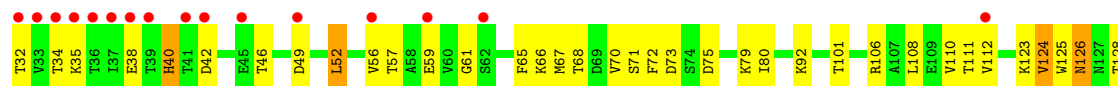
- Molecule 1: 25kDa structural protein VP25



- Molecule 1: 25kDa structural protein VP25

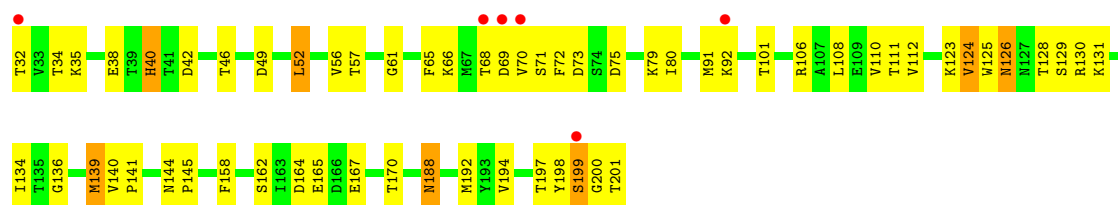


- Molecule 1: 25kDa structural protein VP25



- Molecule 1: 25kDa structural protein VP25





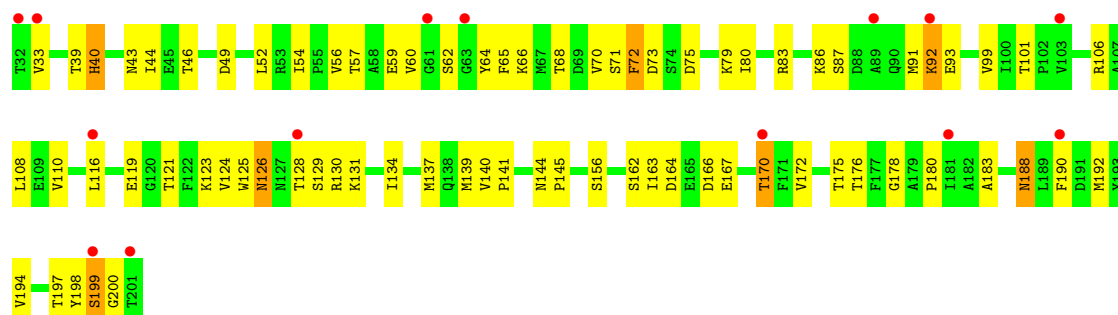
• Molecule 1: 25kDa structural protein VP25

Chain J: 71% 25%



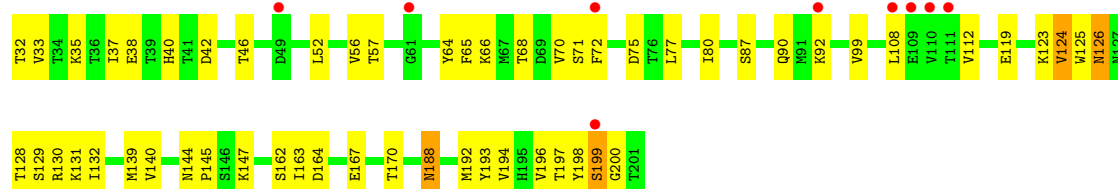
• Molecule 1: 25kDa structural protein VP25

Chain K: 8% 56% 40%



• Molecule 1: 25kDa structural protein VP25

Chain L: 5% 67% 31%





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 105.33Å 106.71Å 200.37Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 45.00 – 2.00<br>49.87 – 2.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | (Not available) (45.00-2.00)<br>99.6 (49.87-2.00)           | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 8.63 (at 2.00Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.248 , 0.281<br>0.252 , 0.256                              | Depositor<br>DCC |
| $R_{free}$ test set   | 7648 reflections (5.02%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 15.3  | Xtriage          |
| Anisotropy  | 0.271   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 57.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction   | 0.020 for k,h,-l  | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 16843   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 21.0  | wwPDB-VP         |

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

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |                | Bond angles |             |
|-----|-------|--------------|----------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$    | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.33         | 0/1309         | 0.61        | 0/1775      |
| 1   | B     | 0.35         | 0/1309         | 0.61        | 0/1775      |
| 1   | C     | 0.34         | 0/1309         | 0.61        | 0/1775      |
| 1   | D     | 0.41         | 1/1309 (0.1%)  | 0.62        | 0/1775      |
| 1   | E     | 0.35         | 0/1309         | 0.61        | 0/1775      |
| 1   | F     | 0.37         | 0/1309         | 0.62        | 0/1775      |
| 1   | G     | 0.37         | 0/1309         | 0.62        | 0/1775      |
| 1   | H     | 0.37         | 0/1309         | 0.61        | 0/1775      |
| 1   | I     | 0.34         | 0/1309         | 0.61        | 0/1775      |
| 1   | J     | 0.37         | 0/1309         | 0.64        | 0/1775      |
| 1   | K     | 0.32         | 0/1309         | 0.57        | 0/1775      |
| 1   | L     | 0.33         | 0/1309         | 0.58        | 0/1775      |
| All | All   | 0.36         | 1/15708 (0.0%) | 0.61        | 0/21300     |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 60  | VAL  | CB-CG1 | -7.91 | 1.36        | 1.52     |

There are no bond angle outliers.

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     | 1288  | 0        | 1256     | 59      | 0            |
| 1   | B     | 1288  | 0        | 1256     | 63      | 0            |
| 1   | C     | 1288  | 0        | 1256     | 62      | 0            |
| 1   | D     | 1288  | 0        | 1256     | 64      | 1            |
| 1   | E     | 1288  | 0        | 1256     | 71      | 0            |
| 1   | F     | 1288  | 0        | 1256     | 62      | 0            |
| 1   | G     | 1288  | 0        | 1256     | 62      | 0            |
| 1   | H     | 1288  | 0        | 1256     | 63      | 1            |
| 1   | I     | 1288  | 0        | 1256     | 73      | 0            |
| 1   | J     | 1288  | 0        | 1256     | 65      | 0            |
| 1   | K     | 1288  | 0        | 1256     | 71      | 0            |
| 1   | L     | 1288  | 0        | 1256     | 54      | 0            |
| 2   | A     | 107   | 0        | 0        | 5       | 0            |
| 2   | B     | 133   | 0        | 0        | 5       | 0            |
| 2   | C     | 124   | 0        | 0        | 8       | 0            |
| 2   | D     | 112   | 0        | 0        | 8       | 0            |
| 2   | E     | 138   | 0        | 0        | 5       | 0            |
| 2   | F     | 154   | 0        | 0        | 5       | 0            |
| 2   | G     | 136   | 0        | 0        | 3       | 0            |
| 2   | H     | 122   | 0        | 0        | 7       | 0            |
| 2   | I     | 125   | 0        | 0        | 6       | 0            |
| 2   | J     | 102   | 0        | 0        | 5       | 0            |
| 2   | K     | 53    | 0        | 0        | 2       | 0            |
| 2   | L     | 81    | 0        | 0        | 2       | 0            |
| All | All   | 16843 | 0        | 15072    | 732     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (732) 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:F:56:VAL:HG11 | 1:F:65:PHE:HB3   | 1.28                     | 1.14              |
| 1:B:56:VAL:HG11 | 1:B:65:PHE:HB3   | 1.29                     | 1.13              |
| 1:D:56:VAL:HG11 | 1:D:65:PHE:HB3   | 1.30                     | 1.13              |
| 1:A:56:VAL:HG11 | 1:A:65:PHE:HB3   | 1.29                     | 1.12              |
| 1:G:56:VAL:HG11 | 1:G:65:PHE:HB3   | 1.27                     | 1.10              |
| 1:E:56:VAL:HG11 | 1:E:65:PHE:HB3   | 1.29                     | 1.09              |
| 1:C:56:VAL:HG11 | 1:C:65:PHE:HB3   | 1.30                     | 1.09              |
| 1:H:56:VAL:HG11 | 1:H:65:PHE:HB3   | 1.29                     | 1.08              |
| 1:I:56:VAL:HG11 | 1:I:65:PHE:HB3   | 1.31                     | 1.07              |
| 1:H:46:THR:HG22 | 1:H:130:ARG:HH22 | 1.19                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:46:THR:HG22  | 1:G:130:ARG:HH22 | 1.23                     | 1.04              |
| 1:D:197:THR:HG22 | 1:D:199:SER:H    | 1.22                     | 1.04              |
| 1:L:46:THR:HG22  | 1:L:130:ARG:HH22 | 1.23                     | 1.03              |
| 1:A:197:THR:HG22 | 1:A:199:SER:H    | 1.23                     | 1.03              |
| 1:L:56:VAL:HG11  | 1:L:65:PHE:HB3   | 1.38                     | 1.03              |
| 1:I:46:THR:HG22  | 1:I:130:ARG:HH22 | 1.21                     | 1.03              |
| 1:F:197:THR:HG22 | 1:F:199:SER:H    | 1.22                     | 1.03              |
| 1:C:46:THR:HG22  | 1:C:130:ARG:HH22 | 1.23                     | 1.03              |
| 1:B:46:THR:HG22  | 1:B:130:ARG:HH22 | 1.22                     | 1.02              |
| 1:B:197:THR:HG22 | 1:B:199:SER:H    | 1.22                     | 1.02              |
| 1:E:46:THR:HG22  | 1:E:130:ARG:HH22 | 1.24                     | 1.02              |
| 1:K:197:THR:HG22 | 1:K:199:SER:H    | 1.17                     | 1.02              |
| 1:C:197:THR:HG22 | 1:C:199:SER:H    | 1.24                     | 1.01              |
| 1:A:46:THR:HG22  | 1:A:130:ARG:HH22 | 1.22                     | 1.01              |
| 1:D:46:THR:HG22  | 1:D:130:ARG:HH22 | 1.21                     | 1.01              |
| 1:H:197:THR:HG22 | 1:H:199:SER:H    | 1.23                     | 1.00              |
| 1:E:197:THR:HG22 | 1:E:199:SER:H    | 1.24                     | 1.00              |
| 1:F:46:THR:HG22  | 1:F:130:ARG:HH22 | 1.21                     | 0.99              |
| 1:I:197:THR:HG22 | 1:I:199:SER:H    | 1.23                     | 0.99              |
| 1:G:197:THR:HG22 | 1:G:199:SER:H    | 1.22                     | 0.99              |
| 1:K:139:MET:HE1  | 1:K:190:PHE:HB2  | 1.44                     | 0.98              |
| 1:J:197:THR:HG22 | 1:J:199:SER:H    | 1.28                     | 0.97              |
| 1:D:126:ASN:HD21 | 1:D:128:THR:HB   | 1.34                     | 0.91              |
| 1:A:126:ASN:HD21 | 1:A:128:THR:HB   | 1.36                     | 0.91              |
| 1:I:126:ASN:HD21 | 1:I:128:THR:HB   | 1.36                     | 0.91              |
| 1:E:126:ASN:HD21 | 1:E:128:THR:HB   | 1.36                     | 0.90              |
| 1:H:126:ASN:HD21 | 1:H:128:THR:HB   | 1.36                     | 0.90              |
| 1:C:126:ASN:HD21 | 1:C:128:THR:HB   | 1.36                     | 0.90              |
| 1:J:126:ASN:HD21 | 1:J:128:THR:HB   | 1.36                     | 0.89              |
| 1:J:46:THR:HG22  | 1:J:130:ARG:HH22 | 1.38                     | 0.89              |
| 1:B:126:ASN:HD21 | 1:B:128:THR:HB   | 1.37                     | 0.89              |
| 1:F:126:ASN:HD21 | 1:F:128:THR:HB   | 1.35                     | 0.89              |
| 1:J:56:VAL:HG11  | 1:J:65:PHE:HB3   | 1.54                     | 0.89              |
| 1:E:49:ASP:HB2   | 2:F:1516:HOH:O   | 1.73                     | 0.89              |
| 1:G:126:ASN:HD21 | 1:G:128:THR:HB   | 1.35                     | 0.88              |
| 1:K:39:THR:HG22  | 1:K:43:ASN:HD21  | 1.38                     | 0.88              |
| 1:K:56:VAL:HG11  | 1:K:65:PHE:HB3   | 1.55                     | 0.88              |
| 1:H:46:THR:HG22  | 1:H:130:ARG:NH2  | 1.90                     | 0.86              |
| 1:L:126:ASN:HD21 | 1:L:128:THR:HB   | 1.41                     | 0.86              |
| 1:F:46:THR:HG22  | 1:F:130:ARG:NH2  | 1.90                     | 0.86              |
| 1:I:46:THR:HG22  | 1:I:130:ARG:NH2  | 1.91                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:197:THR:HG22 | 1:L:199:SER:H    | 1.41                     | 0.85              |
| 1:B:46:THR:HG22  | 1:B:130:ARG:NH2  | 1.91                     | 0.85              |
| 1:G:46:THR:HG22  | 1:G:130:ARG:NH2  | 1.91                     | 0.85              |
| 1:K:46:THR:HG22  | 1:K:130:ARG:HH22 | 1.39                     | 0.85              |
| 1:A:46:THR:HG22  | 1:A:130:ARG:NH2  | 1.91                     | 0.84              |
| 1:C:46:THR:HG22  | 1:C:130:ARG:NH2  | 1.92                     | 0.84              |
| 1:D:46:THR:HG22  | 1:D:130:ARG:NH2  | 1.90                     | 0.84              |
| 1:E:46:THR:HG22  | 1:E:130:ARG:NH2  | 1.92                     | 0.83              |
| 1:L:46:THR:HG22  | 1:L:130:ARG:NH2  | 1.93                     | 0.82              |
| 1:B:49:ASP:HB2   | 2:C:1518:HOH:O   | 1.79                     | 0.82              |
| 1:J:188:ASN:H    | 1:J:188:ASN:HD22 | 1.27                     | 0.81              |
| 1:D:49:ASP:HB2   | 2:D:1519:HOH:O   | 1.81                     | 0.81              |
| 1:L:188:ASN:H    | 1:L:188:ASN:HD22 | 1.29                     | 0.81              |
| 1:J:46:THR:HG22  | 1:J:130:ARG:NH2  | 1.96                     | 0.80              |
| 1:K:141:PRO:HA   | 1:K:190:PHE:HD1  | 1.46                     | 0.80              |
| 1:G:49:ASP:HB2   | 2:I:1515:HOH:O   | 1.80                     | 0.79              |
| 1:F:131:LYS:HE2  | 1:F:162:SER:HB2  | 1.63                     | 0.79              |
| 1:D:131:LYS:HE2  | 1:D:162:SER:HB2  | 1.64                     | 0.79              |
| 1:K:124:VAL:HG11 | 1:K:134:ILE:HD11 | 1.65                     | 0.78              |
| 1:H:131:LYS:HE2  | 1:H:162:SER:HB2  | 1.63                     | 0.78              |
| 1:I:131:LYS:HE2  | 1:I:162:SER:HB2  | 1.64                     | 0.78              |
| 1:E:147:LYS:HE3  | 2:F:2214:HOH:O   | 1.82                     | 0.78              |
| 1:A:131:LYS:HE2  | 1:A:162:SER:HB2  | 1.65                     | 0.77              |
| 1:E:131:LYS:HE2  | 1:E:162:SER:HB2  | 1.65                     | 0.77              |
| 1:G:131:LYS:HE2  | 1:G:162:SER:HB2  | 1.66                     | 0.76              |
| 1:B:131:LYS:HE2  | 1:B:162:SER:HB2  | 1.66                     | 0.76              |
| 1:F:188:ASN:HD22 | 1:F:188:ASN:H    | 1.30                     | 0.76              |
| 1:F:139:MET:HE3  | 1:F:192:MET:HA   | 1.68                     | 0.75              |
| 1:I:188:ASN:H    | 1:I:188:ASN:HD22 | 1.34                     | 0.75              |
| 1:C:131:LYS:HE2  | 1:C:162:SER:HB2  | 1.67                     | 0.75              |
| 2:H:2339:HOH:O   | 1:I:49:ASP:HB2   | 1.87                     | 0.75              |
| 1:E:139:MET:HE3  | 1:E:192:MET:HA   | 1.69                     | 0.75              |
| 1:H:139:MET:HE3  | 1:H:192:MET:HA   | 1.67                     | 0.75              |
| 1:B:188:ASN:HD22 | 1:B:188:ASN:H    | 1.35                     | 0.74              |
| 1:A:188:ASN:HD22 | 1:A:188:ASN:H    | 1.35                     | 0.74              |
| 1:L:128:THR:HG21 | 1:L:198:TYR:OH   | 1.88                     | 0.74              |
| 1:J:68:THR:O     | 1:J:70:VAL:HG23  | 1.88                     | 0.74              |
| 1:H:188:ASN:H    | 1:H:188:ASN:HD22 | 1.32                     | 0.74              |
| 1:K:126:ASN:HD21 | 1:K:128:THR:HB   | 1.52                     | 0.73              |
| 1:C:139:MET:HE3  | 1:C:192:MET:HA   | 1.68                     | 0.73              |
| 1:A:139:MET:HE3  | 1:A:192:MET:HA   | 1.68                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:188:ASN:H    | 1:C:188:ASN:HD22 | 1.35                     | 0.73              |
| 1:G:56:VAL:CG1   | 1:G:65:PHE:HB3   | 2.15                     | 0.73              |
| 1:I:139:MET:HE3  | 1:I:192:MET:HA   | 1.68                     | 0.73              |
| 1:G:188:ASN:HD22 | 1:G:188:ASN:H    | 1.35                     | 0.73              |
| 1:L:68:THR:O     | 1:L:70:VAL:HG23  | 1.89                     | 0.73              |
| 2:G:1517:HOH:O   | 1:H:49:ASP:HB2   | 1.87                     | 0.73              |
| 1:J:144:ASN:HD21 | 1:J:148:ALA:HB3  | 1.54                     | 0.72              |
| 1:E:188:ASN:H    | 1:E:188:ASN:HD22 | 1.37                     | 0.72              |
| 1:D:188:ASN:H    | 1:D:188:ASN:HD22 | 1.36                     | 0.72              |
| 1:K:164:ASP:HB2  | 1:K:167:GLU:OE1  | 1.90                     | 0.72              |
| 1:B:139:MET:HE3  | 1:B:192:MET:HA   | 1.70                     | 0.71              |
| 1:B:139:MET:HA   | 1:B:139:MET:HE3  | 1.72                     | 0.71              |
| 1:D:139:MET:HE3  | 1:D:139:MET:HA   | 1.71                     | 0.71              |
| 1:D:139:MET:HE3  | 1:D:192:MET:HA   | 1.73                     | 0.71              |
| 1:J:52:LEU:HD11  | 1:J:72:PHE:CE1   | 2.25                     | 0.71              |
| 1:G:139:MET:HE3  | 1:G:192:MET:HA   | 1.71                     | 0.70              |
| 1:E:106:ARG:HB3  | 1:I:68:THR:CG2   | 2.21                     | 0.70              |
| 1:K:139:MET:CE   | 1:K:190:PHE:HB2  | 2.20                     | 0.70              |
| 1:L:139:MET:HE2  | 1:L:192:MET:HB2  | 1.74                     | 0.70              |
| 1:B:139:MET:CE   | 1:B:139:MET:HA   | 2.22                     | 0.70              |
| 1:H:199:SER:O    | 1:I:75:ASP:OD2   | 2.09                     | 0.70              |
| 1:F:56:VAL:CG1   | 1:F:65:PHE:HB3   | 2.16                     | 0.69              |
| 1:J:75:ASP:OD2   | 1:K:199:SER:O    | 2.10                     | 0.69              |
| 1:L:52:LEU:HD11  | 1:L:77:LEU:HD12  | 1.73                     | 0.69              |
| 1:G:199:SER:O    | 1:H:75:ASP:OD2   | 2.11                     | 0.69              |
| 1:D:139:MET:CE   | 1:D:139:MET:HA   | 2.22                     | 0.69              |
| 1:I:139:MET:CE   | 1:I:139:MET:HA   | 2.23                     | 0.69              |
| 1:J:139:MET:HE3  | 1:J:192:MET:HA   | 1.74                     | 0.69              |
| 1:F:139:MET:HA   | 1:F:139:MET:CE   | 2.23                     | 0.69              |
| 1:K:197:THR:HG22 | 1:K:199:SER:N    | 2.00                     | 0.68              |
| 1:J:52:LEU:HD11  | 1:J:72:PHE:HE1   | 1.59                     | 0.68              |
| 1:A:139:MET:CE   | 1:A:139:MET:HA   | 2.24                     | 0.68              |
| 1:C:139:MET:HA   | 1:C:139:MET:CE   | 2.23                     | 0.68              |
| 1:K:197:THR:CG2  | 1:K:199:SER:H    | 1.99                     | 0.68              |
| 1:J:199:SER:O    | 1:L:75:ASP:OD2   | 2.12                     | 0.68              |
| 1:G:128:THR:HG21 | 1:G:198:TYR:OH   | 1.94                     | 0.68              |
| 1:H:139:MET:HA   | 1:H:139:MET:CE   | 2.24                     | 0.68              |
| 1:L:131:LYS:HE2  | 1:L:162:SER:HB2  | 1.76                     | 0.67              |
| 1:B:92:LYS:HG3   | 1:B:125:TRP:CZ2  | 2.29                     | 0.67              |
| 1:G:92:LYS:HG3   | 1:G:125:TRP:CZ2  | 2.29                     | 0.67              |
| 1:J:131:LYS:HE2  | 1:J:162:SER:HB2  | 1.76                     | 0.67              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:L:92:LYS:HG3   | 1:L:125:TRP:CZ2 | 2.27                     | 0.67              |
| 1:A:56:VAL:CG1   | 1:A:65:PHE:HB3  | 2.17                     | 0.67              |
| 1:F:197:THR:HG21 | 2:F:1083:HOH:O  | 1.93                     | 0.67              |
| 1:G:197:THR:HG21 | 2:G:1088:HOH:O  | 1.94                     | 0.67              |
| 1:G:139:MET:HA   | 1:G:139:MET:CE  | 2.24                     | 0.67              |
| 1:K:188:ASN:HD22 | 1:K:188:ASN:H   | 1.41                     | 0.67              |
| 1:D:49:ASP:OD2   | 1:E:49:ASP:OD2  | 2.13                     | 0.67              |
| 1:E:106:ARG:HG2  | 1:I:69:ASP:O    | 1.94                     | 0.67              |
| 1:G:68:THR:O     | 1:G:70:VAL:HG23 | 1.95                     | 0.67              |
| 1:E:139:MET:CE   | 1:E:139:MET:HA  | 2.24                     | 0.67              |
| 1:I:139:MET:HE3  | 1:I:139:MET:HA  | 1.77                     | 0.67              |
| 1:I:92:LYS:HG3   | 1:I:125:TRP:CZ2 | 2.30                     | 0.67              |
| 1:E:56:VAL:CG1   | 1:E:65:PHE:HB3  | 2.17                     | 0.66              |
| 1:F:92:LYS:HG3   | 1:F:125:TRP:CZ2 | 2.30                     | 0.66              |
| 1:D:56:VAL:CG1   | 1:D:65:PHE:HB3  | 2.18                     | 0.66              |
| 1:H:92:LYS:HG3   | 1:H:125:TRP:CZ2 | 2.30                     | 0.66              |
| 1:K:39:THR:HG22  | 1:K:43:ASN:ND2  | 2.09                     | 0.66              |
| 1:G:139:MET:HA   | 1:G:139:MET:HE3 | 1.77                     | 0.66              |
| 1:K:46:THR:HG22  | 1:K:130:ARG:NH2 | 2.09                     | 0.66              |
| 1:C:92:LYS:HG3   | 1:C:125:TRP:CZ2 | 2.31                     | 0.66              |
| 1:A:199:SER:O    | 1:C:75:ASP:OD2  | 2.14                     | 0.65              |
| 1:A:75:ASP:OD2   | 1:B:199:SER:O   | 2.13                     | 0.65              |
| 1:L:42:ASP:O     | 1:L:46:THR:HG23 | 1.95                     | 0.65              |
| 1:L:87:SER:OG    | 1:L:90:GLN:HG3  | 1.96                     | 0.65              |
| 1:C:128:THR:HG21 | 1:C:198:TYR:OH  | 1.97                     | 0.65              |
| 1:D:49:ASP:OD2   | 1:F:49:ASP:OD2  | 2.15                     | 0.65              |
| 1:J:124:VAL:HG22 | 1:J:163:ILE:CD1 | 2.25                     | 0.65              |
| 1:A:92:LYS:HG3   | 1:A:125:TRP:CZ2 | 2.31                     | 0.65              |
| 1:C:68:THR:O     | 1:C:70:VAL:HG23 | 1.96                     | 0.64              |
| 1:D:92:LYS:HG3   | 1:D:125:TRP:CZ2 | 2.32                     | 0.64              |
| 1:E:92:LYS:HG3   | 1:E:125:TRP:CZ2 | 2.31                     | 0.64              |
| 1:D:75:ASP:OD2   | 1:E:199:SER:O   | 2.15                     | 0.64              |
| 1:L:52:LEU:HD11  | 1:L:77:LEU:CD1  | 2.27                     | 0.64              |
| 1:A:139:MET:HA   | 1:A:139:MET:HE3 | 1.80                     | 0.64              |
| 1:A:128:THR:HG21 | 1:A:198:TYR:OH  | 1.98                     | 0.64              |
| 1:I:128:THR:HG21 | 1:I:198:TYR:OH  | 1.98                     | 0.64              |
| 1:J:139:MET:CE   | 1:J:139:MET:HA  | 2.28                     | 0.64              |
| 1:F:128:THR:HG21 | 1:F:198:TYR:OH  | 1.97                     | 0.64              |
| 1:I:68:THR:O     | 1:I:70:VAL:HG23 | 1.98                     | 0.64              |
| 1:K:131:LYS:HE2  | 1:K:162:SER:HB2 | 1.80                     | 0.63              |
| 1:F:170:THR:HG23 | 2:F:1304:HOH:O  | 1.98                     | 0.63              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:F:126:ASN:ND2  | 1:F:128:THR:HB  | 2.12                     | 0.63              |
| 1:D:128:THR:HG21 | 1:D:198:TYR:OH  | 1.99                     | 0.63              |
| 1:J:126:ASN:ND2  | 1:J:128:THR:HB  | 2.10                     | 0.63              |
| 1:B:56:VAL:CG1   | 1:B:65:PHE:HB3  | 2.18                     | 0.63              |
| 1:C:197:THR:HG21 | 2:C:1084:HOH:O  | 1.98                     | 0.63              |
| 1:E:128:THR:HG21 | 1:E:198:TYR:OH  | 1.99                     | 0.63              |
| 1:B:128:THR:HG21 | 1:B:198:TYR:OH  | 1.99                     | 0.62              |
| 1:D:197:THR:HG21 | 2:D:1918:HOH:O  | 1.97                     | 0.62              |
| 1:K:75:ASP:OD2   | 1:L:199:SER:O   | 2.15                     | 0.62              |
| 1:G:170:THR:HG23 | 2:G:2286:HOH:O  | 1.99                     | 0.62              |
| 1:H:67:MET:HE3   | 2:H:2129:HOH:O  | 1.99                     | 0.62              |
| 1:K:72:PHE:CE1   | 1:K:80:ILE:HB   | 2.34                     | 0.62              |
| 1:H:56:VAL:CG1   | 1:H:65:PHE:HB3  | 2.17                     | 0.62              |
| 1:L:124:VAL:HG22 | 1:L:163:ILE:CD1 | 2.29                     | 0.62              |
| 1:B:68:THR:O     | 1:B:70:VAL:HG23 | 1.98                     | 0.62              |
| 1:C:32:THR:HG23  | 2:C:2063:HOH:O  | 1.99                     | 0.62              |
| 1:D:126:ASN:ND2  | 1:D:128:THR:HB  | 2.12                     | 0.62              |
| 1:E:139:MET:HE3  | 1:E:139:MET:HA  | 1.80                     | 0.62              |
| 1:A:40:HIS:HD2   | 2:A:1254:HOH:O  | 1.84                     | 0.61              |
| 1:E:49:ASP:OD2   | 1:F:49:ASP:OD2  | 2.19                     | 0.61              |
| 1:G:126:ASN:ND2  | 1:G:128:THR:HB  | 2.12                     | 0.61              |
| 1:F:139:MET:HA   | 1:F:139:MET:HE3 | 1.81                     | 0.61              |
| 1:C:126:ASN:ND2  | 1:C:128:THR:HB  | 2.13                     | 0.61              |
| 1:C:56:VAL:CG1   | 1:C:65:PHE:HB3  | 2.18                     | 0.61              |
| 1:B:70:VAL:HG21  | 2:B:1802:HOH:O  | 1.99                     | 0.61              |
| 1:D:68:THR:O     | 1:D:70:VAL:HG23 | 2.01                     | 0.61              |
| 1:J:37:ILE:CD1   | 1:K:33:VAL:HG13 | 2.31                     | 0.61              |
| 1:A:126:ASN:ND2  | 1:A:128:THR:HB  | 2.13                     | 0.61              |
| 1:C:139:MET:HA   | 1:C:139:MET:HE3 | 1.81                     | 0.60              |
| 1:A:49:ASP:OD2   | 1:B:49:ASP:OD2  | 2.20                     | 0.60              |
| 1:A:68:THR:O     | 1:A:70:VAL:HG23 | 2.01                     | 0.60              |
| 1:H:128:THR:HG21 | 1:H:198:TYR:OH  | 2.00                     | 0.60              |
| 1:J:128:THR:HG21 | 1:J:198:TYR:OH  | 2.02                     | 0.60              |
| 1:K:123:LYS:HA   | 1:K:170:THR:HA  | 1.83                     | 0.60              |
| 1:J:188:ASN:ND2  | 1:J:188:ASN:H   | 1.99                     | 0.59              |
| 1:C:56:VAL:HG12  | 1:C:57:THR:N    | 2.17                     | 0.59              |
| 1:I:56:VAL:CG1   | 1:I:65:PHE:HB3  | 2.19                     | 0.59              |
| 1:L:144:ASN:HB2  | 1:L:145:PRO:CD  | 2.32                     | 0.59              |
| 1:B:126:ASN:ND2  | 1:B:128:THR:HB  | 2.14                     | 0.59              |
| 1:G:56:VAL:HG12  | 1:G:57:THR:N    | 2.18                     | 0.59              |
| 1:H:40:HIS:HD2   | 2:H:1104:HOH:O  | 1.86                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:68:THR:O     | 1:H:70:VAL:HG23  | 2.02                     | 0.59              |
| 1:J:70:VAL:HG12  | 1:J:71:SER:N     | 2.17                     | 0.59              |
| 1:E:56:VAL:HG11  | 1:E:65:PHE:CB    | 2.20                     | 0.59              |
| 1:H:139:MET:HA   | 1:H:139:MET:HE3  | 1.83                     | 0.59              |
| 1:J:56:VAL:CG1   | 1:J:65:PHE:HB3   | 2.31                     | 0.59              |
| 1:A:56:VAL:HG12  | 1:A:57:THR:N     | 2.18                     | 0.59              |
| 1:E:68:THR:O     | 1:E:70:VAL:HG23  | 2.03                     | 0.58              |
| 1:I:56:VAL:HG12  | 1:I:57:THR:N     | 2.18                     | 0.58              |
| 1:J:45:GLU:HG3   | 1:J:130:ARG:HH11 | 1.68                     | 0.58              |
| 1:K:137:MET:HG3  | 1:K:192:MET:HE2  | 1.85                     | 0.58              |
| 1:I:126:ASN:ND2  | 1:I:128:THR:HB   | 2.14                     | 0.58              |
| 1:D:37:ILE:CD1   | 1:E:33:VAL:HG13  | 2.34                     | 0.58              |
| 1:F:56:VAL:HG12  | 1:F:57:THR:N     | 2.19                     | 0.58              |
| 1:H:56:VAL:HG12  | 1:H:57:THR:N     | 2.18                     | 0.58              |
| 1:J:45:GLU:HG3   | 1:J:130:ARG:NH1  | 2.19                     | 0.58              |
| 1:B:56:VAL:HG12  | 1:B:57:THR:N     | 2.19                     | 0.58              |
| 1:K:49:ASP:OD1   | 1:K:197:THR:HG23 | 2.03                     | 0.58              |
| 1:E:75:ASP:OD2   | 1:F:199:SER:O    | 2.22                     | 0.58              |
| 1:K:70:VAL:HG12  | 1:K:71:SER:N     | 2.17                     | 0.58              |
| 1:E:126:ASN:ND2  | 1:E:128:THR:HB   | 2.13                     | 0.57              |
| 1:G:188:ASN:HD22 | 1:G:188:ASN:N    | 2.01                     | 0.57              |
| 1:E:92:LYS:HB2   | 2:E:1525:HOH:O   | 2.04                     | 0.57              |
| 1:A:49:ASP:OD2   | 1:C:49:ASP:OD2   | 2.22                     | 0.57              |
| 1:B:123:LYS:HB3  | 1:B:170:THR:HG22 | 1.86                     | 0.57              |
| 1:H:126:ASN:ND2  | 1:H:128:THR:HB   | 2.14                     | 0.57              |
| 1:K:124:VAL:HG13 | 1:K:163:ILE:CD1  | 2.34                     | 0.57              |
| 1:L:188:ASN:H    | 1:L:188:ASN:ND2  | 2.00                     | 0.57              |
| 1:A:197:THR:HG21 | 2:C:2012:HOH:O   | 2.03                     | 0.57              |
| 1:E:46:THR:CG2   | 1:E:130:ARG:HH12 | 2.18                     | 0.57              |
| 1:C:52:LEU:HD21  | 1:C:80:ILE:HD13  | 1.87                     | 0.57              |
| 1:J:37:ILE:HD11  | 1:K:33:VAL:HG13  | 1.87                     | 0.57              |
| 1:E:56:VAL:HG12  | 1:E:57:THR:N     | 2.20                     | 0.57              |
| 1:I:123:LYS:HB3  | 1:I:170:THR:HG22 | 1.87                     | 0.56              |
| 1:J:126:ASN:ND2  | 1:J:128:THR:H    | 2.02                     | 0.56              |
| 1:H:56:VAL:HG11  | 1:H:65:PHE:CB    | 2.20                     | 0.56              |
| 1:K:73:ASP:OD1   | 1:K:79:LYS:HG3   | 2.04                     | 0.56              |
| 1:B:52:LEU:HD21  | 1:B:80:ILE:HD13  | 1.87                     | 0.56              |
| 1:C:123:LYS:HB3  | 1:C:170:THR:HG22 | 1.87                     | 0.56              |
| 1:F:56:VAL:HG11  | 1:F:65:PHE:CB    | 2.20                     | 0.56              |
| 1:B:56:VAL:HG11  | 1:B:65:PHE:CB    | 2.19                     | 0.56              |
| 1:D:199:SER:O    | 1:F:75:ASP:OD2   | 2.24                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:32:THR:HG23  | 2:I:1412:HOH:O   | 2.05                     | 0.56              |
| 1:A:123:LYS:HB3  | 1:A:170:THR:HG22 | 1.87                     | 0.56              |
| 1:B:170:THR:HG23 | 2:B:2148:HOH:O   | 2.05                     | 0.56              |
| 1:E:170:THR:HG23 | 2:E:2491:HOH:O   | 2.04                     | 0.56              |
| 1:E:70:VAL:HG12  | 1:E:71:SER:N     | 2.21                     | 0.56              |
| 1:E:52:LEU:HD21  | 1:E:80:ILE:HD13  | 1.87                     | 0.56              |
| 1:H:123:LYS:HB3  | 1:H:170:THR:HG22 | 1.88                     | 0.56              |
| 1:G:123:LYS:HB3  | 1:G:170:THR:HG22 | 1.87                     | 0.56              |
| 1:I:68:THR:HG23  | 2:I:1306:HOH:O   | 2.06                     | 0.56              |
| 1:L:52:LEU:HB2   | 1:L:194:VAL:CG2  | 2.36                     | 0.56              |
| 1:C:46:THR:HG21  | 2:C:1470:HOH:O   | 2.05                     | 0.56              |
| 1:D:56:VAL:HG12  | 1:D:57:THR:N     | 2.20                     | 0.56              |
| 1:E:46:THR:HG21  | 2:E:1404:HOH:O   | 2.05                     | 0.56              |
| 1:F:123:LYS:HB3  | 1:F:170:THR:HG22 | 1.87                     | 0.56              |
| 1:H:110:VAL:HG11 | 2:H:1380:HOH:O   | 2.05                     | 0.55              |
| 1:J:129:SER:HA   | 1:J:165:GLU:OE2  | 2.06                     | 0.55              |
| 1:A:56:VAL:HG11  | 1:A:65:PHE:CB    | 2.20                     | 0.55              |
| 1:D:123:LYS:HB3  | 1:D:170:THR:HG22 | 1.87                     | 0.55              |
| 1:D:52:LEU:HD21  | 1:D:80:ILE:HD13  | 1.87                     | 0.55              |
| 1:G:124:VAL:HG11 | 1:G:134:ILE:HD11 | 1.87                     | 0.55              |
| 1:E:123:LYS:HB3  | 1:E:170:THR:HG22 | 1.87                     | 0.55              |
| 1:B:46:THR:CG2   | 1:B:130:ARG:HH12 | 2.19                     | 0.55              |
| 1:A:52:LEU:HD21  | 1:A:80:ILE:HD13  | 1.89                     | 0.55              |
| 1:H:52:LEU:HD21  | 1:H:80:ILE:HD13  | 1.88                     | 0.55              |
| 2:D:1588:HOH:O   | 1:F:147:LYS:HE3  | 2.07                     | 0.55              |
| 1:F:70:VAL:HG12  | 1:F:71:SER:N     | 2.22                     | 0.55              |
| 1:B:75:ASP:OD2   | 1:C:199:SER:O    | 2.24                     | 0.55              |
| 1:F:52:LEU:HD21  | 1:F:80:ILE:HD13  | 1.88                     | 0.55              |
| 1:I:124:VAL:HG11 | 1:I:134:ILE:HD11 | 1.88                     | 0.55              |
| 1:I:188:ASN:HD22 | 1:I:188:ASN:N    | 2.00                     | 0.55              |
| 1:J:46:THR:CG2   | 1:J:130:ARG:HH12 | 2.20                     | 0.55              |
| 1:D:46:THR:CG2   | 1:D:130:ARG:HH12 | 2.20                     | 0.54              |
| 1:D:73:ASP:OD1   | 1:D:79:LYS:HG2   | 2.08                     | 0.54              |
| 1:K:197:THR:HG21 | 2:K:1095:HOH:O   | 2.06                     | 0.54              |
| 1:B:70:VAL:HG12  | 1:B:71:SER:N     | 2.23                     | 0.54              |
| 1:D:124:VAL:HG11 | 1:D:134:ILE:HD11 | 1.89                     | 0.54              |
| 1:H:70:VAL:HG12  | 1:H:71:SER:N     | 2.22                     | 0.54              |
| 1:G:46:THR:CG2   | 1:G:130:ARG:HH12 | 2.21                     | 0.54              |
| 1:I:73:ASP:OD1   | 1:I:79:LYS:HG2   | 2.08                     | 0.54              |
| 1:J:188:ASN:N    | 1:J:188:ASN:HD22 | 1.92                     | 0.54              |
| 1:F:46:THR:CG2   | 1:F:130:ARG:HH12 | 2.20                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:92:LYS:HG3   | 1:J:125:TRP:CZ2  | 2.43                     | 0.54              |
| 1:K:108:LEU:O    | 1:K:110:VAL:HG23 | 2.06                     | 0.54              |
| 1:J:123:LYS:HB3  | 1:J:170:THR:HG22 | 1.90                     | 0.54              |
| 1:L:139:MET:CE   | 1:L:192:MET:HB2  | 2.37                     | 0.54              |
| 1:G:73:ASP:OD1   | 1:G:79:LYS:HG2   | 2.08                     | 0.54              |
| 1:I:52:LEU:HD21  | 1:I:80:ILE:HD13  | 1.90                     | 0.54              |
| 1:K:64:TYR:CD2   | 1:K:119:GLU:HB3  | 2.43                     | 0.54              |
| 1:A:46:THR:CG2   | 1:A:130:ARG:HH12 | 2.21                     | 0.54              |
| 1:E:106:ARG:HB3  | 1:I:68:THR:HG22  | 1.88                     | 0.54              |
| 1:H:73:ASP:OD1   | 1:H:79:LYS:HG2   | 2.08                     | 0.54              |
| 1:K:56:VAL:HG12  | 1:K:57:THR:N     | 2.23                     | 0.54              |
| 1:K:92:LYS:HE3   | 1:K:166:ASP:OD2  | 2.08                     | 0.53              |
| 1:B:73:ASP:OD1   | 1:B:79:LYS:HG2   | 2.09                     | 0.53              |
| 1:D:70:VAL:HG12  | 1:D:71:SER:N     | 2.23                     | 0.53              |
| 1:G:49:ASP:OD2   | 1:H:49:ASP:OD2   | 2.25                     | 0.53              |
| 1:G:70:VAL:HG12  | 1:G:71:SER:N     | 2.23                     | 0.53              |
| 1:G:52:LEU:HD21  | 1:G:80:ILE:HD13  | 1.90                     | 0.53              |
| 1:A:73:ASP:OD1   | 1:A:79:LYS:HG2   | 2.08                     | 0.53              |
| 1:C:70:VAL:HG12  | 1:C:71:SER:N     | 2.23                     | 0.53              |
| 1:G:56:VAL:HG11  | 1:G:65:PHE:CB    | 2.18                     | 0.53              |
| 1:A:70:VAL:HG12  | 1:A:71:SER:N     | 2.23                     | 0.53              |
| 1:H:124:VAL:HG11 | 1:H:134:ILE:HD11 | 1.91                     | 0.53              |
| 1:J:170:THR:HG23 | 2:J:1246:HOH:O   | 2.09                     | 0.53              |
| 1:K:99:VAL:O     | 1:K:124:VAL:HA   | 2.08                     | 0.53              |
| 1:C:73:ASP:OD1   | 1:C:79:LYS:HG2   | 2.08                     | 0.53              |
| 1:F:73:ASP:OD1   | 1:F:79:LYS:HG2   | 2.08                     | 0.53              |
| 1:I:46:THR:CG2   | 1:I:130:ARG:HH12 | 2.22                     | 0.53              |
| 1:I:70:VAL:HG12  | 1:I:71:SER:N     | 2.24                     | 0.52              |
| 1:K:101:THR:CG2  | 1:K:123:LYS:HZ2  | 2.23                     | 0.52              |
| 1:K:83:ARG:HB3   | 1:K:86:LYS:HD2   | 1.91                     | 0.52              |
| 1:F:124:VAL:HG11 | 1:F:134:ILE:HD11 | 1.91                     | 0.52              |
| 1:E:105:GLY:O    | 1:I:68:THR:HG23  | 2.10                     | 0.52              |
| 1:C:164:ASP:HB2  | 1:C:167:GLU:CD   | 2.30                     | 0.52              |
| 1:L:123:LYS:HB3  | 1:L:170:THR:HG22 | 1.92                     | 0.52              |
| 1:E:73:ASP:OD1   | 1:E:79:LYS:HG2   | 2.08                     | 0.52              |
| 1:D:164:ASP:HB2  | 1:D:167:GLU:CD   | 2.30                     | 0.52              |
| 1:B:164:ASP:HB2  | 1:B:167:GLU:CD   | 2.30                     | 0.52              |
| 1:L:126:ASN:ND2  | 1:L:128:THR:HB   | 2.18                     | 0.52              |
| 1:L:56:VAL:HG12  | 1:L:57:THR:N     | 2.25                     | 0.52              |
| 1:A:124:VAL:HG11 | 1:A:134:ILE:HD11 | 1.91                     | 0.52              |
| 1:G:75:ASP:OD2   | 1:I:199:SER:O    | 2.28                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:131:LYS:CE   | 1:J:162:SER:HB2  | 2.40                     | 0.52              |
| 1:J:70:VAL:HG12  | 1:J:71:SER:H     | 1.75                     | 0.52              |
| 1:C:56:VAL:HG11  | 1:C:65:PHE:CB    | 2.21                     | 0.52              |
| 1:L:46:THR:CG2   | 1:L:130:ARG:HH12 | 2.23                     | 0.52              |
| 1:K:139:MET:CE   | 1:K:190:PHE:CB   | 2.88                     | 0.52              |
| 1:L:70:VAL:HG12  | 1:L:71:SER:N     | 2.25                     | 0.52              |
| 1:C:124:VAL:HG11 | 1:C:134:ILE:HD11 | 1.91                     | 0.51              |
| 1:C:46:THR:CG2   | 1:C:130:ARG:HH12 | 2.22                     | 0.51              |
| 1:E:124:VAL:HG11 | 1:E:134:ILE:HD11 | 1.91                     | 0.51              |
| 1:F:68:THR:O     | 1:F:70:VAL:HG23  | 2.09                     | 0.51              |
| 1:J:46:THR:HG22  | 1:J:130:ARG:CZ   | 2.40                     | 0.51              |
| 1:J:42:ASP:O     | 1:J:46:THR:HG23  | 2.11                     | 0.51              |
| 1:I:164:ASP:HB2  | 1:I:167:GLU:CD   | 2.30                     | 0.51              |
| 1:D:56:VAL:HG13  | 1:D:66:LYS:O     | 2.11                     | 0.51              |
| 1:H:56:VAL:HG13  | 1:H:66:LYS:O     | 2.10                     | 0.51              |
| 1:K:46:THR:CG2   | 1:K:130:ARG:HH12 | 2.24                     | 0.51              |
| 1:A:164:ASP:HB2  | 1:A:167:GLU:CD   | 2.31                     | 0.51              |
| 1:A:46:THR:HG21  | 2:A:1673:HOH:O   | 2.10                     | 0.51              |
| 1:L:46:THR:HG21  | 2:L:2137:HOH:O   | 2.11                     | 0.51              |
| 1:D:56:VAL:HG11  | 1:D:65:PHE:CB    | 2.22                     | 0.51              |
| 1:K:106:ARG:HA   | 1:K:106:ARG:NE   | 2.26                     | 0.51              |
| 1:K:54:ILE:O     | 1:K:56:VAL:HG23  | 2.10                     | 0.51              |
| 1:K:60:VAL:HG21  | 1:K:183:ALA:H    | 1.74                     | 0.51              |
| 1:B:124:VAL:HG11 | 1:B:134:ILE:HD11 | 1.93                     | 0.51              |
| 1:H:188:ASN:HD22 | 1:H:188:ASN:N    | 2.00                     | 0.51              |
| 1:E:164:ASP:HB2  | 1:E:167:GLU:CD   | 2.30                     | 0.51              |
| 1:F:86:LYS:HE2   | 2:F:2344:HOH:O   | 2.09                     | 0.51              |
| 1:L:46:THR:HG22  | 1:L:130:ARG:HH12 | 1.75                     | 0.51              |
| 1:B:46:THR:HG21  | 2:B:1396:HOH:O   | 2.11                     | 0.50              |
| 1:C:56:VAL:HG13  | 1:C:66:LYS:O     | 2.12                     | 0.50              |
| 1:K:56:VAL:HG13  | 1:K:66:LYS:O     | 2.12                     | 0.50              |
| 1:K:178:GLY:HA3  | 2:K:2471:HOH:O   | 2.12                     | 0.50              |
| 1:E:92:LYS:HD2   | 2:E:1525:HOH:O   | 2.11                     | 0.50              |
| 1:K:144:ASN:HB2  | 1:K:145:PRO:CD   | 2.42                     | 0.50              |
| 1:L:144:ASN:HB2  | 1:L:145:PRO:HD2  | 1.92                     | 0.50              |
| 1:C:56:VAL:CG1   | 1:C:57:THR:N     | 2.74                     | 0.50              |
| 2:J:1397:HOH:O   | 1:L:147:LYS:HE3  | 2.12                     | 0.50              |
| 1:D:46:THR:HG21  | 2:D:1566:HOH:O   | 2.11                     | 0.50              |
| 2:D:1346:HOH:O   | 1:F:72:PHE:HB2   | 2.11                     | 0.50              |
| 1:G:128:THR:HG22 | 1:G:129:SER:N    | 2.26                     | 0.50              |
| 1:J:45:GLU:CG    | 1:J:130:ARG:HH11 | 2.25                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:132:ILE:HD11 | 1:L:196:VAL:HG11 | 1.94                     | 0.50              |
| 1:E:188:ASN:HD22 | 1:E:188:ASN:N    | 2.03                     | 0.49              |
| 1:J:128:THR:HG22 | 1:J:129:SER:N    | 2.26                     | 0.49              |
| 1:H:128:THR:HG22 | 1:H:129:SER:N    | 2.27                     | 0.49              |
| 1:H:56:VAL:CG1   | 1:H:57:THR:N     | 2.75                     | 0.49              |
| 1:A:56:VAL:CG1   | 1:A:57:THR:N     | 2.75                     | 0.49              |
| 1:G:56:VAL:CG1   | 1:G:57:THR:N     | 2.75                     | 0.49              |
| 1:K:137:MET:HE3  | 1:K:156:SER:HB3  | 1.94                     | 0.49              |
| 1:H:131:LYS:HE2  | 1:H:162:SER:CB   | 2.40                     | 0.49              |
| 2:H:1104:HOH:O   | 1:I:40:HIS:HD2   | 1.95                     | 0.49              |
| 1:I:56:VAL:CG1   | 1:I:57:THR:N     | 2.75                     | 0.49              |
| 1:G:164:ASP:HB2  | 1:G:167:GLU:CD   | 2.32                     | 0.49              |
| 1:B:56:VAL:HG13  | 1:B:66:LYS:O     | 2.13                     | 0.49              |
| 1:I:128:THR:HG22 | 1:I:129:SER:N    | 2.26                     | 0.49              |
| 1:B:56:VAL:CG1   | 1:B:57:THR:N     | 2.76                     | 0.49              |
| 1:E:37:ILE:CD1   | 1:F:33:VAL:HG13  | 2.42                     | 0.49              |
| 1:H:164:ASP:HB2  | 1:H:167:GLU:CD   | 2.32                     | 0.49              |
| 1:I:144:ASN:HB2  | 1:I:145:PRO:CD   | 2.43                     | 0.49              |
| 1:K:199:SER:OG   | 1:K:200:GLY:N    | 2.43                     | 0.49              |
| 1:D:128:THR:HG22 | 1:D:129:SER:N    | 2.28                     | 0.49              |
| 1:E:128:THR:HG22 | 1:E:129:SER:N    | 2.28                     | 0.49              |
| 1:F:128:THR:HG22 | 1:F:129:SER:N    | 2.28                     | 0.49              |
| 1:F:56:VAL:CG1   | 1:F:57:THR:N     | 2.76                     | 0.49              |
| 1:I:188:ASN:ND2  | 1:I:188:ASN:H    | 2.08                     | 0.49              |
| 1:J:139:MET:CE   | 1:J:192:MET:HA   | 2.42                     | 0.49              |
| 1:L:128:THR:HG22 | 1:L:129:SER:N    | 2.27                     | 0.49              |
| 1:E:56:VAL:CG1   | 1:E:57:THR:N     | 2.76                     | 0.48              |
| 1:A:56:VAL:HG13  | 1:A:66:LYS:O     | 2.13                     | 0.48              |
| 1:C:34:THR:O     | 1:C:38:GLU:HG3   | 2.13                     | 0.48              |
| 1:D:56:VAL:CG1   | 1:D:57:THR:N     | 2.76                     | 0.48              |
| 1:H:46:THR:CG2   | 1:H:130:ARG:HH12 | 2.25                     | 0.48              |
| 1:J:139:MET:HE3  | 1:J:192:MET:CA   | 2.43                     | 0.48              |
| 1:F:34:THR:O     | 1:F:38:GLU:HG3   | 2.14                     | 0.48              |
| 1:L:164:ASP:HB2  | 1:L:167:GLU:OE1  | 2.13                     | 0.48              |
| 1:L:132:ILE:HD11 | 1:L:196:VAL:CG1  | 2.43                     | 0.48              |
| 1:L:46:THR:HG22  | 1:L:130:ARG:CZ   | 2.43                     | 0.48              |
| 1:B:128:THR:HG22 | 1:B:129:SER:N    | 2.27                     | 0.48              |
| 1:C:128:THR:HG22 | 1:C:129:SER:N    | 2.28                     | 0.48              |
| 1:D:34:THR:O     | 1:D:38:GLU:HG3   | 2.14                     | 0.48              |
| 1:E:56:VAL:HG13  | 1:E:66:LYS:O     | 2.13                     | 0.48              |
| 1:K:128:THR:HG22 | 1:K:129:SER:N    | 2.28                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:188:ASN:HD22 | 1:K:188:ASN:N    | 2.07                     | 0.48              |
| 1:F:164:ASP:HB2  | 1:F:167:GLU:CD   | 2.33                     | 0.48              |
| 1:F:46:THR:HG23  | 1:F:130:ARG:HH12 | 1.77                     | 0.48              |
| 1:G:49:ASP:OD2   | 1:I:49:ASP:OD2   | 2.32                     | 0.48              |
| 1:C:188:ASN:N    | 1:C:188:ASN:HD22 | 2.01                     | 0.48              |
| 1:G:46:THR:HG22  | 1:G:130:ARG:CZ   | 2.44                     | 0.48              |
| 1:E:101:THR:HB   | 1:E:123:LYS:HZ2  | 1.78                     | 0.48              |
| 1:G:197:THR:HG22 | 1:G:199:SER:N    | 2.07                     | 0.48              |
| 1:H:34:THR:O     | 1:H:38:GLU:HG3   | 2.13                     | 0.48              |
| 1:K:52:LEU:HD11  | 1:K:72:PHE:CE1   | 2.48                     | 0.48              |
| 1:F:56:VAL:HG13  | 1:F:66:LYS:O     | 2.14                     | 0.48              |
| 1:D:37:ILE:HD11  | 1:E:33:VAL:HG13  | 1.96                     | 0.47              |
| 1:E:46:THR:HG22  | 1:E:130:ARG:CZ   | 2.43                     | 0.47              |
| 1:D:201:THR:HG23 | 1:F:73:ASP:O     | 2.14                     | 0.47              |
| 1:K:49:ASP:OD1   | 1:K:197:THR:CG2  | 2.62                     | 0.47              |
| 1:L:32:THR:HG22  | 1:L:35:LYS:H     | 1.79                     | 0.47              |
| 1:A:110:VAL:HG11 | 2:A:1543:HOH:O   | 2.14                     | 0.47              |
| 1:A:128:THR:HG22 | 1:A:129:SER:N    | 2.28                     | 0.47              |
| 1:D:188:ASN:N    | 1:D:188:ASN:HD22 | 2.02                     | 0.47              |
| 1:E:34:THR:O     | 1:E:38:GLU:HG3   | 2.12                     | 0.47              |
| 1:J:49:ASP:HB2   | 1:K:49:ASP:OD2   | 2.14                     | 0.47              |
| 1:A:34:THR:O     | 1:A:38:GLU:HG3   | 2.14                     | 0.47              |
| 1:B:46:THR:HG22  | 1:B:130:ARG:CZ   | 2.44                     | 0.47              |
| 1:D:46:THR:HG22  | 1:D:130:ARG:CZ   | 2.44                     | 0.47              |
| 1:G:61:GLY:O     | 1:G:112:VAL:CG1  | 2.62                     | 0.47              |
| 1:D:42:ASP:O     | 1:D:46:THR:HG23  | 2.15                     | 0.47              |
| 1:F:139:MET:HE3  | 1:F:192:MET:CA   | 2.41                     | 0.47              |
| 1:F:101:THR:HB   | 1:F:123:LYS:HZ2  | 1.79                     | 0.47              |
| 1:B:34:THR:O     | 1:B:38:GLU:HG3   | 2.15                     | 0.47              |
| 2:E:1568:HOH:O   | 1:I:70:VAL:HG22  | 2.14                     | 0.47              |
| 1:B:49:ASP:OD2   | 1:C:49:ASP:OD2   | 2.33                     | 0.47              |
| 1:C:110:VAL:HG11 | 2:C:1316:HOH:O   | 2.15                     | 0.47              |
| 1:C:139:MET:HE3  | 1:C:192:MET:CA   | 2.41                     | 0.47              |
| 1:I:34:THR:O     | 1:I:38:GLU:HG3   | 2.14                     | 0.47              |
| 1:J:50:GLU:HG2   | 1:J:77:LEU:CD1   | 2.45                     | 0.47              |
| 2:A:1254:HOH:O   | 1:C:40:HIS:HD2   | 1.98                     | 0.47              |
| 1:K:140:VAL:O    | 1:K:190:PHE:HB3  | 2.15                     | 0.47              |
| 1:F:131:LYS:HE2  | 1:F:162:SER:CB   | 2.41                     | 0.47              |
| 1:H:61:GLY:O     | 1:H:112:VAL:CG1  | 2.62                     | 0.47              |
| 1:J:32:THR:HG23  | 1:J:35:LYS:H     | 1.80                     | 0.47              |
| 1:J:61:GLY:O     | 1:J:112:VAL:CG1  | 2.63                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:99:VAL:O     | 1:L:124:VAL:HA   | 2.15                     | 0.47              |
| 1:D:114:GLN:HG2  | 2:D:1203:HOH:O   | 2.15                     | 0.46              |
| 1:D:61:GLY:O     | 1:D:112:VAL:CG1  | 2.64                     | 0.46              |
| 1:G:34:THR:O     | 1:G:38:GLU:HG3   | 2.14                     | 0.46              |
| 1:A:79:LYS:HB3   | 2:A:2075:HOH:O   | 2.14                     | 0.46              |
| 1:E:131:LYS:HE2  | 1:E:162:SER:CB   | 2.42                     | 0.46              |
| 1:B:164:ASP:HB2  | 1:B:167:GLU:OE1  | 2.15                     | 0.46              |
| 1:G:56:VAL:HG13  | 1:G:66:LYS:O     | 2.15                     | 0.46              |
| 1:J:139:MET:HE2  | 1:J:139:MET:HA   | 1.96                     | 0.46              |
| 1:K:124:VAL:HG11 | 1:K:134:ILE:CD1  | 2.41                     | 0.46              |
| 1:L:46:THR:HG22  | 1:L:130:ARG:NH1  | 2.30                     | 0.46              |
| 1:I:46:THR:HG23  | 1:I:130:ARG:HH12 | 1.81                     | 0.46              |
| 1:E:106:ARG:CB   | 1:I:68:THR:CG2   | 2.91                     | 0.46              |
| 1:L:64:TYR:CD2   | 1:L:119:GLU:HB3  | 2.50                     | 0.46              |
| 1:A:46:THR:HG22  | 1:A:130:ARG:CZ   | 2.45                     | 0.46              |
| 1:H:101:THR:HB   | 1:H:123:LYS:HZ2  | 1.81                     | 0.46              |
| 1:H:197:THR:HG23 | 2:H:1253:HOH:O   | 2.15                     | 0.46              |
| 1:I:56:VAL:HG13  | 1:I:66:LYS:O     | 2.15                     | 0.46              |
| 1:C:188:ASN:ND2  | 1:C:188:ASN:H    | 2.11                     | 0.46              |
| 1:C:42:ASP:O     | 1:C:46:THR:HG23  | 2.15                     | 0.46              |
| 1:F:72:PHE:CE1   | 1:F:80:ILE:HD12  | 2.51                     | 0.46              |
| 1:G:144:ASN:HB2  | 1:G:145:PRO:CD   | 2.45                     | 0.46              |
| 1:I:164:ASP:HB2  | 1:I:167:GLU:OE1  | 2.16                     | 0.46              |
| 1:J:197:THR:HG23 | 2:J:1534:HOH:O   | 2.15                     | 0.46              |
| 1:K:59:GLU:HB3   | 1:K:62:SER:OG    | 2.16                     | 0.46              |
| 1:L:198:TYR:O    | 1:L:199:SER:O    | 2.33                     | 0.46              |
| 1:C:61:GLY:O     | 1:C:112:VAL:CG1  | 2.64                     | 0.46              |
| 1:C:46:THR:HG22  | 1:C:130:ARG:CZ   | 2.45                     | 0.46              |
| 1:F:46:THR:HG22  | 1:F:130:ARG:CZ   | 2.44                     | 0.46              |
| 1:J:46:THR:HG22  | 1:J:130:ARG:NH1  | 2.30                     | 0.46              |
| 1:J:128:THR:HG22 | 1:J:130:ARG:H    | 1.80                     | 0.46              |
| 1:A:46:THR:HG23  | 1:A:130:ARG:HH12 | 1.80                     | 0.46              |
| 1:B:72:PHE:CE1   | 1:B:80:ILE:HD12  | 2.51                     | 0.46              |
| 1:C:101:THR:HB   | 1:C:123:LYS:HZ2  | 1.80                     | 0.46              |
| 1:E:46:THR:HG23  | 1:E:130:ARG:HH12 | 1.80                     | 0.46              |
| 1:D:144:ASN:HB2  | 1:D:145:PRO:CD   | 2.46                     | 0.46              |
| 1:C:170:THR:HG23 | 2:C:2423:HOH:O   | 2.16                     | 0.45              |
| 1:J:137:MET:HA   | 1:J:193:TYR:O    | 2.15                     | 0.45              |
| 1:C:32:THR:HG22  | 1:C:35:LYS:H     | 1.81                     | 0.45              |
| 1:E:188:ASN:ND2  | 1:E:188:ASN:H    | 2.11                     | 0.45              |
| 1:G:61:GLY:O     | 1:G:112:VAL:HG13 | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:139:MET:HE3  | 1:I:192:MET:CA   | 2.43                     | 0.45              |
| 1:J:128:THR:CG2  | 1:J:129:SER:N    | 2.78                     | 0.45              |
| 1:C:131:LYS:HE2  | 1:C:162:SER:CB   | 2.43                     | 0.45              |
| 1:D:40:HIS:HD2   | 2:D:1558:HOH:O   | 1.99                     | 0.45              |
| 1:G:201:THR:CG2  | 1:H:72:PHE:CD1   | 2.99                     | 0.45              |
| 1:A:61:GLY:O     | 1:A:112:VAL:CG1  | 2.64                     | 0.45              |
| 1:B:199:SER:OG   | 1:B:200:GLY:N    | 2.49                     | 0.45              |
| 1:E:46:THR:HG22  | 1:E:130:ARG:HH12 | 1.81                     | 0.45              |
| 1:E:144:ASN:HB2  | 1:E:145:PRO:CD   | 2.47                     | 0.45              |
| 1:G:128:THR:CG2  | 1:G:129:SER:N    | 2.80                     | 0.45              |
| 1:H:46:THR:HG23  | 1:H:130:ARG:HH12 | 1.82                     | 0.45              |
| 1:J:124:VAL:HG22 | 1:J:163:ILE:HD12 | 1.94                     | 0.45              |
| 1:J:139:MET:HE3  | 1:J:139:MET:HA   | 1.98                     | 0.45              |
| 1:L:197:THR:HG22 | 1:L:199:SER:N    | 2.21                     | 0.45              |
| 1:D:128:THR:O    | 1:D:165:GLU:HG2  | 2.16                     | 0.45              |
| 1:E:42:ASP:O     | 1:E:46:THR:HG23  | 2.17                     | 0.45              |
| 1:L:188:ASN:HD22 | 1:L:188:ASN:N    | 1.95                     | 0.45              |
| 1:A:139:MET:HE3  | 1:A:192:MET:CA   | 2.42                     | 0.45              |
| 1:G:91:MET:SD    | 1:G:123:LYS:NZ   | 2.81                     | 0.45              |
| 1:I:128:THR:CG2  | 1:I:129:SER:N    | 2.79                     | 0.45              |
| 1:L:56:VAL:CG1   | 1:L:57:THR:N     | 2.79                     | 0.45              |
| 1:A:128:THR:O    | 1:A:165:GLU:HG2  | 2.17                     | 0.45              |
| 1:B:46:THR:HG23  | 1:B:130:ARG:HH12 | 1.79                     | 0.45              |
| 1:G:136:GLY:HA2  | 1:G:158:PHE:CZ   | 2.52                     | 0.45              |
| 1:H:197:THR:HG21 | 2:I:1092:HOH:O   | 2.17                     | 0.45              |
| 1:B:144:ASN:HB2  | 1:B:145:PRO:CD   | 2.47                     | 0.45              |
| 1:C:128:THR:O    | 1:C:165:GLU:HG2  | 2.16                     | 0.45              |
| 1:L:139:MET:HE2  | 1:L:192:MET:CB   | 2.46                     | 0.45              |
| 1:B:188:ASN:N    | 1:B:188:ASN:HD22 | 2.01                     | 0.45              |
| 1:E:128:THR:CG2  | 1:E:129:SER:N    | 2.80                     | 0.45              |
| 1:F:140:VAL:HA   | 1:F:141:PRO:HD3  | 1.89                     | 0.45              |
| 1:H:139:MET:HE3  | 1:H:192:MET:CA   | 2.40                     | 0.45              |
| 1:I:56:VAL:HG11  | 1:I:65:PHE:CB    | 2.23                     | 0.45              |
| 1:B:42:ASP:O     | 1:B:46:THR:HG23  | 2.17                     | 0.44              |
| 1:E:139:MET:HE3  | 1:E:192:MET:CA   | 2.43                     | 0.44              |
| 1:G:46:THR:HG23  | 1:G:130:ARG:HH12 | 1.82                     | 0.44              |
| 1:H:61:GLY:O     | 1:H:112:VAL:HG13 | 2.17                     | 0.44              |
| 1:H:128:THR:CG2  | 1:H:129:SER:N    | 2.80                     | 0.44              |
| 1:L:52:LEU:HB2   | 1:L:194:VAL:HG22 | 1.98                     | 0.44              |
| 1:L:56:VAL:HG13  | 1:L:66:LYS:O     | 2.16                     | 0.44              |
| 1:A:144:ASN:HB2  | 1:A:145:PRO:CD   | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:199:SER:OG   | 1:D:200:GLY:N    | 2.50                     | 0.44              |
| 1:G:188:ASN:ND2  | 1:G:188:ASN:H    | 2.10                     | 0.44              |
| 1:J:53:ARG:HG3   | 1:J:193:TYR:CE1  | 2.52                     | 0.44              |
| 1:K:46:THR:HG23  | 1:K:130:ARG:HH12 | 1.82                     | 0.44              |
| 1:D:46:THR:HG23  | 1:D:130:ARG:HH12 | 1.81                     | 0.44              |
| 1:E:164:ASP:HB2  | 1:E:167:GLU:OE1  | 2.17                     | 0.44              |
| 1:I:42:ASP:O     | 1:I:46:THR:HG23  | 2.18                     | 0.44              |
| 1:I:61:GLY:O     | 1:I:112:VAL:CG1  | 2.66                     | 0.44              |
| 1:K:121:THR:HG23 | 1:K:172:VAL:HA   | 2.00                     | 0.44              |
| 1:A:42:ASP:O     | 1:A:46:THR:HG23  | 2.18                     | 0.44              |
| 1:D:61:GLY:O     | 1:D:112:VAL:HG13 | 2.18                     | 0.44              |
| 1:D:128:THR:CG2  | 1:D:129:SER:N    | 2.80                     | 0.44              |
| 1:F:188:ASN:HD22 | 1:F:188:ASN:N    | 1.98                     | 0.44              |
| 1:G:201:THR:HG22 | 1:G:201:THR:O    | 2.17                     | 0.44              |
| 1:I:110:VAL:HG11 | 2:I:1192:HOH:O   | 2.17                     | 0.44              |
| 1:I:32:THR:HG22  | 1:I:35:LYS:H     | 1.82                     | 0.44              |
| 1:A:128:THR:CG2  | 1:A:129:SER:N    | 2.80                     | 0.44              |
| 1:A:188:ASN:HD22 | 1:A:188:ASN:N    | 2.02                     | 0.44              |
| 1:A:72:PHE:CE1   | 1:A:80:ILE:HD12  | 2.52                     | 0.44              |
| 1:B:128:THR:CG2  | 1:B:129:SER:N    | 2.80                     | 0.44              |
| 1:B:92:LYS:HD2   | 2:B:2227:HOH:O   | 2.17                     | 0.44              |
| 1:G:128:THR:O    | 1:G:165:GLU:HG2  | 2.17                     | 0.44              |
| 1:H:72:PHE:CE1   | 1:H:80:ILE:HD12  | 2.52                     | 0.44              |
| 1:I:144:ASN:HB2  | 1:I:145:PRO:HD2  | 2.00                     | 0.44              |
| 1:J:46:THR:HG22  | 1:J:130:ARG:HH12 | 1.83                     | 0.44              |
| 1:K:87:SER:O     | 1:K:91:MET:HG3   | 2.17                     | 0.44              |
| 1:J:46:THR:HG23  | 1:J:130:ARG:HH12 | 1.83                     | 0.44              |
| 1:H:140:VAL:HA   | 1:H:141:PRO:HD3  | 1.89                     | 0.44              |
| 1:I:46:THR:HG22  | 1:I:130:ARG:CZ   | 2.46                     | 0.44              |
| 1:B:128:THR:O    | 1:B:165:GLU:HG2  | 2.18                     | 0.44              |
| 1:E:199:SER:OG   | 1:E:200:GLY:N    | 2.50                     | 0.44              |
| 1:H:144:ASN:HB2  | 1:H:145:PRO:CD   | 2.48                     | 0.44              |
| 1:A:164:ASP:HB2  | 1:A:167:GLU:OE1  | 2.18                     | 0.43              |
| 1:B:61:GLY:O     | 1:B:112:VAL:CG1  | 2.66                     | 0.43              |
| 1:I:131:LYS:HE2  | 1:I:162:SER:CB   | 2.41                     | 0.43              |
| 1:J:144:ASN:HB2  | 1:J:145:PRO:CD   | 2.48                     | 0.43              |
| 1:D:72:PHE:CE1   | 1:D:80:ILE:HD12  | 2.53                     | 0.43              |
| 1:E:46:THR:HG22  | 1:E:130:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:61:GLY:O     | 1:E:112:VAL:CG1  | 2.66                     | 0.43              |
| 1:F:128:THR:CG2  | 1:F:129:SER:N    | 2.81                     | 0.43              |
| 1:H:199:SER:OG   | 1:H:200:GLY:N    | 2.50                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:91:MET:SD    | 1:I:123:LYS:NZ   | 2.85                     | 0.43              |
| 1:K:175:THR:HG22 | 1:K:176:THR:N    | 2.34                     | 0.43              |
| 1:C:128:THR:CG2  | 1:C:129:SER:N    | 2.81                     | 0.43              |
| 1:C:164:ASP:HB2  | 1:C:167:GLU:OE1  | 2.17                     | 0.43              |
| 1:D:37:ILE:HG21  | 1:E:36:THR:HG21  | 2.00                     | 0.43              |
| 1:E:194:VAL:HG23 | 1:E:194:VAL:O    | 2.17                     | 0.43              |
| 1:G:164:ASP:HB2  | 1:G:167:GLU:OE1  | 2.18                     | 0.43              |
| 1:G:199:SER:OG   | 1:G:200:GLY:N    | 2.50                     | 0.43              |
| 1:J:32:THR:CG2   | 1:J:35:LYS:H     | 2.31                     | 0.43              |
| 1:J:45:GLU:OE1   | 1:J:130:ARG:HD2  | 2.18                     | 0.43              |
| 1:K:116:LEU:HD23 | 1:K:180:PRO:HA   | 2.01                     | 0.43              |
| 1:A:61:GLY:O     | 1:A:112:VAL:HG13 | 2.18                     | 0.43              |
| 1:I:199:SER:OG   | 1:I:200:GLY:N    | 2.49                     | 0.43              |
| 1:E:72:PHE:CE1   | 1:E:80:ILE:HD12  | 2.53                     | 0.43              |
| 1:F:128:THR:O    | 1:F:165:GLU:HG2  | 2.19                     | 0.43              |
| 1:I:197:THR:HG21 | 2:I:1086:HOH:O   | 2.18                     | 0.43              |
| 1:D:164:ASP:HB2  | 1:D:167:GLU:OE1  | 2.18                     | 0.43              |
| 1:J:56:VAL:HG11  | 1:J:65:PHE:CB    | 2.38                     | 0.43              |
| 1:C:61:GLY:O     | 1:C:112:VAL:HG13 | 2.19                     | 0.43              |
| 1:C:46:THR:HG23  | 1:C:130:ARG:HH12 | 1.84                     | 0.43              |
| 1:C:144:ASN:HB2  | 1:C:145:PRO:CD   | 2.48                     | 0.43              |
| 1:G:42:ASP:O     | 1:G:46:THR:HG23  | 2.19                     | 0.43              |
| 1:A:101:THR:HB   | 1:A:123:LYS:HZ2  | 1.84                     | 0.43              |
| 1:I:128:THR:O    | 1:I:165:GLU:HG2  | 2.18                     | 0.43              |
| 1:A:32:THR:HG22  | 1:A:35:LYS:H     | 1.84                     | 0.43              |
| 1:E:105:GLY:O    | 1:I:68:THR:CG2   | 2.67                     | 0.43              |
| 1:E:128:THR:O    | 1:E:165:GLU:HG2  | 2.19                     | 0.43              |
| 1:K:40:HIS:O     | 1:K:44:ILE:HG13  | 2.18                     | 0.43              |
| 1:L:33:VAL:HG12  | 1:L:37:ILE:HG13  | 2.01                     | 0.43              |
| 1:F:144:ASN:HB2  | 1:F:145:PRO:CD   | 2.48                     | 0.43              |
| 1:G:72:PHE:CE1   | 1:G:80:ILE:HD12  | 2.53                     | 0.43              |
| 1:I:194:VAL:HG23 | 1:I:194:VAL:O    | 2.19                     | 0.43              |
| 1:D:124:VAL:HG11 | 1:D:134:ILE:CD1  | 2.49                     | 0.42              |
| 1:J:132:ILE:HD12 | 1:J:198:TYR:CZ   | 2.54                     | 0.42              |
| 1:K:68:THR:O     | 1:K:70:VAL:HG23  | 2.19                     | 0.42              |
| 1:G:46:THR:HG22  | 1:G:130:ARG:HH12 | 1.83                     | 0.42              |
| 1:J:40:HIS:O     | 1:J:44:ILE:HG13  | 2.20                     | 0.42              |
| 1:B:46:THR:HG22  | 1:B:130:ARG:NH1  | 2.34                     | 0.42              |
| 1:C:136:GLY:HA2  | 1:C:158:PHE:CZ   | 2.54                     | 0.42              |
| 1:F:136:GLY:HA2  | 1:F:158:PHE:CZ   | 2.54                     | 0.42              |
| 1:I:72:PHE:CE1   | 1:I:80:ILE:HD12  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:194:VAL:O    | 1:D:194:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:201:THR:HG22 | 1:D:201:THR:O    | 2.20                     | 0.42              |
| 1:F:32:THR:HG22  | 1:F:35:LYS:H     | 1.84                     | 0.42              |
| 1:G:144:ASN:HB2  | 1:G:145:PRO:HD2  | 2.00                     | 0.42              |
| 1:I:140:VAL:HA   | 1:I:141:PRO:HD3  | 1.90                     | 0.42              |
| 1:K:52:LEU:HB3   | 1:K:194:VAL:HG22 | 2.02                     | 0.42              |
| 1:L:72:PHE:CE1   | 1:L:80:ILE:HB    | 2.54                     | 0.42              |
| 1:A:199:SER:OG   | 1:A:200:GLY:N    | 2.50                     | 0.42              |
| 1:B:139:MET:CE   | 1:B:139:MET:CA   | 2.96                     | 0.42              |
| 1:B:147:LYS:HE3  | 2:C:1887:HOH:O   | 2.19                     | 0.42              |
| 1:D:110:VAL:HG12 | 1:D:111:THR:N    | 2.34                     | 0.42              |
| 1:D:46:THR:HG22  | 1:D:130:ARG:HH12 | 1.84                     | 0.42              |
| 1:G:124:VAL:HG11 | 1:G:134:ILE:CD1  | 2.50                     | 0.42              |
| 1:A:91:MET:SD    | 1:A:123:LYS:NZ   | 2.88                     | 0.42              |
| 1:B:32:THR:HG22  | 1:B:35:LYS:H     | 1.84                     | 0.42              |
| 1:H:197:THR:HG22 | 1:H:199:SER:N    | 2.09                     | 0.42              |
| 1:E:144:ASN:HB2  | 1:E:145:PRO:HD2  | 2.02                     | 0.42              |
| 1:F:72:PHE:HE1   | 1:F:80:ILE:HD12  | 1.85                     | 0.42              |
| 1:F:42:ASP:O     | 1:F:46:THR:HG23  | 2.20                     | 0.42              |
| 1:H:42:ASP:O     | 1:H:46:THR:HG23  | 2.19                     | 0.42              |
| 1:I:136:GLY:HA2  | 1:I:158:PHE:CZ   | 2.55                     | 0.42              |
| 1:J:53:ARG:HG3   | 1:J:193:TYR:CZ   | 2.55                     | 0.42              |
| 1:K:56:VAL:CG1   | 1:K:57:THR:N     | 2.83                     | 0.42              |
| 1:F:199:SER:OG   | 1:F:200:GLY:N    | 2.52                     | 0.42              |
| 1:H:128:THR:O    | 1:H:165:GLU:HG2  | 2.19                     | 0.42              |
| 1:K:141:PRO:HA   | 1:K:190:PHE:CD1  | 2.38                     | 0.42              |
| 1:K:70:VAL:CG1   | 1:K:71:SER:N     | 2.82                     | 0.42              |
| 1:A:110:VAL:HG12 | 1:A:111:THR:N    | 2.35                     | 0.41              |
| 1:A:136:GLY:HA2  | 1:A:158:PHE:CZ   | 2.55                     | 0.41              |
| 1:B:46:THR:HG22  | 1:B:130:ARG:HH12 | 1.83                     | 0.41              |
| 1:D:136:GLY:HA2  | 1:D:158:PHE:CZ   | 2.54                     | 0.41              |
| 1:E:201:THR:O    | 1:E:201:THR:HG22 | 2.20                     | 0.41              |
| 2:D:1558:HOH:O   | 1:F:40:HIS:HD2   | 2.03                     | 0.41              |
| 1:G:110:VAL:HG12 | 1:G:111:THR:N    | 2.35                     | 0.41              |
| 1:H:106:ARG:HA   | 1:H:106:ARG:NE   | 2.34                     | 0.41              |
| 1:L:128:THR:CG2  | 1:L:129:SER:N    | 2.83                     | 0.41              |
| 1:A:131:LYS:HE2  | 1:A:162:SER:CB   | 2.42                     | 0.41              |
| 1:A:201:THR:O    | 1:A:201:THR:HG22 | 2.20                     | 0.41              |
| 1:B:131:LYS:HE2  | 1:B:162:SER:CB   | 2.43                     | 0.41              |
| 1:C:110:VAL:HG12 | 1:C:111:THR:N    | 2.35                     | 0.41              |
| 1:C:201:THR:O    | 1:C:201:THR:HG22 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:61:GLY:C     | 1:H:112:VAL:HG13 | 2.40                     | 0.41              |
| 1:C:140:VAL:HA   | 1:C:141:PRO:HD3  | 1.88                     | 0.41              |
| 1:K:92:LYS:HG3   | 1:K:125:TRP:CZ2  | 2.55                     | 0.41              |
| 2:J:2246:HOH:O   | 1:L:140:VAL:HG22 | 2.20                     | 0.41              |
| 1:B:61:GLY:O     | 1:B:112:VAL:HG13 | 2.20                     | 0.41              |
| 1:B:197:THR:HG22 | 1:B:199:SER:N    | 2.07                     | 0.41              |
| 1:C:46:THR:HG22  | 1:C:130:ARG:HH12 | 1.84                     | 0.41              |
| 1:D:144:ASN:HB2  | 1:D:145:PRO:HD2  | 2.02                     | 0.41              |
| 1:F:110:VAL:HG12 | 1:F:111:THR:N    | 2.34                     | 0.41              |
| 1:G:194:VAL:O    | 1:G:194:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:32:THR:HG22  | 1:G:35:LYS:H     | 1.86                     | 0.41              |
| 1:J:56:VAL:CG1   | 1:J:57:THR:N     | 2.82                     | 0.41              |
| 1:D:101:THR:HB   | 1:D:123:LYS:HZ2  | 1.85                     | 0.41              |
| 1:F:61:GLY:O     | 1:F:112:VAL:CG1  | 2.68                     | 0.41              |
| 1:F:139:MET:HE2  | 1:F:139:MET:HA   | 2.01                     | 0.41              |
| 1:G:131:LYS:HE2  | 1:G:162:SER:CB   | 2.43                     | 0.41              |
| 1:I:124:VAL:HG11 | 1:I:134:ILE:CD1  | 2.50                     | 0.41              |
| 1:K:144:ASN:HB2  | 1:K:145:PRO:HD2  | 2.01                     | 0.41              |
| 1:K:59:GLU:OE1   | 1:K:66:LYS:HE3   | 2.21                     | 0.41              |
| 1:D:197:THR:HG22 | 1:D:198:TYR:N    | 2.36                     | 0.41              |
| 1:D:61:GLY:C     | 1:D:112:VAL:HG13 | 2.41                     | 0.41              |
| 1:G:46:THR:HG22  | 1:G:130:ARG:NH1  | 2.35                     | 0.41              |
| 1:H:164:ASP:HB2  | 1:H:167:GLU:OE1  | 2.19                     | 0.41              |
| 1:H:32:THR:HG22  | 1:H:35:LYS:H     | 1.86                     | 0.41              |
| 1:L:52:LEU:O     | 1:L:193:TYR:HA   | 2.20                     | 0.41              |
| 1:C:199:SER:OG   | 1:C:200:GLY:N    | 2.50                     | 0.41              |
| 1:C:72:PHE:CE1   | 1:C:80:ILE:HD12  | 2.55                     | 0.41              |
| 1:D:32:THR:HG22  | 1:D:35:LYS:H     | 1.85                     | 0.41              |
| 1:F:201:THR:HG22 | 1:F:201:THR:O    | 2.20                     | 0.41              |
| 1:L:197:THR:HG23 | 2:L:1350:HOH:O   | 2.20                     | 0.41              |
| 1:L:199:SER:OG   | 1:L:200:GLY:N    | 2.50                     | 0.41              |
| 1:E:37:ILE:HD11  | 1:F:33:VAL:HG13  | 2.03                     | 0.41              |
| 1:H:139:MET:HA   | 1:H:139:MET:HE2  | 2.01                     | 0.41              |
| 1:I:106:ARG:NE   | 1:I:106:ARG:HA   | 2.36                     | 0.41              |
| 1:I:110:VAL:HG12 | 1:I:111:THR:N    | 2.34                     | 0.41              |
| 1:K:91:MET:C     | 1:K:93:GLU:H     | 2.22                     | 0.41              |
| 1:I:61:GLY:C     | 1:I:112:VAL:HG13 | 2.41                     | 0.41              |
| 1:A:144:ASN:HB2  | 1:A:145:PRO:HD2  | 2.02                     | 0.41              |
| 1:J:92:LYS:HG2   | 2:J:1873:HOH:O   | 2.21                     | 0.41              |
| 1:K:124:VAL:HG13 | 1:K:163:ILE:HD12 | 2.03                     | 0.41              |
| 1:F:188:ASN:H    | 1:F:188:ASN:ND2  | 2.07                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:110:VAL:HG12 | 1:B:111:THR:N    | 2.35                     | 0.40              |
| 1:B:72:PHE:HE1   | 1:B:80:ILE:HD12  | 1.86                     | 0.40              |
| 1:A:46:THR:HG22  | 1:A:130:ARG:HH12 | 1.86                     | 0.40              |
| 1:B:201:THR:HG22 | 1:B:201:THR:O    | 2.20                     | 0.40              |
| 1:B:70:VAL:HG22  | 2:B:1302:HOH:O   | 2.20                     | 0.40              |
| 1:G:139:MET:HE3  | 1:G:192:MET:CA   | 2.46                     | 0.40              |
| 1:H:144:ASN:HB2  | 1:H:145:PRO:HD2  | 2.04                     | 0.40              |
| 1:H:46:THR:HG22  | 1:H:130:ARG:CZ   | 2.48                     | 0.40              |
| 1:I:61:GLY:O     | 1:I:112:VAL:HG13 | 2.21                     | 0.40              |
| 1:H:49:ASP:OD2   | 1:I:49:ASP:OD2   | 2.40                     | 0.40              |
| 1:B:139:MET:HE3  | 1:B:192:MET:CA   | 2.45                     | 0.40              |
| 1:B:144:ASN:HB2  | 1:B:145:PRO:HD2  | 2.02                     | 0.40              |
| 1:C:46:THR:HG22  | 1:C:130:ARG:NH1  | 2.36                     | 0.40              |
| 1:I:201:THR:O    | 1:I:201:THR:HG22 | 2.21                     | 0.40              |
| 1:B:136:GLY:HA2  | 1:B:158:PHE:CZ   | 2.56                     | 0.40              |
| 1:E:136:GLY:HA2  | 1:E:158:PHE:CZ   | 2.56                     | 0.40              |
| 1:H:110:VAL:HG12 | 1:H:111:THR:N    | 2.35                     | 0.40              |
| 1:H:141:PRO:HG3  | 2:H:1283:HOH:O   | 2.21                     | 0.40              |
| 1:I:139:MET:CA   | 1:I:139:MET:CE   | 2.97                     | 0.40              |
| 1:K:92:LYS:O     | 1:K:92:LYS:HG2   | 2.21                     | 0.40              |
| 1:C:61:GLY:C     | 1:C:112:VAL:HG13 | 2.42                     | 0.40              |
| 1:E:110:VAL:HG12 | 1:E:111:THR:N    | 2.36                     | 0.40              |
| 1:I:101:THR:HB   | 1:I:123:LYS:HZ2  | 1.86                     | 0.40              |
| 1:J:126:ASN:HD22 | 1:J:126:ASN:C    | 2.25                     | 0.40              |
| 1:K:198:TYR:O    | 1:K:199:SER:O    | 2.39                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:D:60:VAL:CG1 | 1:H:59:GLU:OE2[3_656] | 1.92                     | 0.28              |

## 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     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | B     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | C     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | D     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | E     | 168/170 (99%)   | 162 (96%)  | 5 (3%)  | 1 (1%)   | 28          | 21 |
| 1   | F     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | G     | 168/170 (99%)   | 162 (96%)  | 5 (3%)  | 1 (1%)   | 28          | 21 |
| 1   | H     | 168/170 (99%)   | 163 (97%)  | 4 (2%)  | 1 (1%)   | 28          | 21 |
| 1   | I     | 168/170 (99%)   | 162 (96%)  | 5 (3%)  | 1 (1%)   | 28          | 21 |
| 1   | J     | 168/170 (99%)   | 159 (95%)  | 8 (5%)  | 1 (1%)   | 28          | 21 |
| 1   | K     | 168/170 (99%)   | 158 (94%)  | 8 (5%)  | 2 (1%)   | 15          | 8  |
| 1   | L     | 168/170 (99%)   | 163 (97%)  | 3 (2%)  | 2 (1%)   | 15          | 8  |
| All | All   | 2016/2040 (99%) | 1944 (96%) | 58 (3%) | 14 (1%)  | 25          | 18 |

All (14) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 199 | SER  |
| 1   | B     | 199 | SER  |
| 1   | C     | 199 | SER  |
| 1   | D     | 199 | SER  |
| 1   | E     | 199 | SER  |
| 1   | F     | 199 | SER  |
| 1   | G     | 199 | SER  |
| 1   | H     | 199 | SER  |
| 1   | I     | 199 | SER  |
| 1   | K     | 199 | SER  |
| 1   | L     | 199 | SER  |
| 1   | J     | 199 | SER  |
| 1   | L     | 112 | VAL  |
| 1   | K     | 92  | LYS  |

### 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     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | B     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | C     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | D     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | E     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | F     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | G     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | H     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | I     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | J     | 146/146 (100%)   | 139 (95%)  | 7 (5%)   | 30          | 25 |
| 1   | K     | 146/146 (100%)   | 141 (97%)  | 5 (3%)   | 42          | 40 |
| 1   | L     | 146/146 (100%)   | 140 (96%)  | 6 (4%)   | 35          | 31 |
| All | All   | 1752/1752 (100%) | 1671 (95%) | 81 (5%)  | 31          | 27 |

All (81) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | HIS  |
| 1   | A     | 52  | LEU  |
| 1   | A     | 108 | LEU  |
| 1   | A     | 124 | VAL  |
| 1   | A     | 126 | ASN  |
| 1   | A     | 139 | MET  |
| 1   | A     | 188 | ASN  |
| 1   | B     | 40  | HIS  |
| 1   | B     | 52  | LEU  |
| 1   | B     | 108 | LEU  |
| 1   | B     | 124 | VAL  |
| 1   | B     | 126 | ASN  |
| 1   | B     | 139 | MET  |
| 1   | B     | 188 | ASN  |
| 1   | C     | 40  | HIS  |
| 1   | C     | 52  | LEU  |
| 1   | C     | 108 | LEU  |
| 1   | C     | 124 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 126 | ASN  |
| 1   | C     | 139 | MET  |
| 1   | C     | 188 | ASN  |
| 1   | D     | 40  | HIS  |
| 1   | D     | 52  | LEU  |
| 1   | D     | 108 | LEU  |
| 1   | D     | 124 | VAL  |
| 1   | D     | 126 | ASN  |
| 1   | D     | 139 | MET  |
| 1   | D     | 188 | ASN  |
| 1   | E     | 40  | HIS  |
| 1   | E     | 52  | LEU  |
| 1   | E     | 108 | LEU  |
| 1   | E     | 124 | VAL  |
| 1   | E     | 126 | ASN  |
| 1   | E     | 139 | MET  |
| 1   | E     | 188 | ASN  |
| 1   | F     | 40  | HIS  |
| 1   | F     | 52  | LEU  |
| 1   | F     | 108 | LEU  |
| 1   | F     | 124 | VAL  |
| 1   | F     | 126 | ASN  |
| 1   | F     | 139 | MET  |
| 1   | F     | 188 | ASN  |
| 1   | G     | 40  | HIS  |
| 1   | G     | 52  | LEU  |
| 1   | G     | 108 | LEU  |
| 1   | G     | 124 | VAL  |
| 1   | G     | 126 | ASN  |
| 1   | G     | 139 | MET  |
| 1   | G     | 188 | ASN  |
| 1   | H     | 40  | HIS  |
| 1   | H     | 52  | LEU  |
| 1   | H     | 108 | LEU  |
| 1   | H     | 124 | VAL  |
| 1   | H     | 126 | ASN  |
| 1   | H     | 139 | MET  |
| 1   | H     | 188 | ASN  |
| 1   | I     | 40  | HIS  |
| 1   | I     | 52  | LEU  |
| 1   | I     | 108 | LEU  |
| 1   | I     | 124 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 126 | ASN  |
| 1   | I     | 139 | MET  |
| 1   | I     | 188 | ASN  |
| 1   | J     | 32  | THR  |
| 1   | J     | 40  | HIS  |
| 1   | J     | 108 | LEU  |
| 1   | J     | 124 | VAL  |
| 1   | J     | 126 | ASN  |
| 1   | J     | 139 | MET  |
| 1   | J     | 188 | ASN  |
| 1   | K     | 40  | HIS  |
| 1   | K     | 72  | PHE  |
| 1   | K     | 126 | ASN  |
| 1   | K     | 170 | THR  |
| 1   | K     | 188 | ASN  |
| 1   | L     | 38  | GLU  |
| 1   | L     | 40  | HIS  |
| 1   | L     | 108 | LEU  |
| 1   | L     | 124 | VAL  |
| 1   | L     | 126 | ASN  |
| 1   | L     | 188 | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 40  | HIS  |
| 1   | A     | 126 | ASN  |
| 1   | A     | 127 | ASN  |
| 1   | A     | 188 | ASN  |
| 1   | B     | 126 | ASN  |
| 1   | B     | 127 | ASN  |
| 1   | B     | 188 | ASN  |
| 1   | C     | 40  | HIS  |
| 1   | C     | 126 | ASN  |
| 1   | C     | 127 | ASN  |
| 1   | C     | 188 | ASN  |
| 1   | D     | 40  | HIS  |
| 1   | D     | 126 | ASN  |
| 1   | D     | 127 | ASN  |
| 1   | D     | 188 | ASN  |
| 1   | E     | 40  | HIS  |
| 1   | E     | 126 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 127 | ASN  |
| 1   | E     | 188 | ASN  |
| 1   | F     | 40  | HIS  |
| 1   | F     | 126 | ASN  |
| 1   | F     | 127 | ASN  |
| 1   | F     | 188 | ASN  |
| 1   | G     | 40  | HIS  |
| 1   | G     | 126 | ASN  |
| 1   | G     | 127 | ASN  |
| 1   | G     | 188 | ASN  |
| 1   | H     | 40  | HIS  |
| 1   | H     | 126 | ASN  |
| 1   | H     | 127 | ASN  |
| 1   | H     | 188 | ASN  |
| 1   | I     | 40  | HIS  |
| 1   | I     | 126 | ASN  |
| 1   | I     | 127 | ASN  |
| 1   | I     | 188 | ASN  |
| 1   | J     | 40  | HIS  |
| 1   | J     | 126 | ASN  |
| 1   | J     | 127 | ASN  |
| 1   | J     | 188 | ASN  |
| 1   | K     | 40  | HIS  |
| 1   | K     | 43  | ASN  |
| 1   | K     | 126 | ASN  |
| 1   | K     | 127 | ASN  |
| 1   | K     | 188 | ASN  |
| 1   | L     | 126 | ASN  |
| 1   | L     | 127 | ASN  |
| 1   | L     | 138 | GLN  |
| 1   | L     | 188 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|----------------|-----------------------|-------|
| 1   | A     | 170/170 (100%)   | 0.45   | 9 (5%) 27 27   | 8, 17, 47, 74         | 0     |
| 1   | B     | 170/170 (100%)   | 0.45   | 10 (5%) 23 23  | 6, 14, 40, 110        | 0     |
| 1   | C     | 170/170 (100%)   | 0.30   | 7 (4%) 38 38   | 7, 15, 38, 67         | 0     |
| 1   | D     | 170/170 (100%)   | 0.47   | 11 (6%) 20 20  | 6, 16, 39, 87         | 0     |
| 1   | E     | 170/170 (100%)   | 0.42   | 12 (7%) 17 17  | 7, 13, 39, 84         | 0     |
| 1   | F     | 170/170 (100%)   | 0.57   | 17 (10%) 8 8   | 4, 13, 38, 66         | 0     |
| 1   | G     | 170/170 (100%)   | 0.78   | 16 (9%) 9 9    | 5, 13, 48, 124        | 0     |
| 1   | H     | 170/170 (100%)   | 0.76   | 18 (10%) 7 7   | 6, 17, 53, 89         | 0     |
| 1   | I     | 170/170 (100%)   | 0.42   | 6 (3%) 44 45   | 6, 16, 37, 60         | 0     |
| 1   | J     | 170/170 (100%)   | 0.22   | 0 100 100      | 7, 17, 38, 56         | 0     |
| 1   | K     | 170/170 (100%)   | 0.92   | 14 (8%) 12 12  | 12, 29, 51, 68        | 0     |
| 1   | L     | 170/170 (100%)   | 0.49   | 9 (5%) 27 27   | 10, 21, 41, 66        | 0     |
| All | All   | 2040/2040 (100%) | 0.52   | 129 (6%) 21 21 | 4, 17, 45, 124        | 0     |

All (129) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 32  | THR  | 23.1 |
| 1   | G     | 34  | THR  | 19.5 |
| 1   | B     | 32  | THR  | 14.2 |
| 1   | G     | 36  | THR  | 10.1 |
| 1   | G     | 33  | VAL  | 10.1 |
| 1   | G     | 35  | LYS  | 8.8  |
| 1   | H     | 37  | ILE  | 8.8  |
| 1   | G     | 37  | ILE  | 8.7  |
| 1   | F     | 33  | VAL  | 8.6  |
| 1   | H     | 33  | VAL  | 8.6  |
| 1   | H     | 34  | THR  | 8.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 34  | THR  | 7.2  |
| 1   | G     | 38  | GLU  | 7.2  |
| 1   | D     | 35  | LYS  | 5.8  |
| 1   | A     | 34  | THR  | 5.6  |
| 1   | K     | 32  | THR  | 5.4  |
| 1   | F     | 32  | THR  | 5.4  |
| 1   | E     | 32  | THR  | 5.3  |
| 1   | H     | 32  | THR  | 5.3  |
| 1   | B     | 35  | LYS  | 5.3  |
| 1   | E     | 33  | VAL  | 5.1  |
| 1   | F     | 36  | THR  | 5.1  |
| 1   | D     | 201 | THR  | 5.1  |
| 1   | D     | 32  | THR  | 5.0  |
| 1   | H     | 36  | THR  | 5.0  |
| 1   | H     | 35  | LYS  | 4.8  |
| 1   | D     | 33  | VAL  | 4.8  |
| 1   | G     | 39  | THR  | 4.8  |
| 1   | A     | 35  | LYS  | 4.8  |
| 1   | E     | 201 | THR  | 4.7  |
| 1   | F     | 72  | PHE  | 4.5  |
| 1   | F     | 39  | THR  | 4.3  |
| 1   | E     | 36  | THR  | 4.2  |
| 1   | B     | 33  | VAL  | 4.2  |
| 1   | D     | 37  | ILE  | 4.2  |
| 1   | A     | 199 | SER  | 4.2  |
| 1   | L     | 199 | SER  | 4.2  |
| 1   | F     | 110 | VAL  | 4.2  |
| 1   | D     | 199 | SER  | 4.1  |
| 1   | B     | 34  | THR  | 4.1  |
| 1   | F     | 34  | THR  | 4.1  |
| 1   | B     | 199 | SER  | 4.0  |
| 1   | I     | 199 | SER  | 4.0  |
| 1   | H     | 38  | GLU  | 4.0  |
| 1   | K     | 103 | VAL  | 4.0  |
| 1   | H     | 199 | SER  | 3.9  |
| 1   | E     | 199 | SER  | 3.8  |
| 1   | F     | 199 | SER  | 3.7  |
| 1   | A     | 33  | VAL  | 3.6  |
| 1   | E     | 72  | PHE  | 3.6  |
| 1   | A     | 37  | ILE  | 3.5  |
| 1   | B     | 38  | GLU  | 3.5  |
| 1   | A     | 72  | PHE  | 3.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 42  | ASP  | 3.4  |
| 1   | B     | 201 | THR  | 3.4  |
| 1   | D     | 36  | THR  | 3.4  |
| 1   | G     | 92  | LYS  | 3.4  |
| 1   | C     | 199 | SER  | 3.4  |
| 1   | B     | 37  | ILE  | 3.4  |
| 1   | A     | 32  | THR  | 3.4  |
| 1   | F     | 112 | VAL  | 3.4  |
| 1   | I     | 32  | THR  | 3.3  |
| 1   | G     | 199 | SER  | 3.2  |
| 1   | K     | 92  | LYS  | 3.2  |
| 1   | F     | 71  | SER  | 3.2  |
| 1   | K     | 190 | PHE  | 3.2  |
| 1   | F     | 37  | ILE  | 3.2  |
| 1   | D     | 38  | GLU  | 3.1  |
| 1   | B     | 36  | THR  | 3.1  |
| 1   | L     | 72  | PHE  | 3.1  |
| 1   | H     | 201 | THR  | 3.1  |
| 1   | L     | 110 | VAL  | 3.1  |
| 1   | I     | 69  | ASP  | 3.1  |
| 1   | L     | 92  | LYS  | 3.0  |
| 1   | C     | 92  | LYS  | 3.0  |
| 1   | K     | 181 | ILE  | 2.9  |
| 1   | F     | 201 | THR  | 2.9  |
| 1   | K     | 199 | SER  | 2.9  |
| 1   | E     | 34  | THR  | 2.8  |
| 1   | F     | 35  | LYS  | 2.8  |
| 1   | L     | 109 | GLU  | 2.8  |
| 1   | H     | 59  | GLU  | 2.8  |
| 1   | L     | 108 | LEU  | 2.8  |
| 1   | E     | 38  | GLU  | 2.7  |
| 1   | K     | 89  | ALA  | 2.7  |
| 1   | F     | 184 | THR  | 2.7  |
| 1   | K     | 33  | VAL  | 2.6  |
| 1   | K     | 201 | THR  | 2.6  |
| 1   | H     | 41  | THR  | 2.5  |
| 1   | H     | 39  | THR  | 2.5  |
| 1   | K     | 128 | THR  | 2.5  |
| 1   | G     | 128 | THR  | 2.4  |
| 1   | G     | 40  | HIS  | 2.4  |
| 1   | C     | 32  | THR  | 2.4  |
| 1   | E     | 73  | ASP  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 112 | VAL  | 2.4  |
| 1   | C     | 200 | GLY  | 2.4  |
| 1   | G     | 200 | GLY  | 2.4  |
| 1   | F     | 129 | SER  | 2.4  |
| 1   | G     | 201 | THR  | 2.4  |
| 1   | E     | 90  | GLN  | 2.3  |
| 1   | L     | 49  | ASP  | 2.3  |
| 1   | C     | 167 | GLU  | 2.3  |
| 1   | D     | 49  | ASP  | 2.3  |
| 1   | I     | 70  | VAL  | 2.3  |
| 1   | B     | 49  | ASP  | 2.3  |
| 1   | K     | 170 | THR  | 2.2  |
| 1   | I     | 68  | THR  | 2.2  |
| 1   | H     | 62  | SER  | 2.2  |
| 1   | L     | 61  | GLY  | 2.2  |
| 1   | F     | 111 | THR  | 2.2  |
| 1   | C     | 129 | SER  | 2.2  |
| 1   | G     | 42  | ASP  | 2.2  |
| 1   | G     | 49  | ASP  | 2.2  |
| 1   | K     | 63  | GLY  | 2.2  |
| 1   | F     | 49  | ASP  | 2.2  |
| 1   | A     | 79  | LYS  | 2.2  |
| 1   | I     | 92  | LYS  | 2.1  |
| 1   | E     | 71  | SER  | 2.1  |
| 1   | H     | 45  | GLU  | 2.1  |
| 1   | A     | 46  | THR  | 2.1  |
| 1   | H     | 49  | ASP  | 2.1  |
| 1   | C     | 162 | SER  | 2.1  |
| 1   | E     | 37  | ILE  | 2.1  |
| 1   | L     | 111 | THR  | 2.1  |
| 1   | D     | 92  | LYS  | 2.0  |
| 1   | K     | 116 | LEU  | 2.0  |
| 1   | H     | 56  | VAL  | 2.0  |
| 1   | K     | 61  | GLY  | 2.0  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.