



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:05 pm BST

PDB ID : 5BOZ  
Title : Ricin A chain bound to camelid nanobody (VHH9)(E1)  
Authors : Rudolph, M.J.; Mantis, N.  
Deposited on : 2015-05-27  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

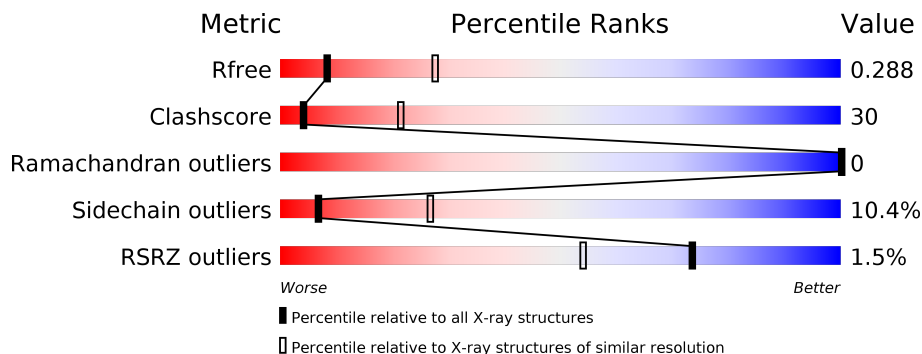
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1094 (3.10-3.10)                                      |
| Clashscore            | 141614                      | 1184 (3.10-3.10)                                      |
| Ramachandran outliers | 138981                      | 1141 (3.10-3.10)                                      |
| Sidechain outliers    | 138945                      | 1141 (3.10-3.10)                                      |
| RSRZ outliers         | 127900                      | 1067 (3.10-3.10)                                      |

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 261    |                  |
| 1   | B     | 261    |                  |
| 1   | C     | 261    |                  |
| 1   | D     | 261    |                  |
| 1   | E     | 261    |                  |
| 1   | F     | 261    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | G     | 127    |                  |
| 2   | H     | 127    |                  |
| 2   | I     | 127    |                  |
| 2   | J     | 127    |                  |
| 2   | K     | 127    |                  |
| 2   | L     | 127    |                  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | SO4  | A     | 301 | -         | -        | X       | -                |
| 3   | SO4  | B     | 301 | -         | -        | X       | -                |
| 3   | SO4  | B     | 304 | -         | -        | X       | -                |
| 3   | SO4  | C     | 301 | -         | -        | X       | -                |
| 3   | SO4  | F     | 301 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18136 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 Ricin.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
|     |       |          | Total         | C         | N        | O        | S      |         |         |       |
| 1   | A     | 259      | Total<br>2046 | C<br>1296 | N<br>362 | O<br>383 | S<br>5 | 0       | 0       | 0     |
| 1   | B     | 260      | Total<br>2052 | C<br>1299 | N<br>363 | O<br>385 | S<br>5 | 0       | 0       | 0     |
| 1   | C     | 259      | Total<br>2046 | C<br>1296 | N<br>362 | O<br>383 | S<br>5 | 0       | 0       | 0     |
| 1   | D     | 259      | Total<br>2046 | C<br>1296 | N<br>362 | O<br>383 | S<br>5 | 0       | 0       | 0     |
| 1   | E     | 259      | Total<br>2068 | C<br>1308 | N<br>370 | O<br>385 | S<br>5 | 0       | 2       | 0     |
| 1   | F     | 260      | Total<br>2052 | C<br>1299 | N<br>363 | O<br>385 | S<br>5 | 0       | 0       | 0     |

- Molecule 2 is a protein called VHH single chain antibody E1.

| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
|     |       |          | Total        | C        | N        | O        | S      |         |         |       |
| 2   | G     | 123      | Total<br>961 | C<br>601 | N<br>173 | O<br>182 | S<br>5 | 0       | 1       | 0     |
| 2   | H     | 125      | Total<br>973 | C<br>607 | N<br>176 | O<br>185 | S<br>5 | 0       | 1       | 0     |
| 2   | I     | 118      | Total<br>911 | C<br>572 | N<br>160 | O<br>174 | S<br>5 | 0       | 0       | 0     |
| 2   | J     | 119      | Total<br>918 | C<br>576 | N<br>161 | O<br>176 | S<br>5 | 0       | 0       | 0     |
| 2   | K     | 125      | Total<br>973 | C<br>607 | N<br>176 | O<br>185 | S<br>5 | 0       | 1       | 0     |
| 2   | L     | 123      | Total<br>961 | C<br>601 | N<br>173 | O<br>182 | S<br>5 | 0       | 1       | 0     |

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
|     |       |          | Total | O | S |         |         |
| 3   | A     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | A     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | G     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | B     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | B     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | B     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | B     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | B     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | C     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | C     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | C     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | I     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | D     | 1        | 5     | 4 | 1 | 0       | 0       |
| 3   | J     | 1        | 5     | 4 | 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 3   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | E     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | F     | 1        | Total O S<br>5 4 1 | 0       | 0       |
| 3   | L     | 1        | Total O S<br>5 4 1 | 0       | 0       |

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | D     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | K     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Cl<br>1 1 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms          | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 5   | G     | 3        | Total O<br>3 3 | 0       | 0       |
| 5   | B     | 1        | Total O<br>1 1 | 0       | 0       |
| 5   | H     | 1        | Total O<br>1 1 | 0       | 0       |
| 5   | C     | 4        | Total O<br>4 4 | 0       | 0       |
| 5   | I     | 1        | Total O<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total O<br>1 1 | 0       | 0       |
| 5   | E     | 5        | Total O<br>5 5 | 0       | 0       |
| 5   | K     | 6        | Total O<br>6 6 | 0       | 0       |

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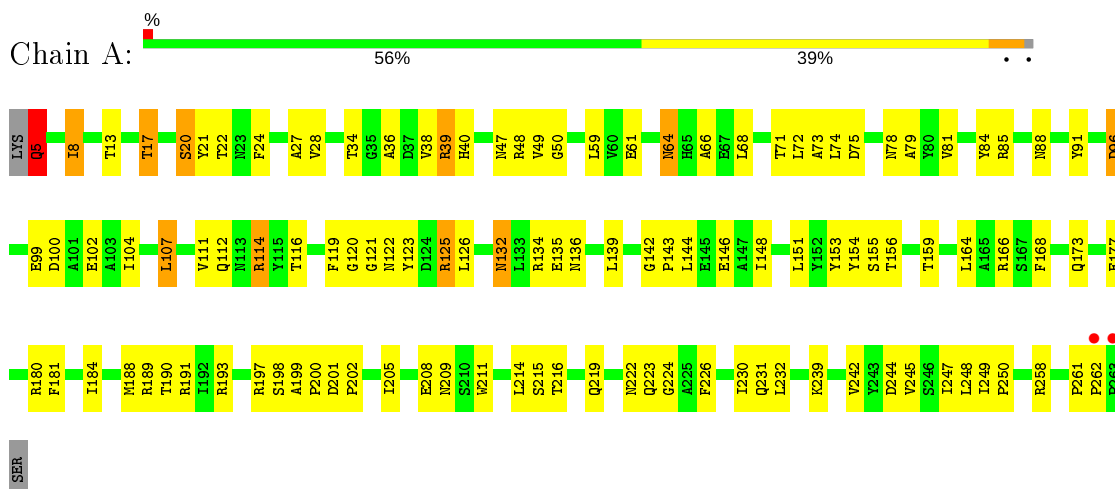
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| <b>Mol</b> | <b>Chain</b> | <b>Residues</b> | <b>Atoms</b>   | <b>ZeroOcc</b> | <b>AltConf</b> |
|------------|--------------|-----------------|----------------|----------------|----------------|
| 5          | F            | 2               | Total O<br>2 2 | 0              | 0              |
| 5          | L            | 2               | Total O<br>2 2 | 0              | 0              |

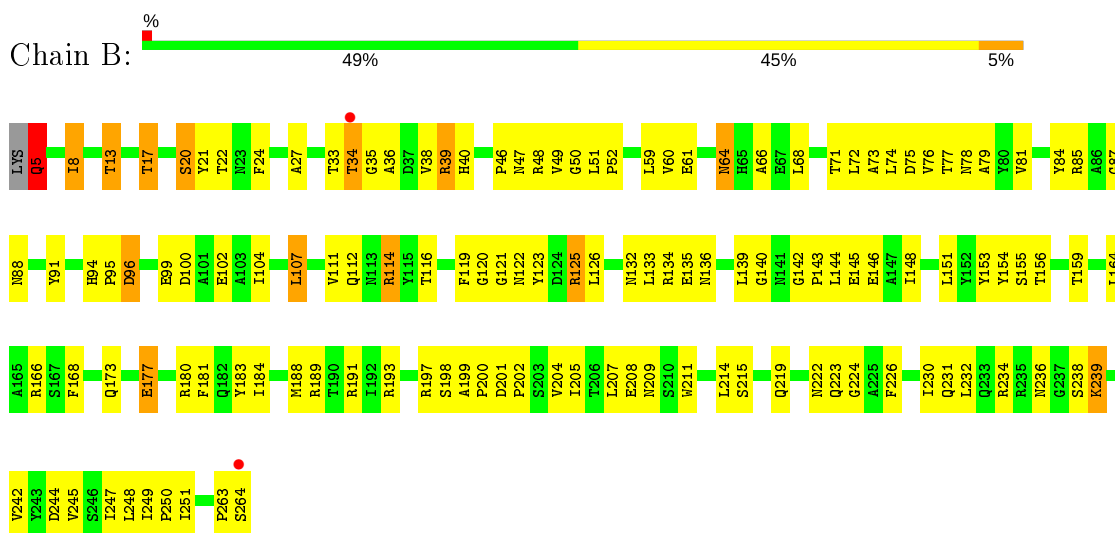
### 3 Residue-property plots [\(i\)](#)

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: Ricin



- Molecule 1: Ricin



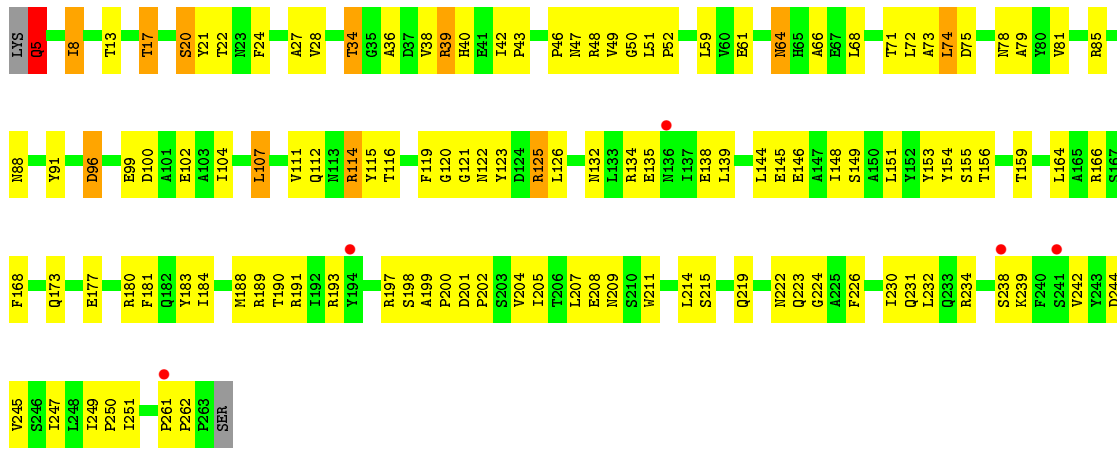
- Molecule 1: Ricin







• Molecule 1: Ricin



• Molecule 1: Ricin

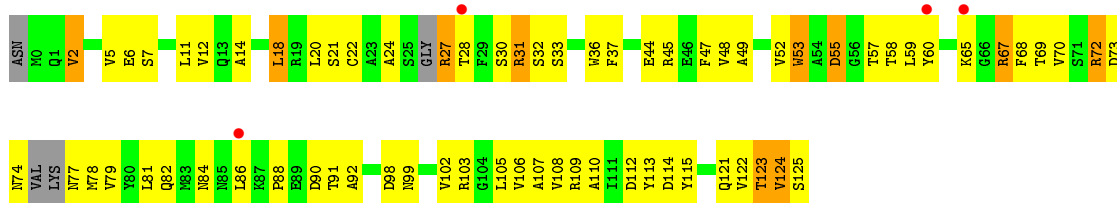
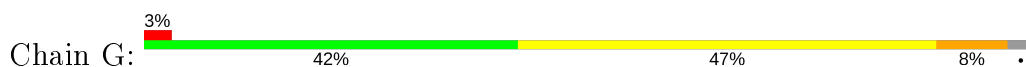


• Molecule 1: Ricin

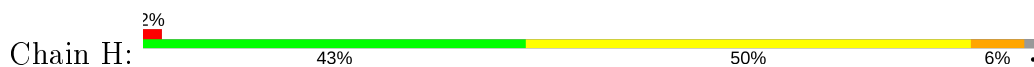




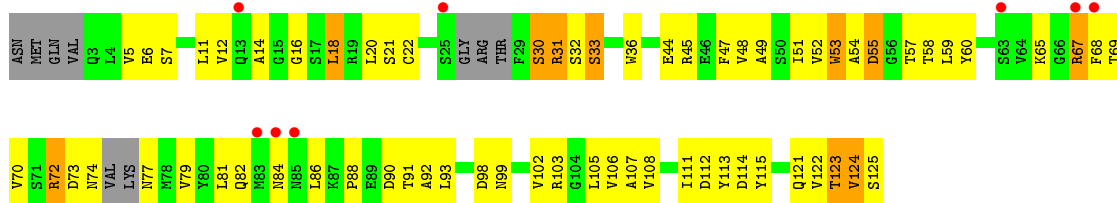
• Molecule 2: VHH single chain antibody E1



• Molecule 2: VHH single chain antibody E1

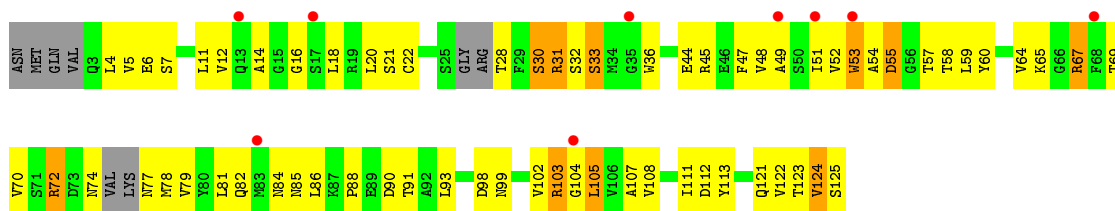


• Molecule 2: VHH single chain antibody E1



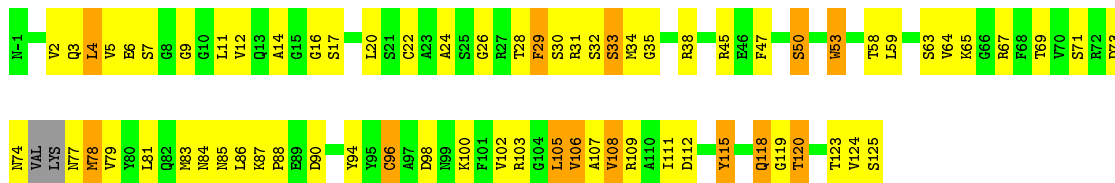
• Molecule 2: VHH single chain antibody E1





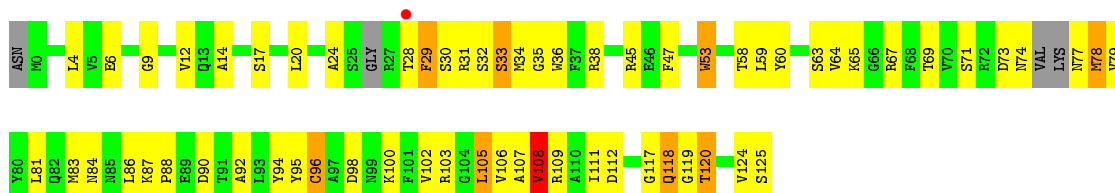
• Molecule 2: VHH single chain antibody E1

Chain K: 43% 45% 10%



• Molecule 2: VHH single chain antibody E1

Chain L: 47% 43% 6%



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | F 2 2 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 239.61Å 242.88Å 355.69Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 49.68 – 3.10<br>49.68 – 3.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (49.68-3.10)<br>99.8 (49.68-3.10)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.20  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.81 (at 3.12Å)   | Xtriage          |
| Refinement program  | PHENIX 1.7.1_743  | Depositor        |
| R, $R_{free}$   | 0.215 , 0.277<br>0.221 , 0.288                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4702 reflections (5.05%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 64.8  | Xtriage          |
| Anisotropy  | 0.664   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 97.9   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction   | 0.000 for -k,-h,-l  | Xtriage          |
| Reported twinning fraction  | 0.017 for -k,-h,-l  | Depositor        |
| Outliers  | 12 of 93146 reflections (0.013%)                            | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 18136   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 89.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6203e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.67         | 0/2091         | 0.83        | 1/2847 (0.0%)   |
| 1   | B     | 0.74         | 1/2097 (0.0%)  | 0.87        | 2/2855 (0.1%)   |
| 1   | C     | 0.70         | 2/2091 (0.1%)  | 0.83        | 1/2847 (0.0%)   |
| 1   | D     | 0.64         | 0/2091         | 0.81        | 1/2847 (0.0%)   |
| 1   | E     | 0.91         | 2/2113 (0.1%)  | 0.99        | 3/2875 (0.1%)   |
| 1   | F     | 0.80         | 0/2097         | 0.89        | 2/2855 (0.1%)   |
| 2   | G     | 0.68         | 0/977          | 0.87        | 0/1317          |
| 2   | H     | 0.74         | 0/990          | 0.93        | 0/1336          |
| 2   | I     | 0.61         | 0/927          | 0.83        | 0/1250          |
| 2   | J     | 0.61         | 0/934          | 0.80        | 0/1260          |
| 2   | K     | 1.16         | 1/990 (0.1%)   | 1.26        | 6/1336 (0.4%)   |
| 2   | L     | 0.90         | 0/977          | 1.09        | 4/1317 (0.3%)   |
| All | All   | 0.77         | 6/18375 (0.0%) | 0.91        | 20/24942 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 2                   |
| 1   | B     | 0                   | 2                   |
| 1   | C     | 0                   | 2                   |
| 1   | D     | 0                   | 2                   |
| 1   | E     | 0                   | 3                   |
| 1   | F     | 0                   | 3                   |
| 2   | H     | 0                   | 1                   |
| 2   | K     | 0                   | 1                   |
| 2   | L     | 0                   | 2                   |
| All | All   | 0                   | 18                  |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 64  | ASN  | CG-ND2 | -8.30 | 1.12        | 1.32     |
| 1   | E     | 64  | ASN  | CG-OD1 | -7.53 | 1.07        | 1.24     |
| 1   | C     | 64  | ASN  | CG-ND2 | -7.48 | 1.14        | 1.32     |
| 1   | C     | 64  | ASN  | CG-OD1 | -7.10 | 1.08        | 1.24     |
| 1   | B     | 177 | GLU  | CG-CD  | 5.76  | 1.60        | 1.51     |
| 2   | K     | 5   | VAL  | CA-CB  | -5.01 | 1.44        | 1.54     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2   | K     | 26  | GLY  | N-CA-C    | -10.52 | 86.79       | 113.10   |
| 2   | L     | 45  | ARG  | NE-CZ-NH2 | -9.31  | 115.65      | 120.30   |
| 2   | K     | 109 | ARG  | NE-CZ-NH1 | 8.04   | 124.32      | 120.30   |
| 2   | K     | 45  | ARG  | NE-CZ-NH2 | -7.78  | 116.41      | 120.30   |
| 1   | E     | 107 | LEU  | CA-CB-CG  | -6.86  | 99.53       | 115.30   |
| 1   | B     | 107 | LEU  | CA-CB-CG  | -6.50  | 100.36      | 115.30   |
| 1   | D     | 107 | LEU  | CA-CB-CG  | -6.18  | 101.09      | 115.30   |
| 1   | C     | 107 | LEU  | CA-CB-CG  | -6.00  | 101.50      | 115.30   |
| 1   | A     | 107 | LEU  | CA-CB-CG  | -6.00  | 101.51      | 115.30   |
| 1   | F     | 107 | LEU  | CA-CB-CG  | -5.71  | 102.17      | 115.30   |
| 2   | L     | 108 | VAL  | N-CA-CB   | -5.48  | 99.44       | 111.50   |
| 1   | E     | 107 | LEU  | C-N-CA    | -5.45  | 108.08      | 121.70   |
| 2   | K     | 4   | LEU  | CB-CG-CD2 | -5.21  | 102.14      | 111.00   |
| 2   | L     | 108 | VAL  | CB-CA-C   | -5.21  | 101.51      | 111.40   |
| 2   | K     | 109 | ARG  | NE-CZ-NH2 | -5.13  | 117.73      | 120.30   |
| 1   | B     | 107 | LEU  | C-N-CA    | -5.12  | 108.89      | 121.70   |
| 2   | K     | 108 | VAL  | N-CA-C    | 5.09   | 124.76      | 111.00   |
| 2   | L     | 117 | GLY  | N-CA-C    | -5.06  | 100.45      | 113.10   |
| 1   | E     | 109 | THR  | CA-CB-CG2 | -5.00  | 105.39      | 112.40   |
| 1   | F     | 107 | LEU  | C-N-CA    | -5.00  | 109.19      | 121.70   |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 36  | ALA  | Peptide |
| 1   | A     | 5   | GLN  | Peptide |
| 1   | B     | 36  | ALA  | Peptide |
| 1   | B     | 5   | GLN  | Peptide |
| 1   | C     | 36  | ALA  | Peptide |
| 1   | C     | 5   | GLN  | Peptide |

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| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | D     | 36  | ALA  | Peptide   |
| 1   | D     | 5   | GLN  | Peptide   |
| 1   | E     | 15  | GLY  | Peptide   |
| 1   | E     | 36  | ALA  | Peptide   |
| 1   | E     | 5   | GLN  | Peptide   |
| 1   | F     | 263 | PRO  | Peptide   |
| 1   | F     | 36  | ALA  | Peptide   |
| 1   | F     | 5   | GLN  | Peptide   |
| 2   | H     | 25  | SER  | Peptide   |
| 2   | K     | 53  | TRP  | Peptide   |
| 2   | L     | 108 | VAL  | Mainchain |
| 2   | L     | 53  | TRP  | Peptide   |

## 5.2 Too-close contacts [i](#)

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     | 2046  | 0        | 2014     | 98      | 1            |
| 1   | B     | 2052  | 0        | 2019     | 125     | 0            |
| 1   | C     | 2046  | 0        | 2014     | 108     | 0            |
| 1   | D     | 2046  | 0        | 2014     | 102     | 1            |
| 1   | E     | 2068  | 0        | 2038     | 143     | 0            |
| 1   | F     | 2052  | 0        | 2019     | 111     | 1            |
| 2   | G     | 961   | 0        | 930      | 73      | 1            |
| 2   | H     | 973   | 0        | 940      | 81      | 1            |
| 2   | I     | 911   | 0        | 876      | 69      | 0            |
| 2   | J     | 918   | 0        | 883      | 71      | 1            |
| 2   | K     | 973   | 0        | 940      | 66      | 0            |
| 2   | L     | 961   | 0        | 930      | 53      | 0            |
| 3   | A     | 10    | 0        | 0        | 3       | 0            |
| 3   | B     | 25    | 0        | 0        | 7       | 0            |
| 3   | C     | 15    | 0        | 0        | 3       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 3   | E     | 15    | 0        | 0        | 1       | 0            |
| 3   | F     | 10    | 0        | 0        | 4       | 0            |
| 3   | G     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 5     | 0        | 0        | 0       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | L     | 5     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 1       | 0            |
| 4   | E     | 1     | 0        | 0        | 1       | 0            |
| 4   | K     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 4     | 0        | 0        | 1       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 5     | 0        | 0        | 1       | 0            |
| 5   | F     | 2     | 0        | 0        | 1       | 0            |
| 5   | G     | 3     | 0        | 0        | 0       | 0            |
| 5   | H     | 1     | 0        | 0        | 0       | 0            |
| 5   | I     | 1     | 0        | 0        | 0       | 0            |
| 5   | K     | 6     | 0        | 0        | 0       | 0            |
| 5   | L     | 2     | 0        | 0        | 0       | 0            |
| All | All   | 18136 | 0        | 17617    | 1058    | 4            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1058) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:E:189:ARG:HH21   | 1:E:193[A]:ARG:NH2  | 1.20                     | 1.37              |
| 1:E:189:ARG:NH2    | 1:E:193[A]:ARG:HH22 | 1.45                     | 1.15              |
| 1:E:189:ARG:NH2    | 1:E:193[A]:ARG:NH2  | 2.00                     | 1.07              |
| 2:H:72[A]:ARG:HH11 | 2:H:72[A]:ARG:HG2   | 1.28                     | 0.99              |
| 2:G:88:PRO:HA      | 2:G:124:VAL:CG2     | 1.93                     | 0.99              |
| 1:C:197:ARG:NH1    | 2:I:30:SER:OG       | 1.96                     | 0.98              |
| 3:C:303:SO4:O1     | 1:D:115:TYR:OH      | 1.81                     | 0.98              |
| 1:E:104:ILE:HG22   | 1:E:114[B]:ARG:HH21 | 1.27                     | 0.96              |
| 1:E:49:VAL:HG23    | 1:E:50:GLY:H        | 1.31                     | 0.96              |
| 2:J:88:PRO:HA      | 2:J:124:VAL:CG2     | 1.96                     | 0.94              |
| 2:K:88:PRO:HA      | 2:K:124:VAL:CG2     | 1.98                     | 0.94              |
| 2:H:88:PRO:HA      | 2:H:124:VAL:CG2     | 1.97                     | 0.94              |
| 2:G:44:GLU:HG3     | 2:G:45:ARG:H        | 1.33                     | 0.92              |
| 1:A:197:ARG:NH1    | 2:G:30:SER:OG       | 2.03                     | 0.91              |
| 2:K:38:ARG:HH12    | 2:K:90:ASP:HA       | 1.35                     | 0.91              |
| 2:L:38:ARG:HH12    | 2:L:90:ASP:HA       | 1.37                     | 0.89              |
| 1:E:189:ARG:HH21   | 1:E:193[A]:ARG:HH22 | 0.92                     | 0.89              |
| 2:K:9:GLY:H        | 2:K:120:THR:HG21    | 1.38                     | 0.88              |
| 1:B:125:ARG:NH2    | 3:B:305:SO4:O1      | 2.07                     | 0.87              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:K:105:LEU:H    | 2:K:105:LEU:HD12    | 1.39                     | 0.87              |
| 1:E:104:ILE:CG2  | 1:E:114[B]:ARG:HH21 | 1.88                     | 0.87              |
| 2:L:88:PRO:HA    | 2:L:124:VAL:CG2     | 2.04                     | 0.87              |
| 2:I:88:PRO:HA    | 2:I:124:VAL:CG2     | 2.05                     | 0.87              |
| 1:B:49:VAL:HG23  | 1:B:50:GLY:H        | 1.39                     | 0.87              |
| 2:I:108:VAL:HG12 | 2:I:108:VAL:O       | 1.73                     | 0.87              |
| 1:F:39:ARG:HH11  | 1:F:39:ARG:HG2      | 1.37                     | 0.86              |
| 2:L:9:GLY:H      | 2:L:120:THR:HG21    | 1.39                     | 0.86              |
| 2:K:108:VAL:HG12 | 2:K:108:VAL:O       | 1.73                     | 0.86              |
| 2:J:108:VAL:O    | 2:J:108:VAL:HG12    | 1.75                     | 0.86              |
| 2:G:108:VAL:HG12 | 2:G:108:VAL:O       | 1.76                     | 0.85              |
| 2:H:108:VAL:HG12 | 2:H:108:VAL:O       | 1.75                     | 0.85              |
| 1:E:191:ARG:NH1  | 1:E:198:SER:O       | 2.10                     | 0.85              |
| 1:B:39:ARG:HG2   | 1:B:39:ARG:HH11     | 1.40                     | 0.84              |
| 1:E:49:VAL:HG23  | 1:E:50:GLY:N        | 1.88                     | 0.84              |
| 1:C:54:ASN:ND2   | 5:C:401:HOH:O       | 2.07                     | 0.84              |
| 1:A:49:VAL:HG23  | 1:A:50:GLY:H        | 1.43                     | 0.84              |
| 2:G:44:GLU:HG3   | 2:G:45:ARG:N        | 1.91                     | 0.84              |
| 2:G:88:PRO:HA    | 2:G:124:VAL:HG21    | 1.59                     | 0.84              |
| 1:B:193:ARG:NH1  | 3:B:304:SO4:O2      | 2.10                     | 0.83              |
| 1:C:8:ILE:HG22   | 1:C:59:LEU:HB2      | 1.59                     | 0.83              |
| 2:I:47:PHE:CG    | 2:I:108:VAL:HG13    | 2.15                     | 0.82              |
| 1:E:39:ARG:HG2   | 1:E:39:ARG:HH11     | 1.44                     | 0.82              |
| 2:K:58:THR:O     | 2:K:59:LEU:HD23     | 1.80                     | 0.82              |
| 1:B:191:ARG:NH1  | 1:B:198:SER:O       | 2.12                     | 0.81              |
| 2:H:88:PRO:HA    | 2:H:124:VAL:HG21    | 1.64                     | 0.80              |
| 1:E:125:ARG:NH2  | 3:E:303:SO4:O2      | 2.14                     | 0.80              |
| 2:G:88:PRO:HA    | 2:G:124:VAL:HG23    | 1.63                     | 0.80              |
| 1:D:197:ARG:NH1  | 2:J:30:SER:OG       | 2.13                     | 0.80              |
| 2:L:108:VAL:O    | 2:L:108:VAL:HG12    | 1.79                     | 0.80              |
| 1:E:96:ASP:OD1   | 1:E:96:ASP:N        | 2.15                     | 0.80              |
| 2:J:47:PHE:CG    | 2:J:108:VAL:HG13    | 2.17                     | 0.79              |
| 1:D:39:ARG:HG2   | 1:D:39:ARG:HH11     | 1.45                     | 0.79              |
| 1:B:197:ARG:NH1  | 2:H:30:SER:OG       | 2.14                     | 0.79              |
| 2:J:88:PRO:HA    | 2:J:124:VAL:HG21    | 1.64                     | 0.79              |
| 1:A:8:ILE:HG22   | 1:A:59:LEU:HB2      | 1.64                     | 0.79              |
| 1:B:173:GLN:NE2  | 1:B:208:GLU:OE2     | 2.15                     | 0.78              |
| 2:I:44:GLU:HG3   | 2:I:45:ARG:H        | 1.48                     | 0.78              |
| 2:J:44:GLU:HG3   | 2:J:45:ARG:H        | 1.49                     | 0.78              |
| 1:A:191:ARG:NH1  | 1:A:198:SER:O       | 2.17                     | 0.78              |
| 2:I:44:GLU:HG3   | 2:I:45:ARG:N        | 1.98                     | 0.78              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:88:PRO:HA    | 2:J:124:VAL:HG23 | 1.64                     | 0.78              |
| 1:A:5:GLN:HA     | 1:A:5:GLN:OE1    | 1.82                     | 0.77              |
| 1:B:159:THR:HG22 | 2:H:115:TYR:CE1  | 2.19                     | 0.77              |
| 1:D:191:ARG:NH1  | 1:D:198:SER:O    | 2.18                     | 0.77              |
| 1:B:193:ARG:NH1  | 3:B:304:SO4:S    | 2.55                     | 0.77              |
| 1:F:49:VAL:HG23  | 1:F:50:GLY:H     | 1.48                     | 0.77              |
| 1:A:39:ARG:HG2   | 1:A:39:ARG:HH11  | 1.46                     | 0.77              |
| 2:I:58:THR:O     | 2:I:59:LEU:HD23  | 1.85                     | 0.77              |
| 2:H:67:ARG:NH2   | 2:H:90:ASP:OD2   | 2.16                     | 0.77              |
| 1:F:96:ASP:OD1   | 1:F:96:ASP:N     | 2.16                     | 0.77              |
| 2:J:47:PHE:CD1   | 2:J:108:VAL:HG13 | 2.19                     | 0.77              |
| 1:C:49:VAL:HG23  | 1:C:50:GLY:H     | 1.50                     | 0.76              |
| 2:J:74:ASN:HB2   | 2:J:77:ASN:HB3   | 1.66                     | 0.76              |
| 1:A:49:VAL:HG23  | 1:A:50:GLY:N     | 1.99                     | 0.76              |
| 2:G:58:THR:O     | 2:G:59:LEU:HD23  | 1.83                     | 0.76              |
| 2:G:52:VAL:HG12  | 2:G:53:TRP:O     | 1.85                     | 0.76              |
| 2:H:44:GLU:HG3   | 2:H:45:ARG:N     | 2.01                     | 0.76              |
| 2:H:58:THR:O     | 2:H:59:LEU:HD23  | 1.86                     | 0.76              |
| 2:J:44:GLU:HG3   | 2:J:45:ARG:N     | 1.99                     | 0.76              |
| 1:B:49:VAL:HG23  | 1:B:50:GLY:N     | 1.96                     | 0.76              |
| 1:D:49:VAL:HG23  | 1:D:50:GLY:H     | 1.49                     | 0.76              |
| 1:F:8:ILE:HG22   | 1:F:59:LEU:HB2   | 1.66                     | 0.76              |
| 1:C:39:ARG:HG2   | 1:C:39:ARG:HH11  | 1.50                     | 0.75              |
| 1:D:5:GLN:OE1    | 1:D:5:GLN:HA     | 1.85                     | 0.75              |
| 1:F:125:ARG:NH1  | 3:F:301:SO4:O4   | 2.18                     | 0.75              |
| 2:G:67:ARG:NH2   | 2:G:90:ASP:OD2   | 2.19                     | 0.74              |
| 2:I:31:ARG:HG2   | 2:I:98:ASP:OD1   | 1.88                     | 0.74              |
| 1:A:120:GLY:N    | 3:A:301:SO4:O4   | 2.20                     | 0.74              |
| 2:I:47:PHE:CD1   | 2:I:108:VAL:HG13 | 2.22                     | 0.74              |
| 1:D:242:VAL:HG13 | 1:D:247:ILE:HD11 | 1.69                     | 0.74              |
| 2:H:88:PRO:HA    | 2:H:124:VAL:HG23 | 1.68                     | 0.74              |
| 2:I:67:ARG:NH2   | 2:I:90:ASP:OD2   | 2.20                     | 0.74              |
| 2:K:4:LEU:CD2    | 2:K:24:ALA:HB2   | 2.18                     | 0.74              |
| 2:K:98:ASP:OD2   | 2:K:100:LYS:NZ   | 2.20                     | 0.74              |
| 1:A:75:ASP:HB3   | 1:A:78:ASN:CB    | 2.18                     | 0.73              |
| 1:D:49:VAL:HG23  | 1:D:50:GLY:N     | 2.03                     | 0.73              |
| 2:L:83:MET:HB3   | 2:L:86:LEU:HD21  | 1.70                     | 0.73              |
| 1:B:5:GLN:HA     | 1:B:5:GLN:OE1    | 1.89                     | 0.73              |
| 2:K:88:PRO:HA    | 2:K:124:VAL:HG22 | 1.68                     | 0.73              |
| 1:C:5:GLN:HA     | 1:C:5:GLN:OE1    | 1.89                     | 0.73              |
| 2:L:58:THR:O     | 2:L:59:LEU:HD23  | 1.88                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:91:THR:HG23  | 2:H:123:THR:HG22 | 1.70                     | 0.73              |
| 2:I:74:ASN:HB2   | 2:I:77:ASN:HB3   | 1.70                     | 0.73              |
| 2:G:74:ASN:HB2   | 2:G:77:ASN:HB3   | 1.70                     | 0.73              |
| 2:L:105:LEU:HD12 | 2:L:105:LEU:H    | 1.53                     | 0.73              |
| 2:J:67:ARG:NH2   | 2:J:90:ASP:OD2   | 2.21                     | 0.72              |
| 1:A:242:VAL:HG13 | 1:A:247:ILE:HD11 | 1.72                     | 0.72              |
| 1:F:104:ILE:HG22 | 1:F:114:ARG:HH21 | 1.54                     | 0.72              |
| 2:H:52:VAL:HG12  | 2:H:53:TRP:O     | 1.90                     | 0.72              |
| 2:L:88:PRO:HA    | 2:L:124:VAL:HG22 | 1.72                     | 0.72              |
| 2:K:83:MET:HB3   | 2:K:86:LEU:HD21  | 1.71                     | 0.72              |
| 1:E:75:ASP:HB3   | 1:E:78:ASN:CB    | 2.21                     | 0.71              |
| 2:I:88:PRO:HA    | 2:I:124:VAL:HG23 | 1.72                     | 0.71              |
| 2:J:52:VAL:HG12  | 2:J:53:TRP:O     | 1.90                     | 0.71              |
| 1:A:17:THR:HB    | 1:A:20:SER:H     | 1.55                     | 0.71              |
| 2:H:20:LEU:HD12  | 2:H:81:LEU:HD23  | 1.71                     | 0.71              |
| 1:E:72:LEU:HD12  | 1:E:72:LEU:N     | 2.04                     | 0.70              |
| 2:G:31:ARG:HG2   | 2:G:98:ASP:OD1   | 1.90                     | 0.70              |
| 2:J:58:THR:O     | 2:J:59:LEU:HD23  | 1.91                     | 0.70              |
| 2:L:6:GLU:OE1    | 2:L:118:GLN:O    | 2.09                     | 0.70              |
| 1:F:191:ARG:NH1  | 1:F:198:SER:O    | 2.24                     | 0.70              |
| 1:E:135:GLU:CD   | 1:E:135:GLU:H    | 1.94                     | 0.70              |
| 1:F:75:ASP:HB3   | 1:F:78:ASN:CB    | 2.21                     | 0.70              |
| 2:H:44:GLU:HG3   | 2:H:45:ARG:H     | 1.54                     | 0.70              |
| 2:G:47:PHE:CD1   | 2:G:108:VAL:HG13 | 2.26                     | 0.70              |
| 1:C:191:ARG:NH1  | 1:C:198:SER:O    | 2.24                     | 0.70              |
| 1:F:17:THR:HB    | 1:F:20:SER:H     | 1.57                     | 0.70              |
| 1:D:135:GLU:CD   | 1:D:135:GLU:H    | 1.95                     | 0.70              |
| 1:B:75:ASP:HB3   | 1:B:78:ASN:CB    | 2.23                     | 0.69              |
| 2:J:31:ARG:HG2   | 2:J:98:ASP:OD1   | 1.92                     | 0.69              |
| 1:D:8:ILE:HG22   | 1:D:59:LEU:HB2   | 1.74                     | 0.69              |
| 1:A:135:GLU:CD   | 1:A:135:GLU:H    | 1.95                     | 0.69              |
| 2:I:91:THR:HG23  | 2:I:123:THR:HG22 | 1.74                     | 0.69              |
| 1:D:17:THR:HB    | 1:D:20:SER:H     | 1.58                     | 0.69              |
| 2:G:47:PHE:CG    | 2:G:108:VAL:HG13 | 2.28                     | 0.69              |
| 1:F:242:VAL:HG13 | 1:F:247:ILE:HD11 | 1.75                     | 0.69              |
| 2:H:74:ASN:HB2   | 2:H:77:ASN:HB3   | 1.75                     | 0.69              |
| 1:D:119:PHE:HB2  | 1:D:125:ARG:HD2  | 1.75                     | 0.69              |
| 1:F:49:VAL:HG23  | 1:F:50:GLY:N     | 2.07                     | 0.69              |
| 2:G:20:LEU:HD12  | 2:G:81:LEU:HD23  | 1.74                     | 0.69              |
| 2:L:4:LEU:CD2    | 2:L:24:ALA:HB2   | 2.23                     | 0.69              |
| 1:B:17:THR:HB    | 1:B:20:SER:H     | 1.58                     | 0.69              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:E:119:PHE:HB2  | 1:E:125:ARG:HD2    | 1.75                     | 0.69              |
| 1:C:135:GLU:CD   | 1:C:135:GLU:H      | 1.96                     | 0.68              |
| 2:I:88:PRO:HA    | 2:I:124:VAL:HG21   | 1.75                     | 0.68              |
| 2:K:105:LEU:H    | 2:K:105:LEU:CD1    | 2.06                     | 0.68              |
| 1:D:75:ASP:HB3   | 1:D:78:ASN:CB      | 2.23                     | 0.68              |
| 1:B:8:ILE:HG22   | 1:B:59:LEU:HB2     | 1.75                     | 0.68              |
| 2:I:52:VAL:HG12  | 2:I:53:TRP:O       | 1.94                     | 0.68              |
| 1:B:75:ASP:HB3   | 1:B:78:ASN:HB3     | 1.76                     | 0.68              |
| 1:D:222:ASN:C    | 1:D:223:GLN:HG2    | 2.14                     | 0.68              |
| 2:J:91:THR:HG23  | 2:J:123:THR:HG22   | 1.74                     | 0.68              |
| 2:J:53:TRP:CZ3   | 2:J:72:ARG:HB2     | 2.29                     | 0.68              |
| 1:A:96:ASP:N     | 1:A:96:ASP:OD1     | 2.26                     | 0.68              |
| 1:E:242:VAL:HG13 | 1:E:247:ILE:HD11   | 1.76                     | 0.68              |
| 1:F:135:GLU:CD   | 1:F:135:GLU:H      | 1.97                     | 0.68              |
| 1:C:49:VAL:HG23  | 1:C:50:GLY:N       | 2.07                     | 0.68              |
| 1:A:224:GLY:O    | 1:A:245:VAL:HG23   | 1.94                     | 0.67              |
| 1:B:231:GLN:O    | 1:B:232:LEU:HD23   | 1.93                     | 0.67              |
| 2:L:12:VAL:O     | 2:L:124:VAL:HA     | 1.94                     | 0.67              |
| 1:E:104:ILE:CG2  | 1:E:114[B]:ARG:NH2 | 2.57                     | 0.67              |
| 1:F:119:PHE:HB2  | 1:F:125:ARG:HD2    | 1.77                     | 0.67              |
| 1:E:173:GLN:NE2  | 1:E:208:GLU:OE2    | 2.22                     | 0.67              |
| 2:L:47:PHE:CG    | 2:L:108:VAL:HG13   | 2.30                     | 0.67              |
| 1:A:75:ASP:HB3   | 1:A:78:ASN:HB3     | 1.76                     | 0.67              |
| 2:I:20:LEU:HD12  | 2:I:81:LEU:HD23    | 1.76                     | 0.67              |
| 1:B:125:ARG:NH1  | 3:B:301:SO4:O1     | 2.27                     | 0.67              |
| 1:F:173:GLN:NE2  | 1:F:208:GLU:OE2    | 2.23                     | 0.67              |
| 1:B:119:PHE:HB2  | 1:B:125:ARG:HD2    | 1.76                     | 0.67              |
| 1:F:75:ASP:HB3   | 1:F:78:ASN:HB3     | 1.77                     | 0.67              |
| 2:K:88:PRO:CA    | 2:K:124:VAL:CG2    | 2.73                     | 0.67              |
| 1:E:49:VAL:CG2   | 1:E:50:GLY:H       | 2.07                     | 0.66              |
| 2:K:67:ARG:NH2   | 2:K:90:ASP:OD2     | 2.27                     | 0.66              |
| 1:A:125:ARG:NH1  | 3:A:301:SO4:O2     | 2.28                     | 0.66              |
| 1:C:222:ASN:C    | 1:C:223:GLN:HG2    | 2.15                     | 0.66              |
| 1:F:125:ARG:NH2  | 3:F:302:SO4:O2     | 2.28                     | 0.66              |
| 2:H:122:VAL:O    | 2:H:123:THR:HG23   | 1.96                     | 0.66              |
| 2:I:123:THR:O    | 2:I:124:VAL:HG13   | 1.95                     | 0.66              |
| 1:B:88:ASN:O     | 1:B:111:VAL:HG13   | 1.95                     | 0.66              |
| 2:K:6:GLU:OE1    | 2:K:118:GLN:O      | 2.14                     | 0.66              |
| 1:F:222:ASN:C    | 1:F:223:GLN:HG2    | 2.16                     | 0.66              |
| 1:B:244:ASP:OD1  | 1:C:244:ASP:OD1    | 2.13                     | 0.66              |
| 1:B:224:GLY:O    | 1:B:245:VAL:HG23   | 1.95                     | 0.66              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:D:72:LEU:N     | 1:D:72:LEU:HD12    | 2.10                     | 0.66              |
| 1:A:119:PHE:HB2  | 1:A:125:ARG:HD2    | 1.78                     | 0.66              |
| 1:C:96:ASP:N     | 1:C:96:ASP:OD1     | 2.22                     | 0.66              |
| 2:H:47:PHE:CG    | 2:H:108:VAL:HG13   | 2.32                     | 0.65              |
| 2:H:11:LEU:HD12  | 2:H:12:VAL:N       | 2.12                     | 0.65              |
| 2:I:53:TRP:CZ3   | 2:I:72:ARG:HB2     | 2.31                     | 0.65              |
| 1:C:75:ASP:HB3   | 1:C:78:ASN:CB      | 2.26                     | 0.65              |
| 2:L:31:ARG:O     | 2:L:32:SER:HB3     | 1.96                     | 0.65              |
| 1:D:231:GLN:O    | 1:D:232:LEU:HD23   | 1.95                     | 0.65              |
| 1:B:193:ARG:NH1  | 3:B:304:SO4:O1     | 2.30                     | 0.65              |
| 2:L:67:ARG:NH2   | 2:L:90:ASP:OD2     | 2.30                     | 0.65              |
| 1:B:135:GLU:CD   | 1:B:135:GLU:H      | 2.00                     | 0.65              |
| 1:C:242:VAL:HG13 | 1:C:247:ILE:HD11   | 1.79                     | 0.65              |
| 1:D:249:ILE:N    | 1:D:250:PRO:HD2    | 2.11                     | 0.65              |
| 1:A:231:GLN:O    | 1:A:232:LEU:HD23   | 1.97                     | 0.65              |
| 1:C:249:ILE:N    | 1:C:250:PRO:HD2    | 2.12                     | 0.65              |
| 1:E:17:THR:HB    | 1:E:20:SER:H       | 1.61                     | 0.65              |
| 2:G:53:TRP:CZ3   | 2:G:72:ARG:HB2     | 2.31                     | 0.65              |
| 2:G:14:ALA:HB2   | 2:G:125:SER:HB3    | 1.79                     | 0.64              |
| 2:H:31:ARG:HG2   | 2:H:98:ASP:OD1     | 1.97                     | 0.64              |
| 2:I:55:ASP:OD1   | 2:I:57:THR:N       | 2.30                     | 0.64              |
| 1:F:74:LEU:HD11  | 1:F:81:VAL:HG22    | 1.79                     | 0.64              |
| 2:L:73:ASP:O     | 2:L:77:ASN:HB3     | 1.96                     | 0.64              |
| 1:A:173:GLN:NE2  | 1:A:208:GLU:OE2    | 2.26                     | 0.64              |
| 1:A:72:LEU:N     | 1:A:72:LEU:HD12    | 2.12                     | 0.64              |
| 1:C:231:GLN:O    | 1:C:232:LEU:HD23   | 1.98                     | 0.64              |
| 2:J:53:TRP:CH2   | 2:J:72:ARG:HB2     | 2.32                     | 0.64              |
| 1:E:222:ASN:C    | 1:E:223:GLN:HG2    | 2.17                     | 0.64              |
| 1:D:75:ASP:HB3   | 1:D:78:ASN:HB3     | 1.80                     | 0.64              |
| 2:L:14:ALA:HB2   | 2:L:125:SER:HB3    | 1.80                     | 0.64              |
| 1:B:222:ASN:C    | 1:B:223:GLN:HG2    | 2.18                     | 0.64              |
| 1:D:104:ILE:HG22 | 1:D:114:ARG:HH21   | 1.63                     | 0.64              |
| 1:D:74:LEU:HD11  | 1:D:81:VAL:HG22    | 1.80                     | 0.64              |
| 1:B:96:ASP:OD1   | 1:B:96:ASP:N       | 2.25                     | 0.63              |
| 1:E:190:THR:HG22 | 1:E:193[A]:ARG:NH1 | 2.12                     | 0.63              |
| 1:E:22:THR:OG1   | 1:E:189:ARG:HD2    | 1.98                     | 0.63              |
| 1:E:75:ASP:HB3   | 1:E:78:ASN:HB3     | 1.80                     | 0.63              |
| 1:E:249:ILE:N    | 1:E:250:PRO:HD2    | 2.13                     | 0.63              |
| 2:K:108:VAL:CG1  | 2:K:108:VAL:O      | 2.46                     | 0.63              |
| 2:I:53:TRP:CH2   | 2:I:72:ARG:HB2     | 2.33                     | 0.63              |
| 2:K:14:ALA:HB2   | 2:K:125:SER:HB3    | 1.81                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:242:VAL:HG13    | 1:B:247:ILE:HD11    | 1.80                     | 0.63              |
| 1:C:17:THR:HB       | 1:C:20:SER:H        | 1.64                     | 0.63              |
| 1:C:119:PHE:HB2     | 1:C:125:ARG:HD2     | 1.81                     | 0.63              |
| 1:A:249:ILE:N       | 1:A:250:PRO:HD2     | 2.14                     | 0.63              |
| 1:C:224:GLY:O       | 1:C:245:VAL:HG23    | 1.99                     | 0.63              |
| 1:E:39:ARG:CG       | 1:E:39:ARG:HH11     | 2.12                     | 0.63              |
| 2:G:91:THR:HG23     | 2:G:123:THR:HG22    | 1.80                     | 0.63              |
| 2:H:55:ASP:OD1      | 2:H:57:THR:N        | 2.32                     | 0.63              |
| 1:B:249:ILE:N       | 1:B:250:PRO:HD2     | 2.13                     | 0.63              |
| 1:E:189:ARG:HH21    | 1:E:193[A]:ARG:HH21 | 1.39                     | 0.62              |
| 2:H:47:PHE:CD1      | 2:H:108:VAL:HG13    | 2.33                     | 0.62              |
| 2:K:20:LEU:HB2      | 2:K:81:LEU:HB3      | 1.81                     | 0.62              |
| 1:E:119:PHE:HB2     | 1:E:125:ARG:CD      | 2.28                     | 0.62              |
| 2:K:31:ARG:O        | 2:K:32:SER:HB3      | 2.00                     | 0.62              |
| 1:C:173:GLN:NE2     | 1:C:208:GLU:OE2     | 2.28                     | 0.62              |
| 1:C:215:SER:O       | 1:C:219:GLN:HG3     | 2.00                     | 0.62              |
| 1:E:49:VAL:CG2      | 1:E:50:GLY:N        | 2.61                     | 0.62              |
| 2:G:103[A]:ARG:HH12 | 2:G:106:VAL:HG21    | 1.64                     | 0.62              |
| 2:H:103:ARG:NH2     | 2:H:106:VAL:HG21    | 2.15                     | 0.62              |
| 2:H:72[A]:ARG:HG2   | 2:H:72[A]:ARG:NH1   | 2.06                     | 0.62              |
| 2:J:12:VAL:O        | 2:J:124:VAL:HA      | 1.99                     | 0.62              |
| 1:A:181:PHE:CZ      | 1:A:211:TRP:HD1     | 2.18                     | 0.62              |
| 1:A:222:ASN:C       | 1:A:223:GLN:HG2     | 2.18                     | 0.62              |
| 1:C:104:ILE:HG22    | 1:C:114:ARG:HH21    | 1.64                     | 0.62              |
| 2:J:20:LEU:HD12     | 2:J:81:LEU:HD23     | 1.79                     | 0.62              |
| 1:D:224:GLY:O       | 1:D:245:VAL:HG23    | 2.00                     | 0.62              |
| 1:F:249:ILE:N       | 1:F:250:PRO:HD2     | 2.15                     | 0.62              |
| 2:J:11:LEU:HD12     | 2:J:12:VAL:N        | 2.15                     | 0.62              |
| 1:F:231:GLN:O       | 1:F:232:LEU:HD23    | 1.98                     | 0.61              |
| 1:B:74:LEU:HD11     | 1:B:81:VAL:HG22     | 1.80                     | 0.61              |
| 1:F:72:LEU:N        | 1:F:72:LEU:HD12     | 2.14                     | 0.61              |
| 1:B:263:PRO:O       | 1:B:264:SER:HB3     | 1.99                     | 0.61              |
| 1:E:189:ARG:CZ      | 1:E:193[A]:ARG:HH22 | 2.13                     | 0.61              |
| 2:J:55:ASP:OD1      | 2:J:57:THR:N        | 2.34                     | 0.61              |
| 1:A:75:ASP:HB3      | 1:A:78:ASN:HB2      | 1.82                     | 0.61              |
| 1:B:119:PHE:HB2     | 1:B:125:ARG:CD      | 2.30                     | 0.61              |
| 1:D:119:PHE:HB2     | 1:D:125:ARG:CD      | 2.30                     | 0.61              |
| 1:E:75:ASP:HB3      | 1:E:78:ASN:HB2      | 1.81                     | 0.61              |
| 2:H:12:VAL:O        | 2:H:124:VAL:HA      | 2.00                     | 0.61              |
| 1:C:121:GLY:HA2     | 1:C:126:LEU:HD11    | 1.83                     | 0.61              |
| 1:E:231:GLN:O       | 1:E:232:LEU:HD23    | 2.01                     | 0.61              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:F:39:ARG:NH1   | 1:F:39:ARG:HG2     | 2.11                     | 0.61              |
| 1:B:72:LEU:N     | 1:B:72:LEU:HD12    | 2.16                     | 0.61              |
| 1:E:190:THR:HA   | 1:E:193[B]:ARG:HB3 | 1.83                     | 0.61              |
| 2:I:49:ALA:HB1   | 2:I:70:VAL:HG21    | 1.83                     | 0.61              |
| 1:E:18:VAL:HG21  | 1:E:193[B]:ARG:HE  | 1.66                     | 0.61              |
| 1:E:224:GLY:O    | 1:E:245:VAL:HG23   | 2.01                     | 0.61              |
| 1:E:8:ILE:HG22   | 1:E:59:LEU:HB2     | 1.83                     | 0.61              |
| 2:G:123:THR:O    | 2:G:124:VAL:HG13   | 2.01                     | 0.61              |
| 2:G:12:VAL:O     | 2:G:124:VAL:HA     | 2.01                     | 0.61              |
| 2:J:14:ALA:HB2   | 2:J:125:SER:HB3    | 1.83                     | 0.61              |
| 2:L:17:SER:HB3   | 2:L:84:ASN:OD1     | 2.01                     | 0.60              |
| 2:H:103:ARG:NH1  | 2:H:103:ARG:HB3    | 2.17                     | 0.60              |
| 2:J:49:ALA:HB1   | 2:J:70:VAL:HG21    | 1.84                     | 0.60              |
| 1:B:49:VAL:CG2   | 1:B:50:GLY:H       | 2.11                     | 0.60              |
| 1:E:247:ILE:HD13 | 1:F:223:GLN:NE2    | 2.16                     | 0.60              |
| 2:G:49:ALA:HB1   | 2:G:70:VAL:HG21    | 1.84                     | 0.60              |
| 2:K:12:VAL:O     | 2:K:124:VAL:HA     | 2.01                     | 0.60              |
| 2:I:11:LEU:HD12  | 2:I:12:VAL:N       | 2.16                     | 0.60              |
| 1:B:214:LEU:HD21 | 1:B:230:ILE:HG21   | 1.84                     | 0.60              |
| 2:L:98:ASP:OD2   | 2:L:100:LYS:NZ     | 2.35                     | 0.60              |
| 2:K:29:PHE:N     | 2:K:29:PHE:CD1     | 2.70                     | 0.60              |
| 1:C:75:ASP:HB3   | 1:C:78:ASN:HB3     | 1.84                     | 0.60              |
| 1:B:189:ARG:NH2  | 3:B:304:SO4:O4     | 2.35                     | 0.60              |
| 2:I:14:ALA:HB2   | 2:I:125:SER:HB3    | 1.82                     | 0.60              |
| 2:H:108:VAL:CG1  | 2:H:108:VAL:O      | 2.47                     | 0.59              |
| 1:C:119:PHE:HB2  | 1:C:125:ARG:CD     | 2.32                     | 0.59              |
| 1:E:74:LEU:HD11  | 1:E:81:VAL:HG22    | 1.84                     | 0.59              |
| 2:H:60:TYR:HB2   | 2:H:65:LYS:HG3     | 1.84                     | 0.59              |
| 1:A:121:GLY:HA2  | 1:A:126:LEU:HD11   | 1.84                     | 0.59              |
| 1:A:119:PHE:HB2  | 1:A:125:ARG:CD     | 2.31                     | 0.59              |
| 1:B:104:ILE:HG22 | 1:B:114:ARG:HH21   | 1.67                     | 0.59              |
| 1:C:214:LEU:HD21 | 1:C:230:ILE:HG21   | 1.85                     | 0.59              |
| 2:K:38:ARG:NH1   | 2:K:90:ASP:HA      | 2.13                     | 0.59              |
| 1:E:104:ILE:HG22 | 1:E:114[B]:ARG:NH2 | 2.09                     | 0.59              |
| 1:F:121:GLY:HA2  | 1:F:126:LEU:HD11   | 1.85                     | 0.59              |
| 2:I:123:THR:C    | 2:I:124:VAL:HG22   | 2.23                     | 0.59              |
| 1:F:119:PHE:HB2  | 1:F:125:ARG:CD     | 2.32                     | 0.59              |
| 1:F:24:PHE:O     | 1:F:27:ALA:HB3     | 2.03                     | 0.59              |
| 2:G:55:ASP:OD1   | 2:G:57:THR:N       | 2.35                     | 0.59              |
| 1:B:99:GLU:CD    | 1:B:99:GLU:H       | 2.06                     | 0.59              |
| 2:K:17:SER:HB3   | 2:K:84:ASN:OD1     | 2.03                     | 0.59              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:E:114[B]:ARG:HG2 | 1:E:114[B]:ARG:HH11 | 1.68                     | 0.58              |
| 1:E:5:GLN:OE1      | 1:E:5:GLN:HA        | 1.97                     | 0.58              |
| 2:K:67:ARG:HH22    | 2:K:90:ASP:CG       | 2.06                     | 0.58              |
| 1:B:39:ARG:HH11    | 1:B:39:ARG:CG       | 2.11                     | 0.58              |
| 1:F:224:GLY:O      | 1:F:245:VAL:HG23    | 2.03                     | 0.58              |
| 2:L:88:PRO:CA      | 2:L:124:VAL:CG2     | 2.79                     | 0.58              |
| 1:D:214:LEU:HD21   | 1:D:230:ILE:HG21    | 1.86                     | 0.58              |
| 1:D:49:VAL:CG2     | 1:D:50:GLY:H        | 2.15                     | 0.58              |
| 1:B:159:THR:HG22   | 2:H:115:TYR:HE1     | 1.67                     | 0.58              |
| 1:D:73:ALA:O       | 1:D:74:LEU:HD12     | 2.04                     | 0.58              |
| 1:E:71:THR:O       | 1:E:84:TYR:HB2      | 2.02                     | 0.58              |
| 2:G:122:VAL:O      | 2:G:123:THR:HG23    | 2.04                     | 0.58              |
| 1:A:189:ARG:HH21   | 1:A:193:ARG:HH22    | 1.52                     | 0.58              |
| 1:A:215:SER:O      | 1:A:219:GLN:HG3     | 2.04                     | 0.58              |
| 2:I:12:VAL:O       | 2:I:124:VAL:HA      | 2.03                     | 0.58              |
| 1:C:74:LEU:HD11    | 1:C:81:VAL:HG22     | 1.86                     | 0.58              |
| 1:D:22:THR:OG1     | 1:D:189:ARG:HD2     | 2.04                     | 0.58              |
| 2:G:108:VAL:CG1    | 2:G:108:VAL:O       | 2.48                     | 0.58              |
| 1:B:39:ARG:HG2     | 1:B:39:ARG:NH1      | 2.14                     | 0.58              |
| 1:B:189:ARG:HH21   | 1:B:193:ARG:HH22    | 1.52                     | 0.58              |
| 1:C:181:PHE:HB2    | 1:C:184:ILE:HG13    | 1.86                     | 0.58              |
| 1:F:215:SER:O      | 1:F:219:GLN:HG3     | 2.04                     | 0.58              |
| 1:A:49:VAL:CG2     | 1:A:50:GLY:H        | 2.15                     | 0.57              |
| 1:B:181:PHE:CZ     | 1:B:211:TRP:HD1     | 2.23                     | 0.57              |
| 2:J:36:TRP:O       | 2:J:48:VAL:HB       | 2.04                     | 0.57              |
| 1:E:51:LEU:HD12    | 1:E:52:PRO:HD2      | 1.86                     | 0.57              |
| 1:B:39:ARG:NH1     | 1:B:39:ARG:CG       | 2.68                     | 0.57              |
| 1:E:108:PHE:N      | 1:E:114[A]:ARG:HH22 | 2.03                     | 0.57              |
| 2:H:53:TRP:CH2     | 2:H:72[B]:ARG:HG3   | 2.39                     | 0.57              |
| 1:B:121:GLY:HA2    | 1:B:126:LEU:HD11    | 1.86                     | 0.57              |
| 1:E:125:ARG:NH1    | 4:E:304:CL:CL       | 2.75                     | 0.57              |
| 1:A:214:LEU:HD21   | 1:A:230:ILE:HG21    | 1.85                     | 0.57              |
| 2:H:49:ALA:HB1     | 2:H:70:VAL:HG21     | 1.87                     | 0.57              |
| 2:J:55:ASP:OD1     | 2:J:57:THR:OG1      | 2.20                     | 0.57              |
| 1:A:85:ARG:HD3     | 1:A:111:VAL:CG2     | 2.35                     | 0.57              |
| 1:B:201:ASP:HB2    | 1:B:202:PRO:CD      | 2.34                     | 0.57              |
| 1:E:99:GLU:H       | 1:E:99:GLU:CD       | 2.09                     | 0.57              |
| 2:G:67:ARG:HB3     | 2:G:84:ASN:O        | 2.04                     | 0.57              |
| 1:B:49:VAL:CG2     | 1:B:50:GLY:N        | 2.66                     | 0.57              |
| 1:C:189:ARG:HH21   | 1:C:193:ARG:HH22    | 1.53                     | 0.57              |
| 1:D:75:ASP:HB3     | 1:D:78:ASN:HB2      | 1.86                     | 0.57              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:F:75:ASP:HB3   | 1:F:78:ASN:HB2     | 1.86                     | 0.57              |
| 2:J:47:PHE:CG    | 2:J:108:VAL:CG1    | 2.87                     | 0.57              |
| 2:K:73:ASP:OD1   | 2:K:74:ASN:N       | 2.38                     | 0.57              |
| 2:L:105:LEU:CD1  | 2:L:105:LEU:H      | 2.18                     | 0.57              |
| 1:F:39:ARG:CG    | 1:F:39:ARG:NH1     | 2.66                     | 0.56              |
| 2:G:53:TRP:CH2   | 2:G:72:ARG:HB2     | 2.40                     | 0.56              |
| 2:H:12:VAL:HG21  | 2:H:86:LEU:HD22    | 1.87                     | 0.56              |
| 1:A:164:LEU:HG   | 1:A:168:PHE:CE2    | 2.40                     | 0.56              |
| 2:I:47:PHE:CG    | 2:I:108:VAL:CG1    | 2.87                     | 0.56              |
| 1:E:214:LEU:HD21 | 1:E:230:ILE:HG21   | 1.86                     | 0.56              |
| 1:F:214:LEU:HD21 | 1:F:230:ILE:HG21   | 1.88                     | 0.56              |
| 1:A:159:THR:HG22 | 2:G:115:TYR:CE1    | 2.39                     | 0.56              |
| 2:G:11:LEU:HD12  | 2:G:12:VAL:N       | 2.20                     | 0.56              |
| 2:I:55:ASP:OD1   | 2:I:57:THR:OG1     | 2.20                     | 0.56              |
| 1:A:188:MET:HA   | 1:A:188:MET:HE2    | 1.88                     | 0.56              |
| 1:A:78:ASN:O     | 1:A:79:ALA:HB3     | 2.06                     | 0.56              |
| 1:D:181:PHE:HB2  | 1:D:184:ILE:HG13   | 1.87                     | 0.56              |
| 1:E:215:SER:O    | 1:E:219:GLN:HG3    | 2.04                     | 0.56              |
| 2:H:67:ARG:HB3   | 2:H:84:ASN:O       | 2.06                     | 0.56              |
| 1:A:104:ILE:HG22 | 1:A:114:ARG:HH21   | 1.70                     | 0.56              |
| 1:E:135:GLU:N    | 1:E:135:GLU:CD     | 2.59                     | 0.56              |
| 1:C:34:THR:HG23  | 1:C:46:PRO:HG3     | 1.88                     | 0.56              |
| 2:J:22:CYS:HB3   | 2:J:79:VAL:HG12    | 1.88                     | 0.56              |
| 1:B:223:GLN:NE2  | 1:C:247:ILE:HD13   | 2.21                     | 0.56              |
| 1:E:188:MET:HA   | 1:E:188:MET:HE2    | 1.87                     | 0.56              |
| 2:L:47:PHE:CD2   | 2:L:108:VAL:HG13   | 2.40                     | 0.56              |
| 2:L:87:LYS:C     | 2:L:124:VAL:HG21   | 2.25                     | 0.56              |
| 2:K:32:SER:O     | 2:K:33:SER:HB3     | 2.05                     | 0.56              |
| 1:A:135:GLU:CD   | 1:A:135:GLU:N      | 2.59                     | 0.56              |
| 1:C:75:ASP:HB3   | 1:C:78:ASN:HB2     | 1.88                     | 0.56              |
| 2:K:73:ASP:O     | 2:K:77:ASN:HB3     | 2.05                     | 0.56              |
| 1:E:108:PHE:O    | 1:E:114[A]:ARG:NH1 | 2.34                     | 0.55              |
| 1:E:39:ARG:NH1   | 1:E:39:ARG:HG2     | 2.19                     | 0.55              |
| 1:B:215:SER:O    | 1:B:219:GLN:HG3    | 2.06                     | 0.55              |
| 1:C:85:ARG:HD3   | 1:C:111:VAL:CG2    | 2.36                     | 0.55              |
| 2:H:14:ALA:HB2   | 2:H:125:SER:HB3    | 1.88                     | 0.55              |
| 2:J:74:ASN:HB2   | 2:J:77:ASN:CB      | 2.36                     | 0.55              |
| 1:D:88:ASN:O     | 1:D:111:VAL:HG13   | 2.07                     | 0.55              |
| 1:D:78:ASN:O     | 1:D:79:ALA:HB3     | 2.06                     | 0.55              |
| 2:I:121:GLN:NE2  | 2:I:122:VAL:O      | 2.39                     | 0.55              |
| 2:L:38:ARG:NH1   | 2:L:90:ASP:HA      | 2.15                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:B:85:ARG:HD3    | 1:B:111:VAL:CG2    | 2.36                     | 0.55              |
| 1:C:8:ILE:HD12    | 1:C:61:GLU:HB2     | 1.88                     | 0.55              |
| 1:D:222:ASN:O     | 1:D:223:GLN:HG2    | 2.06                     | 0.55              |
| 1:E:152:TYR:O     | 1:E:154:TYR:N      | 2.39                     | 0.55              |
| 2:I:36:TRP:NE1    | 2:I:81:LEU:HB2     | 2.22                     | 0.55              |
| 1:D:189:ARG:HH21  | 1:D:193:ARG:HH22   | 1.53                     | 0.55              |
| 1:D:173:GLN:NE2   | 1:D:208:GLU:OE2    | 2.28                     | 0.55              |
| 1:C:24:PHE:O      | 1:C:27:ALA:HB3     | 2.06                     | 0.55              |
| 1:C:125:ARG:NH1   | 3:C:301:SO4:O4     | 2.40                     | 0.55              |
| 1:D:139:LEU:HG    | 1:D:200:PRO:HD3    | 1.88                     | 0.55              |
| 1:D:99:GLU:CD     | 1:D:99:GLU:H       | 2.10                     | 0.55              |
| 2:J:67:ARG:HB3    | 2:J:84:ASN:O       | 2.07                     | 0.55              |
| 1:E:190:THR:HA    | 1:E:193[A]:ARG:HB2 | 1.88                     | 0.55              |
| 1:A:166:ARG:NH2   | 2:G:114:ASP:OD1    | 2.40                     | 0.55              |
| 1:C:72:LEU:N      | 1:C:72:LEU:HD12    | 2.22                     | 0.55              |
| 1:E:154:TYR:HA    | 1:E:159:THR:OG1    | 2.07                     | 0.55              |
| 1:F:139:LEU:HG    | 1:F:200:PRO:HD3    | 1.89                     | 0.55              |
| 2:K:87:LYS:C      | 2:K:124:VAL:HG21   | 2.27                     | 0.55              |
| 1:F:135:GLU:HG3   | 1:F:205:ILE:CD1    | 2.37                     | 0.55              |
| 2:H:103:ARG:NH2   | 2:H:106:VAL:CG2    | 2.70                     | 0.55              |
| 2:H:6:GLU:HA      | 2:H:21:SER:O       | 2.06                     | 0.55              |
| 1:B:177:GLU:OE1   | 1:B:180:ARG:HD2    | 2.07                     | 0.54              |
| 1:E:71:THR:C      | 1:E:72:LEU:HD12    | 2.27                     | 0.54              |
| 1:F:99:GLU:H      | 1:F:99:GLU:CD      | 2.10                     | 0.54              |
| 2:G:6:GLU:HA      | 2:G:21:SER:O       | 2.07                     | 0.54              |
| 1:B:75:ASP:HB3    | 1:B:78:ASN:HB2     | 1.89                     | 0.54              |
| 1:E:144:LEU:O     | 1:E:148:ILE:HG13   | 2.07                     | 0.54              |
| 1:D:135:GLU:N     | 1:D:135:GLU:CD     | 2.61                     | 0.54              |
| 1:E:247:ILE:CD1   | 1:F:223:GLN:NE2    | 2.70                     | 0.54              |
| 2:I:36:TRP:O      | 2:I:48:VAL:HB      | 2.08                     | 0.54              |
| 1:D:135:GLU:HG3   | 1:D:205:ILE:CD1    | 2.38                     | 0.54              |
| 1:C:39:ARG:NH1    | 1:C:39:ARG:HG2     | 2.21                     | 0.54              |
| 1:C:39:ARG:O      | 1:C:40:HIS:C       | 2.46                     | 0.54              |
| 2:H:72[B]:ARG:HG2 | 2:H:73:ASP:N       | 2.22                     | 0.54              |
| 2:H:72[A]:ARG:CG  | 2:H:72[A]:ARG:HH11 | 2.10                     | 0.54              |
| 2:K:9:GLY:H       | 2:K:120:THR:CG2    | 2.15                     | 0.54              |
| 1:D:64:ASN:HB3    | 1:D:66:ALA:H       | 1.73                     | 0.54              |
| 1:E:88:ASN:HD21   | 1:E:112:GLN:CD     | 2.10                     | 0.54              |
| 2:I:12:VAL:HG21   | 2:I:86:LEU:HD22    | 1.90                     | 0.54              |
| 1:D:166:ARG:NH1   | 2:J:111:ILE:O      | 2.38                     | 0.54              |
| 2:K:64:VAL:HA     | 2:K:67:ARG:NH1     | 2.23                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:VAL:CG2   | 1:A:50:GLY:N     | 2.70                     | 0.54              |
| 1:C:135:GLU:HG3  | 1:C:205:ILE:CD1  | 2.38                     | 0.54              |
| 1:F:222:ASN:O    | 1:F:223:GLN:HG2  | 2.07                     | 0.54              |
| 1:F:51:LEU:HD12  | 1:F:52:PRO:HD2   | 1.88                     | 0.54              |
| 1:D:121:GLY:HA2  | 1:D:126:LEU:HD11 | 1.90                     | 0.54              |
| 1:F:64:ASN:HB3   | 1:F:66:ALA:H     | 1.73                     | 0.54              |
| 1:A:181:PHE:CZ   | 1:A:211:TRP:CD1  | 2.96                     | 0.54              |
| 1:B:247:ILE:HD13 | 1:C:223:GLN:NE2  | 2.23                     | 0.54              |
| 1:D:39:ARG:HG2   | 1:D:39:ARG:NH1   | 2.19                     | 0.54              |
| 1:F:71:THR:O     | 1:F:84:TYR:HB2   | 2.08                     | 0.53              |
| 2:I:108:VAL:O    | 2:I:108:VAL:CG1  | 2.45                     | 0.53              |
| 1:D:215:SER:O    | 1:D:219:GLN:HG3  | 2.08                     | 0.53              |
| 1:E:39:ARG:CG    | 1:E:39:ARG:NH1   | 2.69                     | 0.53              |
| 1:C:78:ASN:O     | 1:C:79:ALA:HB3   | 2.08                     | 0.53              |
| 1:E:64:ASN:HB3   | 1:E:66:ALA:H     | 1.73                     | 0.53              |
| 2:H:123:THR:O    | 2:H:124:VAL:HG13 | 2.08                     | 0.53              |
| 1:A:139:LEU:HG   | 1:A:200:PRO:HD3  | 1.91                     | 0.53              |
| 1:B:164:LEU:HG   | 1:B:168:PHE:CE2  | 2.44                     | 0.53              |
| 1:F:47:ASN:ND2   | 1:F:49:VAL:HG22  | 2.23                     | 0.53              |
| 2:I:60:TYR:HB2   | 2:I:65:LYS:HG3   | 1.90                     | 0.53              |
| 1:F:136:ASN:O    | 2:L:102:VAL:HA   | 2.08                     | 0.53              |
| 1:C:139:LEU:HG   | 1:C:200:PRO:HD3  | 1.90                     | 0.53              |
| 1:E:60:VAL:HG12  | 1:E:60:VAL:O     | 2.09                     | 0.53              |
| 2:G:5:VAL:CG1    | 2:G:6:GLU:N      | 2.72                     | 0.53              |
| 1:B:74:LEU:CD1   | 1:B:81:VAL:HG22  | 2.38                     | 0.53              |
| 2:G:58:THR:C     | 2:G:59:LEU:HD23  | 2.28                     | 0.53              |
| 2:H:123:THR:C    | 2:H:124:VAL:HG22 | 2.28                     | 0.53              |
| 1:E:201:ASP:HB2  | 1:E:202:PRO:CD   | 2.38                     | 0.53              |
| 1:B:135:GLU:CD   | 1:B:135:GLU:N    | 2.62                     | 0.53              |
| 1:E:72:LEU:CD1   | 1:E:72:LEU:N     | 2.69                     | 0.53              |
| 1:A:99:GLU:CD    | 1:A:99:GLU:H     | 2.12                     | 0.53              |
| 1:D:39:ARG:HH11  | 1:D:39:ARG:CG    | 2.17                     | 0.53              |
| 2:H:5:VAL:CG1    | 2:H:6:GLU:N      | 2.71                     | 0.53              |
| 1:B:247:ILE:CD1  | 1:C:223:GLN:NE2  | 2.72                     | 0.52              |
| 1:C:190:THR:HG22 | 1:C:193:ARG:HH11 | 1.73                     | 0.52              |
| 1:E:244:ASP:HB3  | 1:F:223:GLN:HG3  | 1.90                     | 0.52              |
| 1:A:39:ARG:HG2   | 1:A:39:ARG:NH1   | 2.19                     | 0.52              |
| 1:B:73:ALA:O     | 1:B:74:LEU:HD12  | 2.10                     | 0.52              |
| 1:F:125:ARG:HD2  | 3:F:301:SO4:O4   | 2.09                     | 0.52              |
| 2:H:72[B]:ARG:CG | 2:H:73:ASP:N     | 2.73                     | 0.52              |
| 2:J:60:TYR:HB2   | 2:J:65:LYS:HG3   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 1:C:222:ASN:O    | 1:C:223:GLN:HG2     | 2.09                     | 0.52              |
| 1:A:201:ASP:HB2  | 1:A:202:PRO:CD      | 2.39                     | 0.52              |
| 1:B:201:ASP:HB2  | 1:B:202:PRO:HD2     | 1.90                     | 0.52              |
| 1:D:164:LEU:HG   | 1:D:168:PHE:CE2     | 2.44                     | 0.52              |
| 1:B:199:ALA:HB1  | 1:B:200:PRO:HD2     | 1.91                     | 0.52              |
| 2:I:22:CYS:HB3   | 2:I:79:VAL:HG12     | 1.90                     | 0.52              |
| 1:F:188:MET:HA   | 1:F:188:MET:HE2     | 1.90                     | 0.52              |
| 1:F:73:ALA:O     | 1:F:74:LEU:HD12     | 2.09                     | 0.52              |
| 1:F:78:ASN:O     | 1:F:79:ALA:HB3      | 2.09                     | 0.52              |
| 2:G:88:PRO:CA    | 2:G:124:VAL:HG21    | 2.36                     | 0.52              |
| 1:E:244:ASP:OD1  | 1:F:244:ASP:OD1     | 2.26                     | 0.52              |
| 1:F:189:ARG:HH21 | 1:F:193:ARG:HH22    | 1.56                     | 0.52              |
| 1:A:74:LEU:HD11  | 1:A:81:VAL:HG22     | 1.91                     | 0.52              |
| 1:E:108:PHE:H    | 1:E:114[A]:ARG:HH22 | 1.56                     | 0.52              |
| 1:E:164:LEU:HG   | 1:E:168:PHE:CE2     | 2.45                     | 0.52              |
| 1:E:135:GLU:HG3  | 1:E:205:ILE:CD1     | 2.40                     | 0.52              |
| 1:E:21:TYR:O     | 1:E:24:PHE:HB3      | 2.10                     | 0.52              |
| 1:F:177:GLU:OE1  | 1:F:180:ARG:HD2     | 2.10                     | 0.52              |
| 1:B:125:ARG:NH1  | 3:B:301:SO4:S       | 2.83                     | 0.52              |
| 1:E:104:ILE:HG21 | 1:E:114[B]:ARG:NH2  | 2.24                     | 0.52              |
| 2:K:88:PRO:N     | 2:K:124:VAL:HG21    | 2.23                     | 0.52              |
| 1:A:24:PHE:O     | 1:A:27:ALA:HB3      | 2.10                     | 0.52              |
| 1:B:244:ASP:HB3  | 1:C:223:GLN:HG3     | 1.91                     | 0.52              |
| 1:B:24:PHE:O     | 1:B:27:ALA:HB3      | 2.10                     | 0.51              |
| 1:C:188:MET:HA   | 1:C:188:MET:HE2     | 1.92                     | 0.51              |
| 1:C:49:VAL:CG2   | 1:C:50:GLY:H        | 2.20                     | 0.51              |
| 1:D:96:ASP:N     | 1:D:96:ASP:OD1      | 2.27                     | 0.51              |
| 1:E:108:PHE:H    | 1:E:114[A]:ARG:NH2  | 2.08                     | 0.51              |
| 1:F:135:GLU:CD   | 1:F:135:GLU:N       | 2.64                     | 0.51              |
| 2:K:73:ASP:N     | 2:K:78:MET:O        | 2.42                     | 0.51              |
| 2:L:32:SER:O     | 2:L:33:SER:HB3      | 2.10                     | 0.51              |
| 1:D:85:ARG:HD3   | 1:D:111:VAL:CG2     | 2.40                     | 0.51              |
| 2:L:9:GLY:HA3    | 2:L:120:THR:HB      | 1.91                     | 0.51              |
| 2:L:20:LEU:HB2   | 2:L:81:LEU:HB3      | 1.90                     | 0.51              |
| 1:A:48:ARG:NH1   | 1:A:100:ASP:OD1     | 2.42                     | 0.51              |
| 1:E:134:ARG:HH22 | 1:E:209:ASN:HD21    | 1.58                     | 0.51              |
| 2:G:123:THR:C    | 2:G:124:VAL:HG22    | 2.30                     | 0.51              |
| 2:H:22:CYS:HB3   | 2:H:79:VAL:HG12     | 1.91                     | 0.51              |
| 1:B:47:ASN:ND2   | 1:B:49:VAL:HG22     | 2.25                     | 0.51              |
| 1:C:154:TYR:HA   | 1:C:159:THR:OG1     | 2.10                     | 0.51              |
| 2:G:102:VAL:CG1  | 2:G:107:ALA:HB2     | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:122:VAL:O    | 2:I:123:THR:HG23 | 2.10                     | 0.51              |
| 1:B:188:MET:HE2  | 1:B:188:MET:HA   | 1.91                     | 0.51              |
| 1:C:177:GLU:OE1  | 1:C:180:ARG:HD2  | 2.11                     | 0.51              |
| 1:E:39:ARG:O     | 1:E:40:HIS:C     | 2.48                     | 0.51              |
| 2:J:103:ARG:HH11 | 2:J:103:ARG:CG   | 2.23                     | 0.51              |
| 1:C:144:LEU:O    | 1:C:148:ILE:HG13 | 2.11                     | 0.51              |
| 1:E:85:ARG:HD3   | 1:E:111:VAL:CG2  | 2.41                     | 0.51              |
| 1:A:135:GLU:HG3  | 1:A:205:ILE:CD1  | 2.41                     | 0.51              |
| 1:A:177:GLU:OE1  | 1:A:180:ARG:HD2  | 2.10                     | 0.51              |
| 1:C:146:GLU:OE1  | 1:C:146:GLU:HA   | 2.11                     | 0.51              |
| 1:F:49:VAL:CG2   | 1:F:50:GLY:H     | 2.18                     | 0.51              |
| 2:J:60:TYR:N     | 2:J:60:TYR:CD1   | 2.79                     | 0.51              |
| 2:L:29:PHE:CD1   | 2:L:29:PHE:N     | 2.78                     | 0.51              |
| 1:B:144:LEU:O    | 1:B:148:ILE:HG13 | 2.11                     | 0.51              |
| 1:C:201:ASP:HB2  | 1:C:202:PRO:CD   | 2.40                     | 0.51              |
| 1:F:85:ARG:HD3   | 1:F:111:VAL:CG2  | 2.40                     | 0.51              |
| 2:I:58:THR:C     | 2:I:59:LEU:HD23  | 2.30                     | 0.51              |
| 2:I:67:ARG:HB3   | 2:I:84:ASN:O     | 2.11                     | 0.51              |
| 2:L:12:VAL:HG22  | 2:L:124:VAL:HG12 | 1.92                     | 0.51              |
| 1:A:144:LEU:O    | 1:A:148:ILE:HG13 | 2.10                     | 0.51              |
| 1:B:181:PHE:HB2  | 1:B:184:ILE:HG13 | 1.93                     | 0.51              |
| 1:C:120:GLY:O    | 1:C:125:ARG:HG2  | 2.10                     | 0.51              |
| 2:G:12:VAL:HG21  | 2:G:86:LEU:HD22  | 1.93                     | 0.51              |
| 1:A:88:ASN:HD21  | 1:A:112:GLN:CD   | 2.14                     | 0.50              |
| 1:C:135:GLU:CD   | 1:C:135:GLU:N    | 2.63                     | 0.50              |
| 1:C:73:ALA:O     | 1:C:74:LEU:HD12  | 2.11                     | 0.50              |
| 1:A:39:ARG:CG    | 1:A:39:ARG:NH1   | 2.73                     | 0.50              |
| 1:B:139:LEU:HG   | 1:B:200:PRO:HD3  | 1.93                     | 0.50              |
| 1:E:236:ASN:ND2  | 1:E:236:ASN:H    | 2.10                     | 0.50              |
| 1:F:166:ARG:NH1  | 2:L:111:ILE:O    | 2.43                     | 0.50              |
| 1:C:159:THR:HG22 | 2:I:115:TYR:CE1  | 2.46                     | 0.50              |
| 1:A:64:ASN:HB2   | 1:A:68:LEU:H     | 1.77                     | 0.50              |
| 1:D:154:TYR:HA   | 1:D:159:THR:OG1  | 2.11                     | 0.50              |
| 1:E:48:ARG:NH1   | 1:E:100:ASP:OD1  | 2.43                     | 0.50              |
| 1:E:136:ASN:O    | 2:K:102:VAL:HA   | 2.11                     | 0.50              |
| 2:G:22:CYS:HB3   | 2:G:79:VAL:HG12  | 1.94                     | 0.50              |
| 2:I:74:ASN:HB2   | 2:I:77:ASN:CB    | 2.39                     | 0.50              |
| 1:A:71:THR:O     | 1:A:84:TYR:HB2   | 2.11                     | 0.50              |
| 1:C:64:ASN:HB3   | 1:C:66:ALA:H     | 1.76                     | 0.50              |
| 2:G:47:PHE:CG    | 2:G:108:VAL:CG1  | 2.95                     | 0.50              |
| 2:H:74:ASN:HB2   | 2:H:77:ASN:CB    | 2.42                     | 0.50              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:L:67:ARG:HH22  | 2:L:90:ASP:CG      | 2.14                     | 0.50              |
| 1:B:181:PHE:CZ   | 1:B:211:TRP:CD1    | 3.00                     | 0.50              |
| 1:C:184:ILE:HD13 | 1:C:204:VAL:HG13   | 1.93                     | 0.50              |
| 1:E:121:GLY:HA2  | 1:E:126:LEU:HD11   | 1.94                     | 0.50              |
| 1:E:152:TYR:C    | 1:E:154:TYR:H      | 2.14                     | 0.50              |
| 1:F:125:ARG:NH1  | 3:F:301:SO4:S      | 2.85                     | 0.50              |
| 1:F:21:TYR:O     | 1:F:24:PHE:HB3     | 2.12                     | 0.50              |
| 2:G:52:VAL:C     | 2:G:53:TRP:O       | 2.49                     | 0.50              |
| 1:D:74:LEU:CD1   | 1:D:81:VAL:HG22    | 2.42                     | 0.50              |
| 2:G:36:TRP:O     | 2:G:48:VAL:HB      | 2.11                     | 0.50              |
| 2:G:36:TRP:NE1   | 2:G:81:LEU:HB2     | 2.27                     | 0.50              |
| 2:H:58:THR:C     | 2:H:59:LEU:HD23    | 2.32                     | 0.50              |
| 1:F:39:ARG:O     | 1:F:40:HIS:C       | 2.48                     | 0.49              |
| 2:L:102:VAL:CG1  | 2:L:107:ALA:HB2    | 2.42                     | 0.49              |
| 2:L:109:ARG:HB2  | 2:L:112:ASP:OD2    | 2.12                     | 0.49              |
| 1:A:21:TYR:O     | 1:A:24:PHE:HB3     | 2.12                     | 0.49              |
| 1:D:88:ASN:HD21  | 1:D:112:GLN:CD     | 2.15                     | 0.49              |
| 1:D:24:PHE:O     | 1:D:27:ALA:HB3     | 2.11                     | 0.49              |
| 2:G:74:ASN:HB2   | 2:G:77:ASN:CB      | 2.40                     | 0.49              |
| 1:A:47:ASN:ND2   | 1:A:49:VAL:HG22    | 2.27                     | 0.49              |
| 1:A:8:ILE:HD12   | 1:A:61:GLU:HB2     | 1.95                     | 0.49              |
| 1:D:177:GLU:OE1  | 1:D:180:ARG:HD2    | 2.12                     | 0.49              |
| 1:E:189:ARG:CZ   | 1:E:193[A]:ARG:NH2 | 2.71                     | 0.49              |
| 1:B:21:TYR:O     | 1:B:24:PHE:HB3     | 2.13                     | 0.49              |
| 1:B:78:ASN:O     | 1:B:79:ALA:HB3     | 2.13                     | 0.49              |
| 1:B:91:TYR:OH    | 1:B:155:SER:HA     | 2.11                     | 0.49              |
| 2:G:121:GLN:NE2  | 2:G:122:VAL:O      | 2.42                     | 0.49              |
| 1:A:181:PHE:HB2  | 1:A:184:ILE:HG13   | 1.95                     | 0.49              |
| 1:B:123:TYR:CD1  | 1:B:134:ARG:HD3    | 2.47                     | 0.49              |
| 2:I:5:VAL:CG1    | 2:I:6:GLU:N        | 2.75                     | 0.49              |
| 1:D:39:ARG:NH1   | 1:D:39:ARG:CG      | 2.73                     | 0.49              |
| 1:D:72:LEU:N     | 1:D:72:LEU:CD1     | 2.74                     | 0.49              |
| 1:B:166:ARG:NH2  | 2:H:114:ASP:OD1    | 2.46                     | 0.49              |
| 2:I:103:ARG:NH1  | 2:I:106:VAL:HG21   | 2.28                     | 0.49              |
| 2:J:58:THR:C     | 2:J:59:LEU:HD23    | 2.32                     | 0.49              |
| 2:L:88:PRO:N     | 2:L:124:VAL:HG21   | 2.28                     | 0.49              |
| 1:B:135:GLU:HG3  | 1:B:205:ILE:CD1    | 2.42                     | 0.49              |
| 1:F:154:TYR:HA   | 1:F:159:THR:OG1    | 2.13                     | 0.49              |
| 1:F:88:ASN:HD21  | 1:F:112:GLN:CD     | 2.16                     | 0.49              |
| 2:H:16:GLY:O     | 2:H:86:LEU:HD13    | 2.12                     | 0.49              |
| 1:A:91:TYR:OH    | 1:A:155:SER:HA     | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:134:ARG:HH22 | 1:D:209:ASN:HD21 | 1.61                     | 0.49              |
| 1:E:248:LEU:N    | 1:E:248:LEU:HD23 | 2.28                     | 0.49              |
| 2:J:6:GLU:HA     | 2:J:21:SER:O     | 2.13                     | 0.49              |
| 1:C:99:GLU:H     | 1:C:99:GLU:CD    | 2.16                     | 0.48              |
| 1:D:201:ASP:HB2  | 1:D:202:PRO:CD   | 2.43                     | 0.48              |
| 1:E:153:TYR:HB3  | 1:E:159:THR:HG23 | 1.94                     | 0.48              |
| 1:F:144:LEU:O    | 1:F:148:ILE:HG13 | 2.13                     | 0.48              |
| 2:G:60:TYR:HB2   | 2:G:65:LYS:HG3   | 1.95                     | 0.48              |
| 2:J:123:THR:O    | 2:J:124:VAL:HG13 | 2.13                     | 0.48              |
| 1:A:72:LEU:N     | 1:A:72:LEU:CD1   | 2.76                     | 0.48              |
| 1:B:71:THR:O     | 1:B:84:TYR:HB2   | 2.13                     | 0.48              |
| 1:C:39:ARG:HH11  | 1:C:39:ARG:CG    | 2.20                     | 0.48              |
| 2:I:73:ASP:O     | 2:I:74:ASN:O     | 2.31                     | 0.48              |
| 1:B:223:GLN:NE2  | 1:C:247:ILE:CD1  | 2.76                     | 0.48              |
| 1:D:64:ASN:HB2   | 1:D:68:LEU:H     | 1.79                     | 0.48              |
| 1:E:12:THR:HG23  | 1:E:12:THR:O     | 2.11                     | 0.48              |
| 1:F:13:THR:HG22  | 1:F:64:ASN:HA    | 1.95                     | 0.48              |
| 2:H:102:VAL:CG1  | 2:H:107:ALA:HB2  | 2.44                     | 0.48              |
| 2:L:9:GLY:H      | 2:L:120:THR:CG2  | 2.18                     | 0.48              |
| 1:E:12:THR:CG2   | 1:E:12:THR:O     | 2.61                     | 0.48              |
| 1:F:123:TYR:O    | 1:F:124:ASP:C    | 2.52                     | 0.48              |
| 1:C:136:ASN:O    | 2:I:102:VAL:HA   | 2.13                     | 0.48              |
| 1:F:201:ASP:HB2  | 1:F:202:PRO:CD   | 2.43                     | 0.48              |
| 1:F:5:GLN:HA     | 1:F:5:GLN:OE1    | 2.08                     | 0.48              |
| 1:A:125:ARG:NH1  | 3:A:301:SO4:S    | 2.86                     | 0.48              |
| 1:B:134:ARG:HH22 | 1:B:209:ASN:HD21 | 1.62                     | 0.48              |
| 1:B:51:LEU:HD12  | 1:B:52:PRO:HD2   | 1.95                     | 0.48              |
| 1:C:49:VAL:CG2   | 1:C:50:GLY:N     | 2.76                     | 0.48              |
| 1:D:47:ASN:ND2   | 1:D:49:VAL:HG22  | 2.28                     | 0.48              |
| 1:F:123:TYR:CD1  | 1:F:134:ARG:HD3  | 2.48                     | 0.48              |
| 1:B:166:ARG:NH2  | 2:H:112:ASP:O    | 2.47                     | 0.48              |
| 2:K:22:CYS:O     | 2:K:78:MET:HE2   | 2.14                     | 0.48              |
| 1:A:190:THR:HG22 | 1:A:193:ARG:HH11 | 1.78                     | 0.48              |
| 1:D:39:ARG:O     | 1:D:40:HIS:C     | 2.51                     | 0.48              |
| 1:F:74:LEU:CD1   | 1:F:81:VAL:HG22  | 2.44                     | 0.48              |
| 1:A:39:ARG:O     | 1:A:40:HIS:C     | 2.51                     | 0.48              |
| 1:C:13:THR:HG22  | 1:C:64:ASN:HA    | 1.96                     | 0.48              |
| 1:D:64:ASN:HB3   | 1:D:66:ALA:N     | 2.29                     | 0.48              |
| 2:G:44:GLU:CG    | 2:G:45:ARG:N     | 2.73                     | 0.48              |
| 1:B:48:ARG:NH1   | 1:B:100:ASP:OD1  | 2.47                     | 0.47              |
| 1:E:159:THR:HG22 | 2:K:115:TYR:HE2  | 1.78                     | 0.47              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:223:GLN:NE2    | 1:F:247:ILE:HD13 | 2.29                     | 0.47              |
| 1:E:73:ALA:O       | 1:E:74:LEU:HD12  | 2.14                     | 0.47              |
| 1:F:49:VAL:CG2     | 1:F:50:GLY:N     | 2.75                     | 0.47              |
| 1:A:73:ALA:O       | 1:A:74:LEU:HD12  | 2.14                     | 0.47              |
| 1:B:263:PRO:O      | 1:B:264:SER:CB   | 2.57                     | 0.47              |
| 1:D:181:PHE:CZ     | 1:D:211:TRP:HD1  | 2.31                     | 0.47              |
| 1:B:154:TYR:HA     | 1:B:159:THR:OG1  | 2.13                     | 0.47              |
| 1:D:144:LEU:O      | 1:D:148:ILE:HG13 | 2.14                     | 0.47              |
| 2:I:47:PHE:CD2     | 2:I:108:VAL:HG13 | 2.49                     | 0.47              |
| 1:C:21:TYR:O       | 1:C:24:PHE:HB3   | 2.15                     | 0.47              |
| 1:D:188:MET:HA     | 1:D:188:MET:HE2  | 1.95                     | 0.47              |
| 1:C:47:ASN:ND2     | 1:C:49:VAL:HG22  | 2.29                     | 0.47              |
| 1:E:152:TYR:C      | 1:E:154:TYR:N    | 2.65                     | 0.47              |
| 2:I:6:GLU:HA       | 2:I:21:SER:O     | 2.14                     | 0.47              |
| 2:L:73:ASP:N       | 2:L:78:MET:O     | 2.46                     | 0.47              |
| 1:E:26:ARG:NH2     | 5:E:402:HOH:O    | 2.46                     | 0.47              |
| 1:E:74:LEU:CD1     | 1:E:81:VAL:HG22  | 2.44                     | 0.47              |
| 1:F:120:GLY:O      | 1:F:125:ARG:HG2  | 2.15                     | 0.47              |
| 1:F:64:ASN:HB3     | 1:F:66:ALA:N     | 2.29                     | 0.47              |
| 2:H:51:ILE:O       | 2:H:51:ILE:HG23  | 2.15                     | 0.47              |
| 2:I:93:LEU:HA      | 2:I:93:LEU:HD12  | 1.68                     | 0.47              |
| 2:L:64:VAL:HA      | 2:L:67:ARG:NH1   | 2.30                     | 0.47              |
| 1:B:222:ASN:O      | 1:B:223:GLN:HG2  | 2.15                     | 0.47              |
| 1:B:39:ARG:O       | 1:B:40:HIS:C     | 2.53                     | 0.47              |
| 1:C:39:ARG:NH1     | 1:C:39:ARG:CG    | 2.74                     | 0.47              |
| 1:D:226:PHE:HE1    | 1:D:245:VAL:HG22 | 1.79                     | 0.47              |
| 1:F:226:PHE:HE1    | 1:F:245:VAL:HG22 | 1.79                     | 0.47              |
| 1:F:34:THR:HG23    | 1:F:46:PRO:HG3   | 1.96                     | 0.47              |
| 2:H:55:ASP:OD1     | 2:H:57:THR:OG1   | 2.23                     | 0.47              |
| 2:I:102:VAL:HB     | 2:I:107:ALA:HB2  | 1.95                     | 0.47              |
| 2:J:103:ARG:HB2    | 2:J:103:ARG:HH11 | 1.78                     | 0.47              |
| 2:J:12:VAL:HG21    | 2:J:86:LEU:HD22  | 1.95                     | 0.47              |
| 2:K:14:ALA:H       | 2:K:125:SER:CB   | 2.28                     | 0.47              |
| 1:A:189:ARG:NH2    | 1:A:193:ARG:HH22 | 2.11                     | 0.47              |
| 1:A:64:ASN:HB3     | 1:A:66:ALA:H     | 1.80                     | 0.47              |
| 2:K:102:VAL:CG1    | 2:K:107:ALA:HB2  | 2.45                     | 0.47              |
| 1:F:104:ILE:CG2    | 1:F:114:ARG:HH21 | 2.25                     | 0.47              |
| 2:H:82:GLN:HA      | 2:H:82:GLN:OE1   | 2.15                     | 0.47              |
| 2:J:122:VAL:O      | 2:J:123:THR:HG23 | 2.14                     | 0.47              |
| 2:K:103[A]:ARG:HB3 | 2:K:106:VAL:CG2  | 2.45                     | 0.47              |
| 1:D:107:LEU:HA     | 1:D:107:LEU:HD23 | 1.57                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:94:HIS:HA    | 1:F:95:PRO:HD2   | 1.81                     | 0.47              |
| 2:H:121:GLN:NE2  | 2:H:122:VAL:O    | 2.44                     | 0.47              |
| 2:H:36:TRP:NE1   | 2:H:81:LEU:HB2   | 2.30                     | 0.47              |
| 2:J:93:LEU:HD12  | 2:J:93:LEU:HA    | 1.67                     | 0.47              |
| 2:K:9:GLY:HA3    | 2:K:120:THR:HB   | 1.96                     | 0.47              |
| 2:L:73:ASP:OD1   | 2:L:74:ASN:N     | 2.47                     | 0.47              |
| 1:D:21:TYR:O     | 1:D:24:PHE:HB3   | 2.15                     | 0.47              |
| 1:E:139:LEU:HG   | 1:E:200:PRO:HD3  | 1.97                     | 0.47              |
| 1:E:177:GLU:OE1  | 1:E:180:ARG:HD2  | 2.15                     | 0.47              |
| 1:F:261:PRO:HA   | 1:F:262:PRO:HD3  | 1.69                     | 0.47              |
| 1:C:166:ARG:NH2  | 2:I:114:ASP:OD1  | 2.48                     | 0.46              |
| 2:K:31:ARG:HD3   | 2:K:34:MET:SD    | 2.55                     | 0.46              |
| 1:C:226:PHE:HE1  | 1:C:245:VAL:HG22 | 1.80                     | 0.46              |
| 1:A:136:ASN:O    | 2:G:102:VAL:HA   | 2.15                     | 0.46              |
| 2:H:36:TRP:O     | 2:H:48:VAL:HB    | 2.15                     | 0.46              |
| 2:K:4:LEU:CD2    | 2:K:24:ALA:CB    | 2.91                     | 0.46              |
| 2:K:77:ASN:HB3   | 2:K:78:MET:H     | 1.51                     | 0.46              |
| 2:K:94:TYR:O     | 2:K:119:GLY:HA2  | 2.15                     | 0.46              |
| 1:D:261:PRO:HA   | 1:D:262:PRO:HD3  | 1.72                     | 0.46              |
| 1:F:134:ARG:HH22 | 1:F:209:ASN:HD21 | 1.63                     | 0.46              |
| 2:J:102:VAL:HB   | 2:J:107:ALA:HB2  | 1.96                     | 0.46              |
| 1:A:107:LEU:HA   | 1:A:107:LEU:HD23 | 1.64                     | 0.46              |
| 1:A:71:THR:C     | 1:A:72:LEU:HD12  | 2.35                     | 0.46              |
| 1:B:64:ASN:HB2   | 1:B:68:LEU:H     | 1.80                     | 0.46              |
| 2:H:91:THR:O     | 2:H:92:ALA:HB2   | 2.16                     | 0.46              |
| 2:J:51:ILE:HG23  | 2:J:51:ILE:O     | 2.16                     | 0.46              |
| 1:A:261:PRO:HA   | 1:A:262:PRO:HD3  | 1.66                     | 0.46              |
| 1:C:74:LEU:CD1   | 1:C:81:VAL:HG22  | 2.46                     | 0.46              |
| 2:I:60:TYR:CD1   | 2:I:60:TYR:N     | 2.82                     | 0.46              |
| 2:J:123:THR:C    | 2:J:124:VAL:HG22 | 2.36                     | 0.46              |
| 2:K:58:THR:C     | 2:K:59:LEU:HD23  | 2.35                     | 0.46              |
| 2:L:58:THR:C     | 2:L:59:LEU:HD23  | 2.36                     | 0.46              |
| 1:E:122:ASN:O    | 1:E:126:LEU:HD13 | 2.15                     | 0.46              |
| 1:E:181:PHE:CZ   | 1:E:211:TRP:HD1  | 2.34                     | 0.46              |
| 1:F:245:VAL:O    | 1:F:245:VAL:HG12 | 2.14                     | 0.46              |
| 1:F:8:ILE:HD12   | 1:F:61:GLU:HB2   | 1.96                     | 0.46              |
| 1:F:64:ASN:HB2   | 1:F:68:LEU:H     | 1.81                     | 0.46              |
| 2:L:94:TYR:O     | 2:L:119:GLY:HA2  | 2.16                     | 0.46              |
| 2:G:44:GLU:CG    | 2:G:45:ARG:H     | 2.16                     | 0.46              |
| 2:H:37:PHE:CD2   | 2:H:47:PHE:HA    | 2.51                     | 0.46              |
| 2:I:53:TRP:O     | 2:I:54:ALA:HB3   | 2.15                     | 0.46              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 2:L:124:VAL:O      | 2:L:125:SER:C       | 2.54                     | 0.46              |
| 1:B:72:LEU:N       | 1:B:72:LEU:CD1      | 2.79                     | 0.46              |
| 1:F:204:VAL:O      | 1:F:208:GLU:HG3     | 2.16                     | 0.46              |
| 2:G:102:VAL:HB     | 2:G:107:ALA:HB2     | 1.98                     | 0.46              |
| 2:I:31:ARG:O       | 2:I:99:ASN:O        | 2.34                     | 0.46              |
| 1:A:78:ASN:O       | 1:A:79:ALA:CB       | 2.64                     | 0.46              |
| 1:B:151:LEU:HD23   | 1:B:164:LEU:CD1     | 2.46                     | 0.46              |
| 1:E:159:THR:HG22   | 2:K:115:TYR:CE2     | 2.51                     | 0.46              |
| 1:F:136:ASN:O      | 2:L:103[B]:ARG:N    | 2.38                     | 0.46              |
| 1:F:17:THR:OG1     | 1:F:20:SER:HB3      | 2.16                     | 0.46              |
| 2:G:124:VAL:O      | 2:G:125:SER:C       | 2.54                     | 0.46              |
| 2:K:103[B]:ARG:HG2 | 2:K:103[B]:ARG:HH11 | 1.81                     | 0.46              |
| 2:L:74:ASN:HB2     | 2:L:77:ASN:HB2      | 1.98                     | 0.46              |
| 1:B:140:GLY:C      | 1:B:143:PRO:HD2     | 2.37                     | 0.46              |
| 1:C:48:ARG:NH1     | 1:C:100:ASP:OD1     | 2.49                     | 0.46              |
| 1:C:134:ARG:HH22   | 1:C:209:ASN:HD21    | 1.63                     | 0.46              |
| 1:E:181:PHE:HB2    | 1:E:184:ILE:HG13    | 1.98                     | 0.46              |
| 2:H:102:VAL:HB     | 2:H:107:ALA:HB2     | 1.98                     | 0.46              |
| 2:J:44:GLU:CG      | 2:J:45:ARG:H        | 2.26                     | 0.46              |
| 1:B:22:THR:OG1     | 1:B:189:ARG:HD2     | 2.16                     | 0.45              |
| 1:D:34:THR:HG23    | 1:D:46:PRO:HG3      | 1.98                     | 0.45              |
| 2:G:28:THR:HG23    | 2:G:28:THR:O        | 2.15                     | 0.45              |
| 2:G:31:ARG:O       | 2:G:99:ASN:O        | 2.34                     | 0.45              |
| 1:A:123:TYR:CD1    | 1:A:134:ARG:HD3     | 2.52                     | 0.45              |
| 1:A:201:ASP:HB2    | 1:A:202:PRO:HD2     | 1.97                     | 0.45              |
| 1:A:134:ARG:NH2    | 1:A:209:ASN:OD1     | 2.49                     | 0.45              |
| 1:B:94:HIS:HA      | 1:B:95:PRO:HD2      | 1.81                     | 0.45              |
| 1:C:85:ARG:HD2     | 1:C:87:GLY:O        | 2.16                     | 0.45              |
| 2:J:108:VAL:O      | 2:J:108:VAL:CG1     | 2.47                     | 0.45              |
| 2:J:36:TRP:NE1     | 2:J:81:LEU:HB2      | 2.30                     | 0.45              |
| 1:A:120:GLY:O      | 1:A:125:ARG:HG2     | 2.16                     | 0.45              |
| 1:A:199:ALA:HB1    | 1:A:200:PRO:HD2     | 1.99                     | 0.45              |
| 1:B:184:ILE:HD13   | 1:B:204:VAL:HG13    | 1.98                     | 0.45              |
| 1:B:33:THR:O       | 1:B:35:GLY:N        | 2.50                     | 0.45              |
| 1:E:190:THR:HG22   | 1:E:193[A]:ARG:HH11 | 1.82                     | 0.45              |
| 1:E:64:ASN:HB3     | 1:E:66:ALA:N        | 2.31                     | 0.45              |
| 1:E:166:ARG:NH1    | 2:K:111:ILE:O       | 2.49                     | 0.45              |
| 2:K:47:PHE:CG      | 2:K:108:VAL:HG13    | 2.51                     | 0.45              |
| 1:B:151:LEU:HD23   | 1:B:164:LEU:HD12    | 1.98                     | 0.45              |
| 1:C:64:ASN:HB3     | 1:C:66:ALA:N        | 2.31                     | 0.45              |
| 1:D:8:ILE:HD12     | 1:D:61:GLU:HB2      | 1.96                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:K:14:ALA:CB      | 2:K:125:SER:HB3    | 2.45                     | 0.45              |
| 1:A:22:THR:OG1     | 1:A:189:ARG:HD2    | 2.15                     | 0.45              |
| 1:B:142:GLY:N      | 1:B:143:PRO:CD     | 2.80                     | 0.45              |
| 1:C:153:TYR:HB3    | 1:C:159:THR:HG23   | 1.97                     | 0.45              |
| 1:F:181:PHE:CZ     | 1:F:211:TRP:HD1    | 2.33                     | 0.45              |
| 2:H:107:ALA:HB1    | 2:H:112:ASP:HB3    | 1.98                     | 0.45              |
| 1:C:181:PHE:CZ     | 1:C:211:TRP:HD1    | 2.35                     | 0.45              |
| 1:E:114[B]:ARG:HG2 | 1:E:114[B]:ARG:NH1 | 2.32                     | 0.45              |
| 2:G:91:THR:O       | 2:G:92:ALA:HB2     | 2.15                     | 0.45              |
| 2:H:53:TRP:O       | 2:H:54:ALA:HB3     | 2.17                     | 0.45              |
| 2:G:102:VAL:HG11   | 2:G:107:ALA:HB2    | 1.99                     | 0.45              |
| 2:L:36:TRP:HA      | 2:L:95:TYR:O       | 2.16                     | 0.45              |
| 1:B:226:PHE:HE1    | 1:B:245:VAL:HG22   | 1.82                     | 0.45              |
| 1:D:48:ARG:NH1     | 1:D:100:ASP:OD1    | 2.50                     | 0.45              |
| 1:D:78:ASN:O       | 1:D:79:ALA:CB      | 2.65                     | 0.45              |
| 2:J:53:TRP:O       | 2:J:54:ALA:HB3     | 2.17                     | 0.45              |
| 2:K:12:VAL:HG22    | 2:K:124:VAL:HG12   | 1.98                     | 0.45              |
| 1:B:239:LYS:HE3    | 1:B:239:LYS:HB3    | 1.54                     | 0.45              |
| 1:C:91:TYR:OH      | 1:C:155:SER:HA     | 2.17                     | 0.45              |
| 1:C:68:LEU:HD11    | 1:C:149:SER:HA     | 1.99                     | 0.45              |
| 1:D:51:LEU:HD12    | 1:D:52:PRO:HD2     | 1.98                     | 0.45              |
| 1:E:91:TYR:OH      | 1:E:155:SER:HA     | 2.17                     | 0.45              |
| 1:E:8:ILE:HD12     | 1:E:61:GLU:HB2     | 1.99                     | 0.45              |
| 1:F:164:LEU:HG     | 1:F:168:PHE:CE2    | 2.52                     | 0.45              |
| 1:F:48:ARG:NH1     | 1:F:100:ASP:OD1    | 2.49                     | 0.45              |
| 1:F:72:LEU:N       | 1:F:72:LEU:CD1     | 2.79                     | 0.45              |
| 2:G:2:VAL:CG1      | 2:G:2:VAL:O        | 2.64                     | 0.45              |
| 2:J:88:PRO:CA      | 2:J:124:VAL:HG21   | 2.40                     | 0.45              |
| 2:J:121:GLN:NE2    | 2:J:122:VAL:O      | 2.46                     | 0.44              |
| 1:A:146:GLU:OE1    | 1:A:146:GLU:HA     | 2.17                     | 0.44              |
| 1:B:64:ASN:HB3     | 1:B:66:ALA:H       | 1.82                     | 0.44              |
| 1:E:24:PHE:O       | 1:E:27:ALA:HB3     | 2.17                     | 0.44              |
| 2:H:31:ARG:O       | 2:H:99:ASN:O       | 2.34                     | 0.44              |
| 1:B:71:THR:C       | 1:B:72:LEU:HD12    | 2.38                     | 0.44              |
| 2:G:103[A]:ARG:NH1 | 2:G:106:VAL:HG21   | 2.32                     | 0.44              |
| 2:I:121:GLN:HG3    | 2:I:122:VAL:N      | 2.33                     | 0.44              |
| 2:I:99:ASN:HB2     | 2:I:113:TYR:CD2    | 2.52                     | 0.44              |
| 2:J:28:THR:O       | 2:J:28:THR:HG23    | 2.17                     | 0.44              |
| 1:A:134:ARG:HH22   | 1:A:209:ASN:HD21   | 1.65                     | 0.44              |
| 1:C:173:GLN:O      | 1:C:177:GLU:HB2    | 2.17                     | 0.44              |
| 2:H:88:PRO:CA      | 2:H:124:VAL:HG21   | 2.41                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 2:K:102:VAL:HG21    | 2:K:112:ASP:HB3    | 1.99                     | 0.44              |
| 1:C:164:LEU:HG      | 1:C:168:PHE:CE2    | 2.53                     | 0.44              |
| 1:C:88:ASN:HD21     | 1:C:112:GLN:CD     | 2.21                     | 0.44              |
| 1:D:120:GLY:O       | 1:D:125:ARG:HG2    | 2.17                     | 0.44              |
| 1:E:47:ASN:ND2      | 1:E:49:VAL:HG22    | 2.33                     | 0.44              |
| 2:J:121:GLN:HG3     | 2:J:122:VAL:N      | 2.33                     | 0.44              |
| 2:J:5:VAL:CG1       | 2:J:6:GLU:N        | 2.79                     | 0.44              |
| 1:C:64:ASN:HD22     | 1:C:68:LEU:HD12    | 1.82                     | 0.44              |
| 1:C:94:HIS:HA       | 1:C:95:PRO:HD2     | 1.85                     | 0.44              |
| 1:D:123:TYR:CD1     | 1:D:134:ARG:HD3    | 2.52                     | 0.44              |
| 1:D:189:ARG:NH2     | 1:D:193:ARG:HH22   | 2.15                     | 0.44              |
| 1:D:49:VAL:CG2      | 1:D:50:GLY:N       | 2.71                     | 0.44              |
| 1:E:123:TYR:CD1     | 1:E:134:ARG:HD3    | 2.53                     | 0.44              |
| 1:E:25:ILE:O        | 1:E:26:ARG:C       | 2.56                     | 0.44              |
| 1:F:232:LEU:HA      | 1:F:232:LEU:HD23   | 1.62                     | 0.44              |
| 2:G:18:LEU:HA       | 2:G:18:LEU:HD23    | 1.69                     | 0.44              |
| 2:G:2:VAL:O         | 2:G:2:VAL:HG13     | 2.16                     | 0.44              |
| 2:G:60:TYR:CD1      | 2:G:60:TYR:N       | 2.84                     | 0.44              |
| 1:A:222:ASN:O       | 1:A:223:GLN:HG2    | 2.17                     | 0.44              |
| 2:I:51:ILE:HG23     | 2:I:51:ILE:O       | 2.18                     | 0.44              |
| 2:I:91:THR:O        | 2:I:92:ALA:HB2     | 2.18                     | 0.44              |
| 2:J:103:ARG:NH1     | 2:J:103:ARG:CG     | 2.81                     | 0.44              |
| 2:J:103:ARG:HG3     | 2:J:103:ARG:NH1    | 2.31                     | 0.44              |
| 2:K:4:LEU:HD23      | 2:K:24:ALA:CB      | 2.48                     | 0.44              |
| 1:B:153:TYR:HB3     | 1:B:159:THR:HG23   | 1.99                     | 0.44              |
| 1:D:190:THR:HG22    | 1:D:193:ARG:HH11   | 1.82                     | 0.44              |
| 2:H:103:ARG:HH22    | 2:H:106:VAL:CG2    | 2.31                     | 0.44              |
| 2:L:103[B]:ARG:HH11 | 2:L:103[B]:ARG:HG2 | 1.83                     | 0.44              |
| 1:B:120:GLY:O       | 1:B:125:ARG:HG2    | 2.18                     | 0.44              |
| 1:D:153:TYR:HB3     | 1:D:159:THR:HG23   | 1.98                     | 0.44              |
| 2:K:83:MET:CB       | 2:K:86:LEU:HD21    | 2.44                     | 0.44              |
| 1:A:248:LEU:HD23    | 1:A:248:LEU:N      | 2.33                     | 0.43              |
| 1:B:207:LEU:HA      | 1:B:207:LEU:HD23   | 1.87                     | 0.43              |
| 1:C:71:THR:O        | 1:C:84:TYR:HB2     | 2.18                     | 0.43              |
| 1:D:201:ASP:HB2     | 1:D:202:PRO:HD2    | 1.98                     | 0.43              |
| 1:E:222:ASN:O       | 1:E:223:GLN:HG2    | 2.17                     | 0.43              |
| 1:F:188:MET:HA      | 1:F:188:MET:CE     | 2.48                     | 0.43              |
| 1:F:22:THR:OG1      | 1:F:189:ARG:HD2    | 2.18                     | 0.43              |
| 2:G:121:GLN:HG3     | 2:G:122:VAL:N      | 2.33                     | 0.43              |
| 2:G:5:VAL:O         | 2:G:22:CYS:HA      | 2.18                     | 0.43              |
| 2:G:82:GLN:OE1      | 2:G:82:GLN:HA      | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:99:ASN:HB2   | 2:J:113:TYR:CD2  | 2.53                     | 0.43              |
| 2:K:35:GLY:O     | 2:K:96:CYS:HA    | 2.18                     | 0.43              |
| 1:B:214:LEU:HD23 | 1:B:214:LEU:HA   | 1.82                     | 0.43              |
| 1:D:17:THR:OG1   | 1:D:20:SER:HB3   | 2.18                     | 0.43              |
| 1:F:91:TYR:OH    | 1:F:155:SER:HA   | 2.17                     | 0.43              |
| 1:C:64:ASN:HB2   | 1:C:68:LEU:H     | 1.83                     | 0.43              |
| 1:D:207:LEU:HD23 | 1:D:207:LEU:HA   | 1.84                     | 0.43              |
| 1:A:64:ASN:HB3   | 1:A:66:ALA:N     | 2.33                     | 0.43              |
| 1:B:223:GLN:HG3  | 1:C:244:ASP:HB3  | 2.00                     | 0.43              |
| 1:E:34:THR:HG23  | 1:E:46:PRO:HG3   | 2.00                     | 0.43              |
| 2:H:86:LEU:HD12  | 2:H:86:LEU:N     | 2.33                     | 0.43              |
| 2:I:12:VAL:HG23  | 2:I:124:VAL:HG12 | 2.01                     | 0.43              |
| 2:L:14:ALA:CB    | 2:L:125:SER:HB3  | 2.47                     | 0.43              |
| 2:I:31:ARG:CG    | 2:I:98:ASP:OD1   | 2.64                     | 0.43              |
| 2:L:35:GLY:O     | 2:L:96:CYS:HA    | 2.18                     | 0.43              |
| 1:A:188:MET:HA   | 1:A:188:MET:CE   | 2.48                     | 0.43              |
| 1:C:239:LYS:HB3  | 1:C:239:LYS:HE3  | 1.57                     | 0.43              |
| 1:C:64:ASN:HD22  | 1:C:68:LEU:CD1   | 2.30                     | 0.43              |
| 1:D:183:TYR:HB2  | 1:D:251:ILE:HG23 | 2.00                     | 0.43              |
| 1:E:134:ARG:HH22 | 1:E:209:ASN:ND2  | 2.16                     | 0.43              |
| 1:E:204:VAL:O    | 1:E:208:GLU:HG3  | 2.19                     | 0.43              |
| 2:L:60:TYR:N     | 2:L:60:TYR:CD1   | 2.87                     | 0.43              |
| 1:C:151:LEU:HD23 | 1:C:164:LEU:CD1  | 2.49                     | 0.43              |
| 1:E:199:ALA:HB1  | 1:E:200:PRO:HD2  | 2.01                     | 0.43              |
| 1:F:263:PRO:O    | 1:F:264:SER:C    | 2.57                     | 0.43              |
| 2:I:60:TYR:CE2   | 2:I:70:VAL:HG23  | 2.53                     | 0.43              |
| 1:B:34:THR:HG23  | 1:B:46:PRO:HG3   | 2.01                     | 0.43              |
| 1:C:78:ASN:O     | 1:C:79:ALA:CB    | 2.66                     | 0.43              |
| 1:E:223:GLN:NE2  | 1:F:247:ILE:CD1  | 2.82                     | 0.43              |
| 1:E:234:ARG:HD2  | 1:E:238:SER:OG   | 2.19                     | 0.43              |
| 1:E:85:ARG:HD2   | 1:E:87:GLY:O     | 2.19                     | 0.43              |
| 2:G:107:ALA:HB1  | 2:G:112:ASP:HB3  | 2.00                     | 0.43              |
| 2:G:86:LEU:HB3   | 2:G:124:VAL:HG11 | 2.00                     | 0.43              |
| 2:H:124:VAL:O    | 2:H:125:SER:C    | 2.56                     | 0.43              |
| 2:J:103:ARG:HD3  | 2:J:105:LEU:HD12 | 2.00                     | 0.43              |
| 2:J:47:PHE:CD2   | 2:J:108:VAL:HG13 | 2.53                     | 0.43              |
| 2:J:52:VAL:C     | 2:J:53:TRP:O     | 2.57                     | 0.43              |
| 1:A:104:ILE:O    | 1:A:107:LEU:HB2  | 2.19                     | 0.43              |
| 1:A:232:LEU:HD23 | 1:A:232:LEU:HA   | 1.69                     | 0.43              |
| 1:D:166:ARG:NH2  | 2:J:112:ASP:O    | 2.52                     | 0.43              |
| 1:D:239:LYS:HB3  | 1:D:239:LYS:HE3  | 1.53                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:E:201:ASP:HB2    | 1:E:202:PRO:HD2   | 1.99                     | 0.43              |
| 1:F:107:LEU:HA     | 1:F:107:LEU:HD23  | 1.69                     | 0.43              |
| 2:I:44:GLU:CG      | 2:I:45:ARG:H      | 2.25                     | 0.43              |
| 2:J:103:ARG:CB     | 2:J:103:ARG:HH11  | 2.31                     | 0.43              |
| 2:J:77:ASN:OD1     | 2:J:78:MET:HG3    | 2.19                     | 0.43              |
| 1:B:189:ARG:NH2    | 1:B:193:ARG:HH22  | 2.15                     | 0.43              |
| 1:B:197:ARG:O      | 1:B:197:ARG:HG3   | 2.19                     | 0.43              |
| 1:B:8:ILE:HD12     | 1:B:61:GLU:HB2    | 2.00                     | 0.43              |
| 1:C:189:ARG:NH2    | 1:C:193:ARG:HH22  | 2.14                     | 0.43              |
| 1:C:204:VAL:O      | 1:C:208:GLU:HG3   | 2.19                     | 0.43              |
| 1:D:184:ILE:O      | 1:D:188:MET:HG2   | 2.19                     | 0.43              |
| 2:K:103[A]:ARG:HB3 | 2:K:106:VAL:HG23  | 2.01                     | 0.43              |
| 2:L:14:ALA:H       | 2:L:125:SER:CB    | 2.32                     | 0.43              |
| 1:A:153:TYR:HB3    | 1:A:159:THR:HG23  | 2.00                     | 0.42              |
| 1:B:136:ASN:O      | 2:H:102:VAL:HA    | 2.19                     | 0.42              |
| 1:C:123:TYR:CD1    | 1:C:134:ARG:HD3   | 2.53                     | 0.42              |
| 1:C:51:LEU:HD12    | 1:C:52:PRO:HD2    | 1.99                     | 0.42              |
| 1:D:204:VAL:O      | 1:D:208:GLU:HG3   | 2.19                     | 0.42              |
| 1:D:125:ARG:NH1    | 4:D:302:CL:CL     | 2.89                     | 0.42              |
| 1:E:190:THR:HA     | 1:E:193[A]:ARG:CB | 2.47                     | 0.42              |
| 1:F:60:VAL:HG12    | 1:F:60:VAL:O      | 2.19                     | 0.42              |
| 2:K:47:PHE:CD2     | 2:K:108:VAL:HG13  | 2.55                     | 0.42              |
| 1:C:183:TYR:HB2    | 1:C:251:ILE:HG23  | 2.00                     | 0.42              |
| 1:D:71:THR:C       | 1:D:72:LEU:HD12   | 2.40                     | 0.42              |
| 1:F:68:LEU:HD11    | 1:F:149:SER:HA    | 2.01                     | 0.42              |
| 2:I:33:SER:HB3     | 2:I:99:ASN:HD22   | 1.84                     | 0.42              |
| 2:K:64:VAL:HA      | 2:K:67:ARG:HH11   | 1.83                     | 0.42              |
| 1:B:88:ASN:HD21    | 1:B:112:GLN:CD    | 2.23                     | 0.42              |
| 1:C:201:ASP:HB2    | 1:C:202:PRO:HD2   | 1.99                     | 0.42              |
| 2:J:102:VAL:O      | 2:J:104:GLY:N     | 2.52                     | 0.42              |
| 2:K:85:ASN:C       | 2:K:85:ASN:OD1    | 2.55                     | 0.42              |
| 1:D:234:ARG:HD2    | 1:D:238:SER:OG    | 2.18                     | 0.42              |
| 1:F:181:PHE:HB2    | 1:F:184:ILE:HG13  | 2.01                     | 0.42              |
| 2:H:121:GLN:HG3    | 2:H:122:VAL:N     | 2.34                     | 0.42              |
| 2:J:16:GLY:O       | 2:J:86:LEU:HD13   | 2.20                     | 0.42              |
| 2:L:20:LEU:HD23    | 2:L:20:LEU:HA     | 1.56                     | 0.42              |
| 1:B:183:TYR:HB2    | 1:B:251:ILE:HG23  | 2.02                     | 0.42              |
| 1:D:42:ILE:HA      | 1:D:43:PRO:HD3    | 1.88                     | 0.42              |
| 1:E:142:GLY:N      | 1:E:143:PRO:CD    | 2.82                     | 0.42              |
| 1:F:190:THR:HG22   | 1:F:193:ARG:HH11  | 1.84                     | 0.42              |
| 1:F:71:THR:C       | 1:F:72:LEU:HD12   | 2.40                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:H:4:LEU:O      | 2:H:5:VAL:HG23     | 2.19                     | 0.42              |
| 1:B:48:ARG:HA    | 1:B:77:THR:HG21    | 2.02                     | 0.42              |
| 1:E:226:PHE:HE1  | 1:E:245:VAL:HG22   | 1.83                     | 0.42              |
| 1:F:207:LEU:HA   | 1:F:207:LEU:HD23   | 1.93                     | 0.42              |
| 1:B:64:ASN:HB3   | 1:B:66:ALA:N       | 2.34                     | 0.42              |
| 1:D:151:LEU:HD23 | 1:D:164:LEU:CD1    | 2.49                     | 0.42              |
| 1:D:91:TYR:OH    | 1:D:155:SER:HA     | 2.19                     | 0.42              |
| 1:E:144:LEU:HG   | 1:E:144:LEU:O      | 2.18                     | 0.42              |
| 1:E:68:LEU:HD12  | 1:E:68:LEU:C       | 2.40                     | 0.42              |
| 1:F:199:ALA:HB1  | 1:F:200:PRO:HD2    | 2.02                     | 0.42              |
| 2:G:37:PHE:CD2   | 2:G:47:PHE:HA      | 2.54                     | 0.42              |
| 2:H:73:ASP:O     | 2:H:74:ASN:O       | 2.37                     | 0.42              |
| 2:J:74:ASN:OD1   | 2:J:77:ASN:OD1     | 2.38                     | 0.42              |
| 2:K:14:ALA:H     | 2:K:125:SER:HB3    | 1.85                     | 0.42              |
| 1:D:138:GLU:HG3  | 2:J:103:ARG:HA     | 2.00                     | 0.42              |
| 1:D:181:PHE:CB   | 1:D:184:ILE:HG13   | 2.49                     | 0.42              |
| 1:D:13:THR:HG22  | 1:D:64:ASN:HA      | 2.01                     | 0.42              |
| 1:E:205:ILE:O    | 1:E:208:GLU:N      | 2.53                     | 0.42              |
| 1:E:245:VAL:HG12 | 1:E:245:VAL:O      | 2.18                     | 0.42              |
| 1:E:64:ASN:HB2   | 1:E:68:LEU:H       | 1.84                     | 0.42              |
| 2:H:52:VAL:C     | 2:H:53:TRP:O       | 2.57                     | 0.42              |
| 2:I:82:GLN:OE1   | 2:I:82:GLN:HA      | 2.20                     | 0.42              |
| 2:J:102:VAL:CG1  | 2:J:107:ALA:HB2    | 2.50                     | 0.42              |
| 1:E:189:ARG:HE   | 1:E:193[A]:ARG:NH2 | 2.17                     | 0.42              |
| 1:F:25:ILE:O     | 1:F:26:ARG:C       | 2.58                     | 0.42              |
| 1:A:132:ASN:OD1  | 1:A:132:ASN:N      | 2.53                     | 0.42              |
| 1:D:181:PHE:CZ   | 1:D:211:TRP:CD1    | 3.07                     | 0.42              |
| 1:D:199:ALA:HB1  | 1:D:200:PRO:HD2    | 2.02                     | 0.42              |
| 1:D:68:LEU:HD11  | 1:D:149:SER:HA     | 2.01                     | 0.42              |
| 1:E:145:GLU:O    | 1:E:146:GLU:C      | 2.58                     | 0.42              |
| 1:E:261:PRO:HA   | 1:E:262:PRO:HD3    | 1.74                     | 0.42              |
| 1:F:183:TYR:HB2  | 1:F:251:ILE:HG23   | 2.01                     | 0.42              |
| 1:F:189:ARG:NH2  | 1:F:193:ARG:HH22   | 2.18                     | 0.42              |
| 2:H:60:TYR:CE2   | 2:H:70:VAL:HG23    | 2.55                     | 0.42              |
| 1:A:197:ARG:HG3  | 1:A:197:ARG:O      | 2.19                     | 0.41              |
| 1:A:214:LEU:HD23 | 1:A:214:LEU:HA     | 1.87                     | 0.41              |
| 1:A:39:ARG:NH2   | 1:A:261:PRO:HD3    | 2.35                     | 0.41              |
| 1:B:60:VAL:HG12  | 1:B:60:VAL:O       | 2.19                     | 0.41              |
| 1:B:13:THR:HG22  | 1:B:64:ASN:HA      | 2.02                     | 0.41              |
| 1:F:239:LYS:HE3  | 1:F:239:LYS:HB3    | 1.46                     | 0.41              |
| 1:F:42:ILE:HA    | 1:F:43:PRO:HD3     | 1.88                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:86:LEU:CD1   | 2:H:86:LEU:N      | 2.82                     | 0.41              |
| 2:J:82:GLN:OE1   | 2:J:82:GLN:HA     | 2.19                     | 0.41              |
| 1:B:107:LEU:HD23 | 1:B:107:LEU:HA    | 1.58                     | 0.41              |
| 1:E:94:HIS:HA    | 1:E:95:PRO:HD2    | 1.74                     | 0.41              |
| 1:F:94:HIS:HB2   | 1:F:117:PHE:O     | 2.20                     | 0.41              |
| 2:G:68:PHE:N     | 2:G:68:PHE:CD1    | 2.88                     | 0.41              |
| 2:H:47:PHE:CG    | 2:H:108:VAL:CG1   | 3.02                     | 0.41              |
| 2:H:72[A]:ARG:CG | 2:H:72[A]:ARG:NH1 | 2.75                     | 0.41              |
| 2:K:20:LEU:HA    | 2:K:20:LEU:HD23   | 1.59                     | 0.41              |
| 2:J:12:VAL:HG23  | 2:J:124:VAL:HG12  | 2.02                     | 0.41              |
| 2:K:88:PRO:CA    | 2:K:124:VAL:HG21  | 2.48                     | 0.41              |
| 1:C:151:LEU:HD23 | 1:C:164:LEU:HD12  | 2.02                     | 0.41              |
| 1:E:107:LEU:HD23 | 1:E:107:LEU:HA    | 1.58                     | 0.41              |
| 1:E:239:LYS:HB3  | 1:E:239:LYS:HE3   | 1.55                     | 0.41              |
| 1:F:169:ILE:O    | 1:F:173:GLN:HG3   | 2.20                     | 0.41              |
| 1:F:78:ASN:O     | 1:F:79:ALA:CB     | 2.68                     | 0.41              |
| 2:G:60:TYR:CE2   | 2:G:70:VAL:HG23   | 2.55                     | 0.41              |
| 2:H:68:PHE:HD1   | 2:H:68:PHE:N      | 2.18                     | 0.41              |
| 1:B:189:ARG:HB3  | 1:B:189:ARG:HE    | 1.66                     | 0.41              |
| 1:C:166:ARG:NH2  | 2:I:112:ASP:O     | 2.52                     | 0.41              |
| 1:C:199:ALA:HB1  | 1:C:200:PRO:HD2   | 2.03                     | 0.41              |
| 1:E:88:ASN:OD1   | 1:E:112:GLN:HG3   | 2.20                     | 0.41              |
| 1:E:13:THR:HG22  | 1:E:64:ASN:HA     | 2.01                     | 0.41              |
| 1:E:247:ILE:HG13 | 1:E:248:LEU:HD23  | 2.03                     | 0.41              |
| 2:G:77:ASN:OD1   | 2:G:78:MET:HG3    | 2.20                     | 0.41              |
| 2:G:99:ASN:HB2   | 2:G:113:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:151:LEU:HD23 | 1:A:164:LEU:CD1   | 2.51                     | 0.41              |
| 1:C:48:ARG:HA    | 1:C:77:THR:HG21   | 2.01                     | 0.41              |
| 1:E:140:GLY:C    | 1:E:143:PRO:HD2   | 2.40                     | 0.41              |
| 1:E:134:ARG:NH2  | 1:E:209:ASN:OD1   | 2.53                     | 0.41              |
| 1:F:153:TYR:HB3  | 1:F:159:THR:HG23  | 2.01                     | 0.41              |
| 2:G:73:ASP:O     | 2:G:74:ASN:O      | 2.38                     | 0.41              |
| 2:H:102:VAL:HG11 | 2:H:107:ALA:HB2   | 2.03                     | 0.41              |
| 2:I:124:VAL:O    | 2:I:125:SER:C     | 2.59                     | 0.41              |
| 2:K:11:LEU:HA    | 2:K:123:THR:O     | 2.19                     | 0.41              |
| 2:L:31:ARG:HD3   | 2:L:34:MET:SD     | 2.61                     | 0.41              |
| 1:A:142:GLY:N    | 1:A:143:PRO:CD    | 2.83                     | 0.41              |
| 1:A:154:TYR:HA   | 1:A:159:THR:OG1   | 2.20                     | 0.41              |
| 1:A:226:PHE:HE1  | 1:A:245:VAL:HG22  | 1.85                     | 0.41              |
| 1:D:146:GLU:OE1  | 1:D:146:GLU:HA    | 2.21                     | 0.41              |
| 1:D:189:ARG:HE   | 1:D:189:ARG:HB3   | 1.63                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:106:VAL:HG12 | 2:G:106:VAL:O    | 2.21                     | 0.41              |
| 2:I:18:LEU:HA    | 2:I:18:LEU:HD23  | 1.76                     | 0.41              |
| 2:I:16:GLY:O     | 2:I:86:LEU:HD13  | 2.20                     | 0.41              |
| 1:D:188:MET:HA   | 1:D:188:MET:CE   | 2.51                     | 0.41              |
| 1:E:188:MET:CE   | 1:E:188:MET:HA   | 2.51                     | 0.41              |
| 2:H:68:PHE:N     | 2:H:68:PHE:CD1   | 2.89                     | 0.41              |
| 2:I:68:PHE:CD1   | 2:I:68:PHE:N     | 2.88                     | 0.41              |
| 1:A:216:THR:HG23 | 1:A:258:ARG:NE   | 2.36                     | 0.41              |
| 1:E:39:ARG:O     | 1:E:41:GLU:N     | 2.54                     | 0.41              |
| 1:E:247:ILE:CD1  | 1:F:223:GLN:HE22 | 2.33                     | 0.41              |
| 2:G:68:PHE:N     | 2:G:68:PHE:HD1   | 2.19                     | 0.41              |
| 2:H:18:LEU:HA    | 2:H:18:LEU:HD23  | 1.73                     | 0.41              |
| 2:H:28:THR:O     | 2:H:28:THR:HG23  | 2.21                     | 0.41              |
| 2:I:86:LEU:HB3   | 2:I:124:VAL:HG11 | 2.03                     | 0.41              |
| 2:J:64:VAL:O     | 2:J:65:LYS:C     | 2.58                     | 0.41              |
| 2:J:4:LEU:HD11   | 2:J:98:ASP:HB2   | 2.03                     | 0.41              |
| 2:J:33:SER:HB3   | 2:J:99:ASN:HD22  | 1.86                     | 0.41              |
| 2:K:2:VAL:O      | 2:K:3:GLN:HB2    | 2.21                     | 0.41              |
| 2:K:47:PHE:CZ    | 2:K:50:SER:HB3   | 2.56                     | 0.41              |
| 2:L:67:ARG:NE    | 2:L:87:LYS:HE3   | 2.36                     | 0.41              |
| 1:A:164:LEU:HG   | 1:A:168:PHE:HE2  | 1.85                     | 0.41              |
| 1:D:184:ILE:HD13 | 1:D:204:VAL:HG13 | 2.03                     | 0.41              |
| 1:E:17:THR:OG1   | 1:E:20:SER:HB3   | 2.20                     | 0.41              |
| 1:E:205:ILE:O    | 1:E:208:GLU:HB2  | 2.21                     | 0.41              |
| 2:H:5:VAL:HG12   | 2:H:6:GLU:N      | 2.35                     | 0.41              |
| 2:I:68:PHE:HD1   | 2:I:68:PHE:N     | 2.19                     | 0.41              |
| 2:K:2:VAL:CG1    | 2:K:2:VAL:O      | 2.69                     | 0.41              |
| 2:L:38:ARG:HB2   | 2:L:92:ALA:HB1   | 2.02                     | 0.41              |
| 1:A:13:THR:HG22  | 1:A:64:ASN:HA    | 2.02                     | 0.41              |
| 1:B:133:LEU:HD23 | 1:B:133:LEU:HA   | 1.77                     | 0.41              |
| 1:B:146:GLU:HA   | 1:B:146:GLU:OE1  | 2.21                     | 0.41              |
| 1:C:125:ARG:NH1  | 3:C:301:SO4:S    | 2.93                     | 0.41              |
| 1:C:133:LEU:HD23 | 1:C:133:LEU:HA   | 1.85                     | 0.41              |
| 2:H:91:THR:CG2   | 2:H:123:THR:HG22 | 2.46                     | 0.41              |
| 2:H:77:ASN:OD1   | 2:H:78:MET:HG3   | 2.21                     | 0.41              |
| 1:B:188:MET:CE   | 1:B:188:MET:HA   | 2.51                     | 0.40              |
| 1:A:74:LEU:CD1   | 1:A:81:VAL:HG22  | 2.50                     | 0.40              |
| 1:B:17:THR:OG1   | 1:B:20:SER:HB3   | 2.21                     | 0.40              |
| 1:B:232:LEU:HA   | 1:B:232:LEU:HD23 | 1.69                     | 0.40              |
| 1:F:189:ARG:NH2  | 5:F:401:HOH:O    | 2.54                     | 0.40              |
| 1:C:166:ARG:NH1  | 2:I:111:ILE:O    | 2.53                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:103[B]:ARG:O | 2:K:106:VAL:HG23 | 2.21                     | 0.40              |
| 2:K:16:GLY:O     | 2:K:86:LEU:HD12  | 2.22                     | 0.40              |
| 1:B:248:LEU:N    | 1:B:248:LEU:HD23 | 2.36                     | 0.40              |
| 1:C:232:LEU:HA   | 1:C:232:LEU:HD23 | 1.68                     | 0.40              |
| 1:C:92:PHE:HB3   | 1:C:104:ILE:HD13 | 2.03                     | 0.40              |
| 1:D:249:ILE:N    | 1:D:250:PRO:CD   | 2.83                     | 0.40              |
| 1:B:236:ASN:H    | 1:B:236:ASN:ND2  | 2.20                     | 0.40              |
| 1:B:46:PRO:HG2   | 1:B:76:VAL:CG1   | 2.52                     | 0.40              |
| 1:B:85:ARG:HD2   | 1:B:87:GLY:O     | 2.22                     | 0.40              |
| 1:C:72:LEU:N     | 1:C:72:LEU:CD1   | 2.83                     | 0.40              |
| 1:E:223:GLN:HG3  | 1:F:244:ASP:HB3  | 2.03                     | 0.40              |
| 1:E:51:LEU:HD12  | 1:E:51:LEU:HA    | 1.90                     | 0.40              |
| 1:B:234:ARG:HD2  | 1:B:238:SER:OG   | 2.22                     | 0.40              |
| 2:G:109:ARG:O    | 2:G:110:ALA:C    | 2.58                     | 0.40              |

All (4) 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) |
|-----------------|-------------------------|--------------------------|-------------------|
| 2:G:24:ALA:O    | 2:G:27:ARG:NH2[8_544]   | 1.85                     | 0.35              |
| 2:H:3:GLN:NE2   | 2:H:3:GLN:NE2[8_544]    | 1.96                     | 0.24              |
| 2:J:85:ASN:ND2  | 1:F:239:LYS:NZ[15_545]  | 2.17                     | 0.03              |
| 1:A:244:ASP:OD1 | 1:D:244:ASP:OD1[13_455] | 2.18                     | 0.02              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 257/261 (98%) | 244 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | B     | 258/261 (99%) | 244 (95%) | 14 (5%) | 0        | 100         | 100 |
| 1   | C     | 257/261 (98%) | 243 (95%) | 14 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | D     | 257/261 (98%)   | 244 (95%)  | 13 (5%)  | 0        | 100         | 100 |
| 1   | E     | 259/261 (99%)   | 248 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 1   | F     | 258/261 (99%)   | 244 (95%)  | 14 (5%)  | 0        | 100         | 100 |
| 2   | G     | 118/127 (93%)   | 105 (89%)  | 13 (11%) | 0        | 100         | 100 |
| 2   | H     | 122/127 (96%)   | 108 (88%)  | 14 (12%) | 0        | 100         | 100 |
| 2   | I     | 112/127 (88%)   | 100 (89%)  | 12 (11%) | 0        | 100         | 100 |
| 2   | J     | 113/127 (89%)   | 99 (88%)   | 14 (12%) | 0        | 100         | 100 |
| 2   | K     | 122/127 (96%)   | 112 (92%)  | 10 (8%)  | 0        | 100         | 100 |
| 2   | L     | 118/127 (93%)   | 106 (90%)  | 12 (10%) | 0        | 100         | 100 |
| All | All   | 2251/2328 (97%) | 2097 (93%) | 154 (7%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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     | 218/220 (99%)  | 200 (92%) | 18 (8%)  | 11          | 38 |
| 1   | B     | 219/220 (100%) | 200 (91%) | 19 (9%)  | 10          | 36 |
| 1   | C     | 218/220 (99%)  | 201 (92%) | 17 (8%)  | 12          | 40 |
| 1   | D     | 218/220 (99%)  | 199 (91%) | 19 (9%)  | 10          | 36 |
| 1   | E     | 220/220 (100%) | 204 (93%) | 16 (7%)  | 14          | 43 |
| 1   | F     | 219/220 (100%) | 202 (92%) | 17 (8%)  | 12          | 40 |
| 2   | G     | 100/103 (97%)  | 85 (85%)  | 15 (15%) | 3           | 12 |
| 2   | H     | 101/103 (98%)  | 86 (85%)  | 15 (15%) | 3           | 13 |
| 2   | I     | 95/103 (92%)   | 81 (85%)  | 14 (15%) | 3           | 13 |
| 2   | J     | 96/103 (93%)   | 82 (85%)  | 14 (15%) | 3           | 13 |
| 2   | K     | 101/103 (98%)  | 82 (81%)  | 19 (19%) | 1           | 6  |
| 2   | L     | 100/103 (97%)  | 84 (84%)  | 16 (16%) | 2           | 11 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |
|-----|-------|-----------------|------------|-----------|-------------|
| All | All   | 1905/1938 (98%) | 1706 (90%) | 199 (10%) | 7 27        |

All (199) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 5   | GLN  |
| 1   | A     | 8   | ILE  |
| 1   | A     | 17  | THR  |
| 1   | A     | 20  | SER  |
| 1   | A     | 28  | VAL  |
| 1   | A     | 34  | THR  |
| 1   | A     | 38  | VAL  |
| 1   | A     | 39  | ARG  |
| 1   | A     | 64  | ASN  |
| 1   | A     | 96  | ASP  |
| 1   | A     | 102 | GLU  |
| 1   | A     | 114 | ARG  |
| 1   | A     | 116 | THR  |
| 1   | A     | 122 | ASN  |
| 1   | A     | 125 | ARG  |
| 1   | A     | 132 | ASN  |
| 1   | A     | 156 | THR  |
| 1   | A     | 239 | LYS  |
| 2   | G     | 2   | VAL  |
| 2   | G     | 7   | SER  |
| 2   | G     | 18  | LEU  |
| 2   | G     | 27  | ARG  |
| 2   | G     | 31  | ARG  |
| 2   | G     | 32  | SER  |
| 2   | G     | 33  | SER  |
| 2   | G     | 53  | TRP  |
| 2   | G     | 55  | ASP  |
| 2   | G     | 67  | ARG  |
| 2   | G     | 69  | THR  |
| 2   | G     | 72  | ARG  |
| 2   | G     | 105 | LEU  |
| 2   | G     | 123 | THR  |
| 2   | G     | 124 | VAL  |
| 1   | B     | 5   | GLN  |
| 1   | B     | 8   | ILE  |
| 1   | B     | 13  | THR  |
| 1   | B     | 17  | THR  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 20         | SER         |
| 1          | B            | 34         | THR         |
| 1          | B            | 38         | VAL         |
| 1          | B            | 39         | ARG         |
| 1          | B            | 64         | ASN         |
| 1          | B            | 96         | ASP         |
| 1          | B            | 102        | GLU         |
| 1          | B            | 114        | ARG         |
| 1          | B            | 116        | THR         |
| 1          | B            | 122        | ASN         |
| 1          | B            | 125        | ARG         |
| 1          | B            | 132        | ASN         |
| 1          | B            | 145        | GLU         |
| 1          | B            | 156        | THR         |
| 1          | B            | 239        | LYS         |
| 2          | H            | 7          | SER         |
| 2          | H            | 18         | LEU         |
| 2          | H            | 27         | ARG         |
| 2          | H            | 31         | ARG         |
| 2          | H            | 32         | SER         |
| 2          | H            | 33         | SER         |
| 2          | H            | 53         | TRP         |
| 2          | H            | 55         | ASP         |
| 2          | H            | 67         | ARG         |
| 2          | H            | 69         | THR         |
| 2          | H            | 72[A]      | ARG         |
| 2          | H            | 72[B]      | ARG         |
| 2          | H            | 105        | LEU         |
| 2          | H            | 123        | THR         |
| 2          | H            | 124        | VAL         |
| 1          | C            | 5          | GLN         |
| 1          | C            | 8          | ILE         |
| 1          | C            | 17         | THR         |
| 1          | C            | 28         | VAL         |
| 1          | C            | 34         | THR         |
| 1          | C            | 38         | VAL         |
| 1          | C            | 39         | ARG         |
| 1          | C            | 74         | LEU         |
| 1          | C            | 96         | ASP         |
| 1          | C            | 102        | GLU         |
| 1          | C            | 114        | ARG         |
| 1          | C            | 116        | THR         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | C            | 122        | ASN         |
| 1          | C            | 125        | ARG         |
| 1          | C            | 145        | GLU         |
| 1          | C            | 156        | THR         |
| 1          | C            | 239        | LYS         |
| 2          | I            | 7          | SER         |
| 2          | I            | 18         | LEU         |
| 2          | I            | 30         | SER         |
| 2          | I            | 31         | ARG         |
| 2          | I            | 32         | SER         |
| 2          | I            | 33         | SER         |
| 2          | I            | 53         | TRP         |
| 2          | I            | 55         | ASP         |
| 2          | I            | 67         | ARG         |
| 2          | I            | 69         | THR         |
| 2          | I            | 72         | ARG         |
| 2          | I            | 105        | LEU         |
| 2          | I            | 123        | THR         |
| 2          | I            | 124        | VAL         |
| 1          | D            | 5          | GLN         |
| 1          | D            | 8          | ILE         |
| 1          | D            | 17         | THR         |
| 1          | D            | 20         | SER         |
| 1          | D            | 28         | VAL         |
| 1          | D            | 34         | THR         |
| 1          | D            | 38         | VAL         |
| 1          | D            | 39         | ARG         |
| 1          | D            | 64         | ASN         |
| 1          | D            | 74         | LEU         |
| 1          | D            | 96         | ASP         |
| 1          | D            | 102        | GLU         |
| 1          | D            | 114        | ARG         |
| 1          | D            | 116        | THR         |
| 1          | D            | 122        | ASN         |
| 1          | D            | 125        | ARG         |
| 1          | D            | 132        | ASN         |
| 1          | D            | 145        | GLU         |
| 1          | D            | 156        | THR         |
| 2          | J            | 7          | SER         |
| 2          | J            | 18         | LEU         |
| 2          | J            | 30         | SER         |
| 2          | J            | 31         | ARG         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | J            | 32         | SER         |
| 2          | J            | 33         | SER         |
| 2          | J            | 53         | TRP         |
| 2          | J            | 55         | ASP         |
| 2          | J            | 67         | ARG         |
| 2          | J            | 69         | THR         |
| 2          | J            | 72         | ARG         |
| 2          | J            | 103        | ARG         |
| 2          | J            | 105        | LEU         |
| 2          | J            | 124        | VAL         |
| 1          | E            | 5          | GLN         |
| 1          | E            | 8          | ILE         |
| 1          | E            | 13         | THR         |
| 1          | E            | 17         | THR         |
| 1          | E            | 20         | SER         |
| 1          | E            | 34         | THR         |
| 1          | E            | 38         | VAL         |
| 1          | E            | 39         | ARG         |
| 1          | E            | 96         | ASP         |
| 1          | E            | 102        | GLU         |
| 1          | E            | 116        | THR         |
| 1          | E            | 122        | ASN         |
| 1          | E            | 125        | ARG         |
| 1          | E            | 145        | GLU         |
| 1          | E            | 156        | THR         |
| 1          | E            | 239        | LYS         |
| 2          | K            | 7          | SER         |
| 2          | K            | 28         | THR         |
| 2          | K            | 29         | PHE         |
| 2          | K            | 30         | SER         |
| 2          | K            | 33         | SER         |
| 2          | K            | 50         | SER         |
| 2          | K            | 53         | TRP         |
| 2          | K            | 63         | SER         |
| 2          | K            | 65         | LYS         |
| 2          | K            | 69         | THR         |
| 2          | K            | 71         | SER         |
| 2          | K            | 78         | MET         |
| 2          | K            | 79         | VAL         |
| 2          | K            | 96         | CYS         |
| 2          | K            | 105        | LEU         |
| 2          | K            | 106        | VAL         |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 2          | K            | 115        | TYR         |
| 2          | K            | 118        | GLN         |
| 2          | K            | 120        | THR         |
| 1          | F            | 5          | GLN         |
| 1          | F            | 8          | ILE         |
| 1          | F            | 17         | THR         |
| 1          | F            | 28         | VAL         |
| 1          | F            | 34         | THR         |
| 1          | F            | 38         | VAL         |
| 1          | F            | 39         | ARG         |
| 1          | F            | 64         | ASN         |
| 1          | F            | 96         | ASP         |
| 1          | F            | 102        | GLU         |
| 1          | F            | 114        | ARG         |
| 1          | F            | 116        | THR         |
| 1          | F            | 122        | ASN         |
| 1          | F            | 125        | ARG         |
| 1          | F            | 132        | ASN         |
| 1          | F            | 145        | GLU         |
| 1          | F            | 156        | THR         |
| 2          | L            | 28         | THR         |
| 2          | L            | 29         | PHE         |
| 2          | L            | 30         | SER         |
| 2          | L            | 33         | SER         |
| 2          | L            | 53         | TRP         |
| 2          | L            | 63         | SER         |
| 2          | L            | 65         | LYS         |
| 2          | L            | 69         | THR         |
| 2          | L            | 71         | SER         |
| 2          | L            | 78         | MET         |
| 2          | L            | 79         | VAL         |
| 2          | L            | 96         | CYS         |
| 2          | L            | 105        | LEU         |
| 2          | L            | 106        | VAL         |
| 2          | L            | 118        | GLN         |
| 2          | L            | 120        | THR         |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 1          | B            | 10         | ASN         |
| 1          | B            | 223        | GLN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 64  | ASN  |
| 1   | C     | 223 | GLN  |
| 1   | E     | 223 | GLN  |
| 1   | F     | 160 | GLN  |
| 1   | F     | 223 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | SO4  | B     | 302 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.38 | 0           |
| 3   | SO4  | B     | 301 | -    | 4,4,4        | 0.25 | 0           | 6,6,6       | 1.10 | 0           |
| 3   | SO4  | L     | 201 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.30 | 0           |
| 3   | SO4  | C     | 303 | -    | 4,4,4        | 0.07 | 0           | 6,6,6       | 0.42 | 0           |
| 3   | SO4  | E     | 303 | -    | 4,4,4        | 0.27 | 0           | 6,6,6       | 0.68 | 0           |
| 3   | SO4  | I     | 201 | -    | 4,4,4        | 0.16 | 0           | 6,6,6       | 0.34 | 0           |
| 3   | SO4  | G     | 201 | -    | 4,4,4        | 0.15 | 0           | 6,6,6       | 0.40 | 0           |
| 3   | SO4  | A     | 302 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.33 | 0           |
| 3   | SO4  | B     | 304 | -    | 4,4,4        | 0.13 | 0           | 6,6,6       | 0.16 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | B     | 303 | -    | 4,4,4        | 0.22 | 0        | 6,6,6       | 0.31 | 0        |
| 3   | SO4  | F     | 301 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.43 | 0        |
| 3   | SO4  | E     | 302 | -    | 4,4,4        | 0.19 | 0        | 6,6,6       | 0.39 | 0        |
| 3   | SO4  | C     | 301 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 1.00 | 0        |
| 3   | SO4  | D     | 301 | -    | 4,4,4        | 0.08 | 0        | 6,6,6       | 0.29 | 0        |
| 3   | SO4  | A     | 301 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.33 | 0        |
| 3   | SO4  | F     | 302 | -    | 4,4,4        | 0.22 | 0        | 6,6,6       | 0.39 | 0        |
| 3   | SO4  | C     | 302 | -    | 4,4,4        | 0.17 | 0        | 6,6,6       | 0.35 | 0        |
| 3   | SO4  | E     | 301 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.74 | 0        |
| 3   | SO4  | B     | 305 | -    | 4,4,4        | 0.09 | 0        | 6,6,6       | 0.34 | 0        |
| 3   | SO4  | J     | 201 | -    | 4,4,4        | 0.19 | 0        | 6,6,6       | 0.21 | 0        |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 301 | SO4  | 2       | 0            |
| 3   | C     | 303 | SO4  | 1       | 0            |
| 3   | E     | 303 | SO4  | 1       | 0            |
| 3   | B     | 304 | SO4  | 4       | 0            |
| 3   | F     | 301 | SO4  | 3       | 0            |
| 3   | C     | 301 | SO4  | 2       | 0            |
| 3   | A     | 301 | SO4  | 3       | 0            |
| 3   | F     | 302 | SO4  | 1       | 0            |
| 3   | B     | 305 | SO4  | 1       | 0            |

## 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 i

### 6.1 Protein, DNA and RNA chains i

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 259/261 (99%)   | -0.15  | 2 (0%) 86 72  | 62, 93, 122, 145      | 0     |
| 1   | B     | 260/261 (99%)   | -0.21  | 2 (0%) 86 72  | 48, 80, 111, 147      | 0     |
| 1   | C     | 259/261 (99%)   | -0.17  | 0 100 100     | 60, 90, 119, 140      | 0     |
| 1   | D     | 259/261 (99%)   | -0.02  | 5 (1%) 66 46  | 74, 101, 128, 154     | 0     |
| 1   | E     | 259/261 (99%)   | -0.23  | 0 100 100     | 33, 66, 102, 134      | 0     |
| 1   | F     | 260/261 (99%)   | -0.27  | 0 100 100     | 45, 77, 116, 130      | 0     |
| 2   | G     | 123/127 (96%)   | 0.38   | 4 (3%) 46 24  | 78, 108, 137, 179     | 0     |
| 2   | H     | 125/127 (98%)   | 0.33   | 3 (2%) 59 37  | 60, 93, 120, 171      | 0     |
| 2   | I     | 118/127 (92%)   | 0.33   | 8 (6%) 17 7   | 77, 104, 135, 156     | 0     |
| 2   | J     | 119/127 (93%)   | 0.75   | 9 (7%) 13 5   | 96, 121, 144, 171     | 0     |
| 2   | K     | 125/127 (98%)   | -0.18  | 0 100 100     | 26, 58, 98, 111       | 0     |
| 2   | L     | 123/127 (96%)   | -0.02  | 1 (0%) 86 72  | 52, 84, 120, 139      | 0     |
| All | All   | 2289/2328 (98%) | -0.03  | 34 (1%) 73 54 | 26, 89, 128, 179      | 0     |

All (34) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | I     | 85  | ASN  | 3.8  |
| 2   | I     | 67  | ARG  | 3.3  |
| 2   | G     | 28  | THR  | 3.1  |
| 2   | G     | 65  | LYS  | 3.1  |
| 2   | I     | 84  | ASN  | 3.1  |
| 1   | D     | 136 | ASN  | 3.0  |
| 2   | I     | 63  | SER  | 2.9  |
| 1   | A     | 263 | PRO  | 2.8  |
| 2   | J     | 35  | GLY  | 2.8  |
| 1   | D     | 238 | SER  | 2.7  |
| 1   | B     | 264 | SER  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | J     | 68  | PHE  | 2.5  |
| 2   | J     | 104 | GLY  | 2.5  |
| 2   | J     | 17  | SER  | 2.5  |
| 1   | A     | 262 | PRO  | 2.5  |
| 2   | I     | 13  | GLN  | 2.5  |
| 2   | L     | 28  | THR  | 2.3  |
| 2   | J     | 49  | ALA  | 2.3  |
| 2   | I     | 68  | PHE  | 2.3  |
| 2   | H     | 71  | SER  | 2.2  |
| 1   | D     | 194 | TYR  | 2.1  |
| 1   | D     | 241 | SER  | 2.1  |
| 1   | D     | 261 | PRO  | 2.1  |
| 2   | H     | 26  | GLY  | 2.1  |
| 2   | J     | 51  | ILE  | 2.1  |
| 2   | I     | 25  | SER  | 2.1  |
| 2   | J     | 53  | TRP  | 2.1  |
| 2   | J     | 83  | MET  | 2.1  |
| 2   | I     | 83  | MET  | 2.1  |
| 2   | J     | 13  | GLN  | 2.0  |
| 2   | G     | 60  | TYR  | 2.0  |
| 1   | B     | 34  | THR  | 2.0  |
| 2   | H     | 74  | ASN  | 2.0  |
| 2   | G     | 86  | LEU  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | SO4  | C     | 303 | 5/5   | 0.73 | 0.33 | 109,132,166,186            | 0     |
| 3   | SO4  | D     | 301 | 5/5   | 0.77 | 0.23 | 89,122,180,197             | 0     |
| 3   | SO4  | B     | 304 | 5/5   | 0.79 | 0.32 | 149,162,186,206            | 0     |
| 3   | SO4  | G     | 201 | 5/5   | 0.80 | 0.29 | 57,87,160,182              | 0     |
| 3   | SO4  | B     | 302 | 5/5   | 0.84 | 0.23 | 54,130,184,193             | 0     |
| 3   | SO4  | J     | 201 | 5/5   | 0.86 | 0.22 | 60,119,163,174             | 0     |
| 3   | SO4  | B     | 305 | 5/5   | 0.89 | 0.14 | 84,119,120,156             | 0     |
| 3   | SO4  | A     | 302 | 5/5   | 0.89 | 0.20 | 58,95,185,235              | 0     |
| 3   | SO4  | B     | 303 | 5/5   | 0.90 | 0.22 | 30,74,172,189              | 0     |
| 3   | SO4  | I     | 201 | 5/5   | 0.92 | 0.21 | 48,90,150,162              | 0     |
| 4   | CL   | K     | 201 | 1/1   | 0.93 | 0.21 | 42,42,42,42                | 0     |
| 3   | SO4  | E     | 302 | 5/5   | 0.94 | 0.26 | 28,70,183,217              | 0     |
| 3   | SO4  | C     | 302 | 5/5   | 0.94 | 0.15 | 98,104,154,156             | 0     |
| 3   | SO4  | E     | 303 | 5/5   | 0.94 | 0.12 | 38,66,138,203              | 0     |
| 3   | SO4  | L     | 201 | 5/5   | 0.95 | 0.21 | 87,97,114,115              | 0     |
| 3   | SO4  | E     | 301 | 5/5   | 0.95 | 0.27 | 16,52,139,160              | 0     |
| 4   | CL   | D     | 302 | 1/1   | 0.95 | 0.16 | 46,46,46,46                | 0     |
| 3   | SO4  | F     | 302 | 5/5   | 0.95 | 0.14 | 54,97,156,163              | 0     |
| 3   | SO4  | C     | 301 | 5/5   | 0.96 | 0.13 | 12,42,80,124               | 0     |
| 3   | SO4  | F     | 301 | 5/5   | 0.97 | 0.11 | 11,25,74,146               | 0     |
| 3   | SO4  | A     | 301 | 5/5   | 0.97 | 0.16 | 40,47,104,133              | 0     |
| 4   | CL   | E     | 304 | 1/1   | 0.98 | 0.34 | 30,30,30,30                | 0     |
| 3   | SO4  | B     | 301 | 5/5   | 0.98 | 0.10 | 40,44,58,115               | 0     |

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

There are no such residues in this entry.