



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:02 PM GMT

PDB ID : 4NG2  
Title : Crystal structure of LasR LBD-QslA complex from *Pseudomonas aeruginosa*  
Authors : Fan, H.; Wu, D.H.; Song, H.  
Deposited on : 2013-11-01  
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

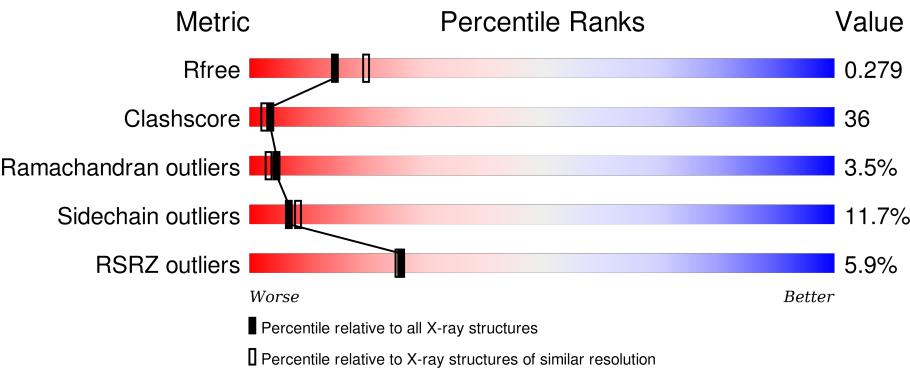
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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 <sub>free</sub>     | 91344                       | 3386 (2.44-2.40)                                      |
| Clashscore            | 102246                      | 3897 (2.44-2.40)                                      |
| Ramachandran outliers | 100387                      | 3837 (2.44-2.40)                                      |
| Sidechain outliers    | 100360                      | 3838 (2.44-2.40)                                      |
| RSRZ outliers         | 91569                       | 3396 (2.44-2.40)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | A     | 184    | <div><div>2%</div><div>66%</div><div>20%</div><div>•</div><div>10%</div></div>               |
| 1   | B     | 184    | <div><div>60%</div><div>27%</div><div>•</div><div>10%</div></div>                            |
| 1   | C     | 184    | <div><div>6%</div><div>49%</div><div>36%</div><div>• •</div><div>10%</div></div>             |
| 1   | D     | 184    | <div><div>2%</div><div>67%</div><div>19%</div><div>•</div><div>10%</div></div>               |
| 2   | E     | 113    | <div><div>4%</div><div>39%</div><div>32%</div><div>12%</div><div>•</div><div>17%</div></div> |

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| Mol | Chain | Length | Quality of chain           |
|-----|-------|--------|----------------------------|
| 2   | F     | 113    | <p>7% 35% 29% 9% 27%</p>   |
| 2   | G     | 113    | <p>8% 31% 33% 8% 27%</p>   |
| 2   | H     | 113    | <p>8% 44% 28% 10% 17%</p>  |
| 2   | I     | 113    | <p>10% 29% 41% 13% 17%</p> |
| 2   | J     | 113    | <p>12% 24% 34% 14% 27%</p> |
| 2   | K     | 113    | <p>1% 46% 20% 6% 27%</p>   |
| 2   | L     | 113    | <p>5% 45% 26% 11% 17%</p>  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11158 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 Transcriptional activator protein LasR.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 217 | 242 | 5 |         |         |       |
| 1   | B     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 217 | 242 | 5 |         |         |       |
| 1   | C     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 217 | 242 | 5 |         |         |       |
| 1   | D     | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 834 | 217 | 242 | 5 |         |         |       |

There are 56 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -13     | MET      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -12     | GLY      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -11     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -10     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -9      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -8      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -7      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -6      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -5      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -4      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -3      | SER      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -2      | GLN      | -      | EXPRESSION TAG | UNP P25084 |
| A     | -1      | ASP      | -      | EXPRESSION TAG | UNP P25084 |
| A     | 0       | PRO      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -13     | MET      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -12     | GLY      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -11     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -10     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -9      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -8      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -7      | HIS      | -      | EXPRESSION TAG | UNP P25084 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -6      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -5      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -4      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -3      | SER      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -2      | GLN      | -      | EXPRESSION TAG | UNP P25084 |
| B     | -1      | ASP      | -      | EXPRESSION TAG | UNP P25084 |
| B     | 0       | PRO      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -13     | MET      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -12     | GLY      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -11     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -10     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -9      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -8      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -7      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -6      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -5      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -4      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -3      | SER      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -2      | GLN      | -      | EXPRESSION TAG | UNP P25084 |
| C     | -1      | ASP      | -      | EXPRESSION TAG | UNP P25084 |
| C     | 0       | PRO      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -13     | MET      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -12     | GLY      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -11     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -10     | SER      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -9      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -8      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -7      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -6      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -5      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -4      | HIS      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -3      | SER      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -2      | GLN      | -      | EXPRESSION TAG | UNP P25084 |
| D     | -1      | ASP      | -      | EXPRESSION TAG | UNP P25084 |
| D     | 0       | PRO      | -      | EXPRESSION TAG | UNP P25084 |

- Molecule 2 is a protein called Uncharacterized protein.

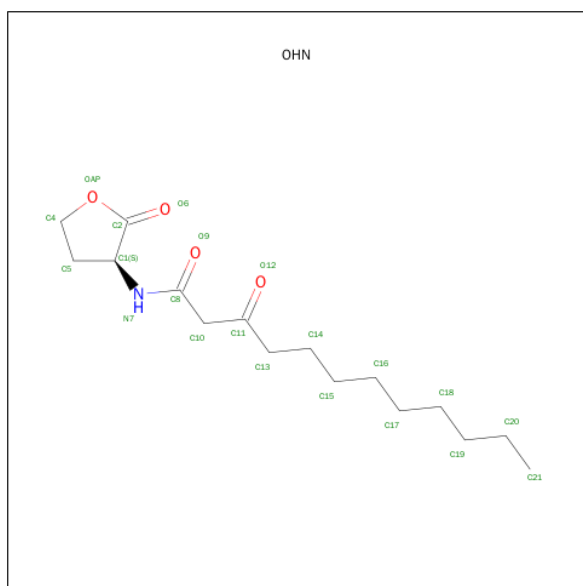
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | E     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 751   | 483 | 133 | 133 | 2 |         |         |       |
| 2   | F     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 417 | 114 | 115 | 2 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | G     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 417 | 114 | 115 | 2 |         |         |       |
| 2   | H     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 751   | 483 | 133 | 133 | 2 |         |         |       |
| 2   | I     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 751   | 483 | 133 | 133 | 2 |         |         |       |
| 2   | J     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 417 | 114 | 115 | 2 |         |         |       |
| 2   | K     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 417 | 114 | 115 | 2 |         |         |       |
| 2   | L     | 94       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 751   | 483 | 133 | 133 | 2 |         |         |       |

- Molecule 3 is N-3-OXO-DODECANOYL-L-HOMOSERINE LACTONE (three-letter code: OHN) (formula: C<sub>16</sub>H<sub>27</sub>NO<sub>4</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 3   | A     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |
| 3   | B     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |
| 3   | C     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |
| 3   | D     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 21    | 16 | 1 | 4 |         |         |

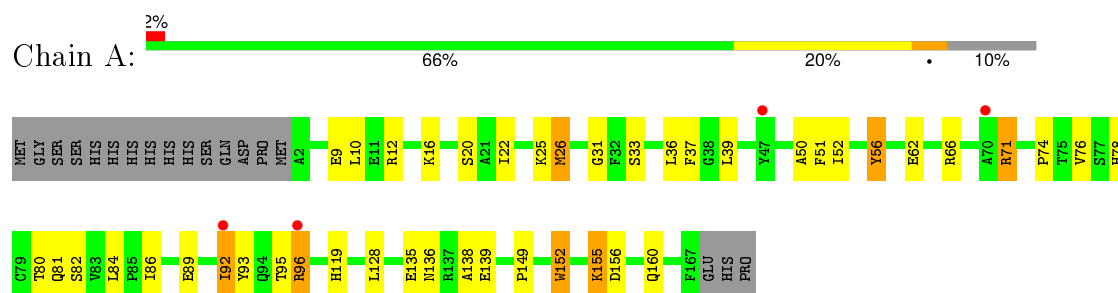
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 4   | A     | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 4   | B     | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 4   | C     | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 4   | D     | 52       | Total<br>52 | O<br>52 | 0       | 0       |
| 4   | E     | 29       | Total<br>29 | O<br>29 | 0       | 0       |
| 4   | F     | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 4   | G     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 4   | H     | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 4   | I     | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 4   | J     | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 4   | K     | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 4   | L     | 33       | Total<br>33 | O<br>33 | 0       | 0       |

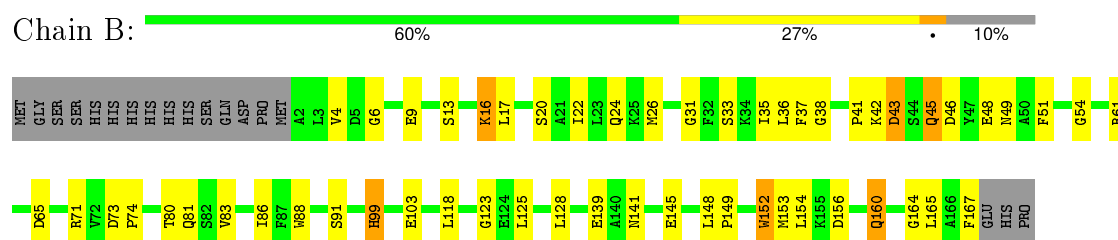
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

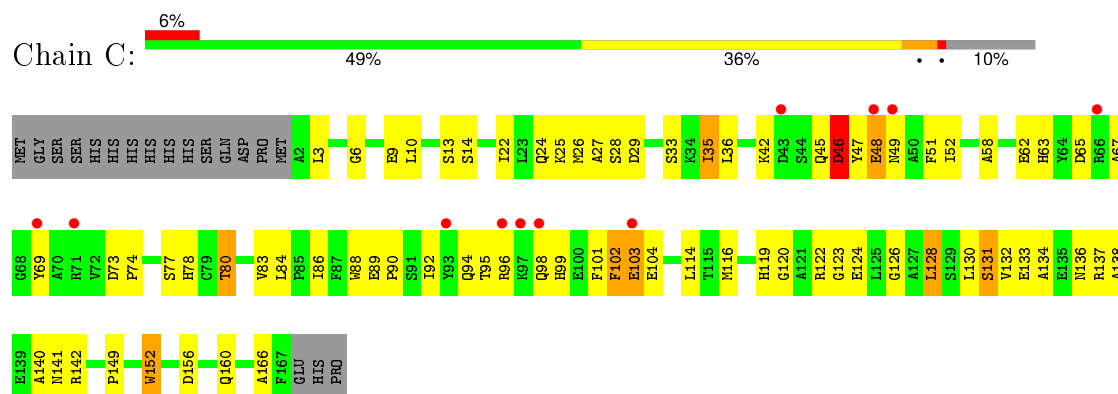
- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR



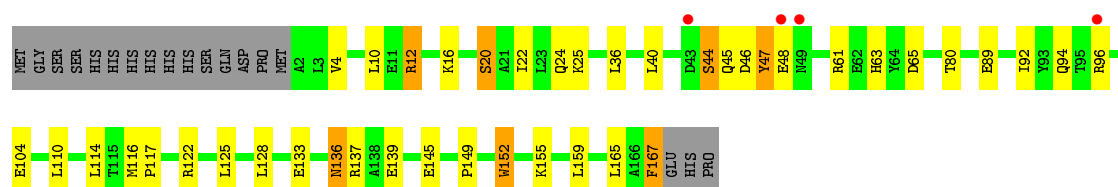
- Molecule 1: Transcriptional activator protein LasR



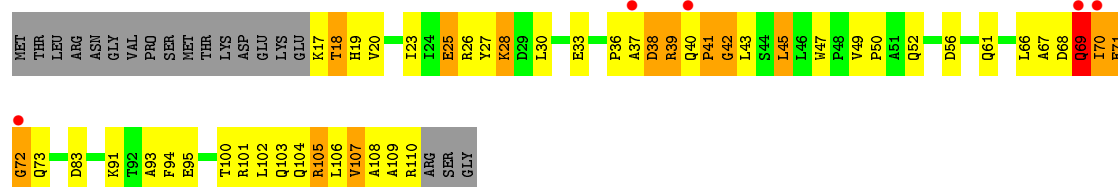
- Molecule 1: Transcriptional activator protein LasR







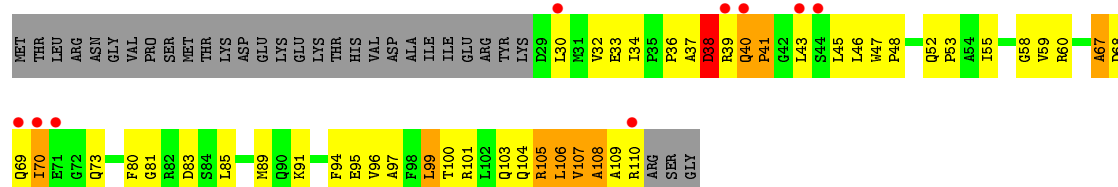
- Molecule 2: Uncharacterized protein



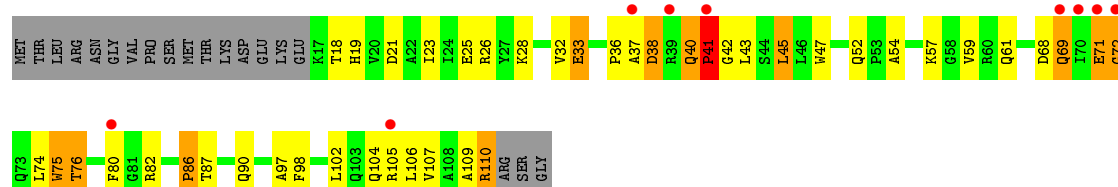
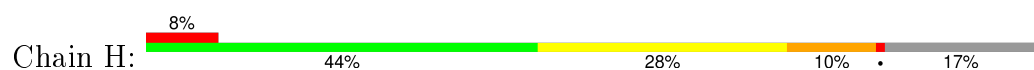
- Molecule 2: Uncharacterized protein



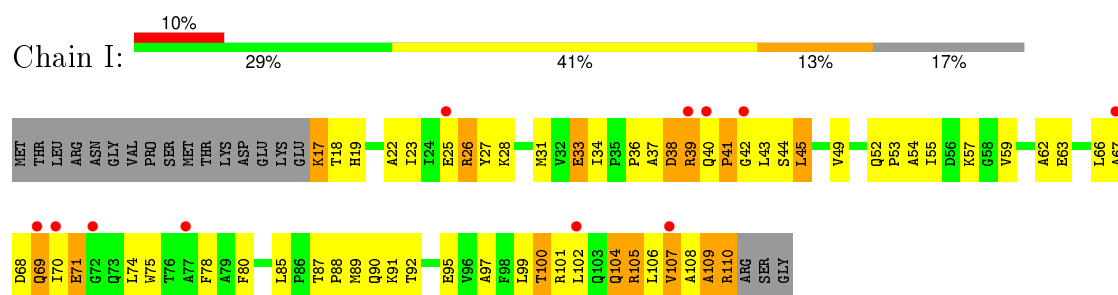
- Molecule 2: Uncharacterized protein



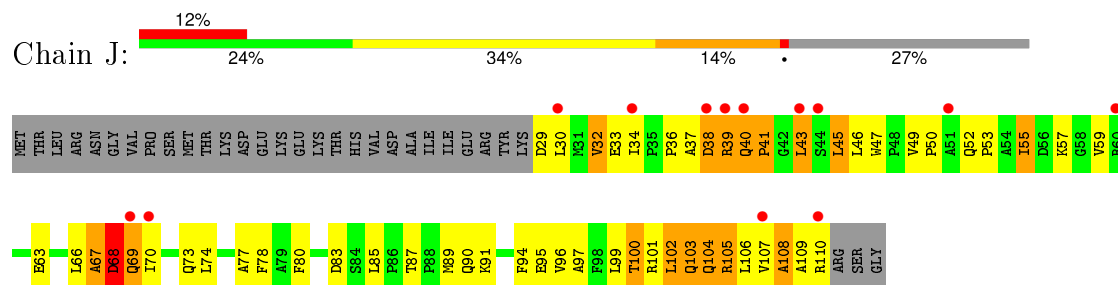
- Molecule 2: Uncharacterized protein



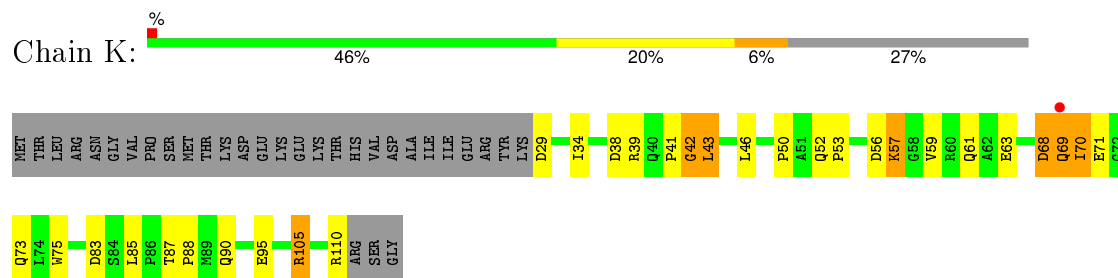
- Molecule 2: Uncharacterized protein



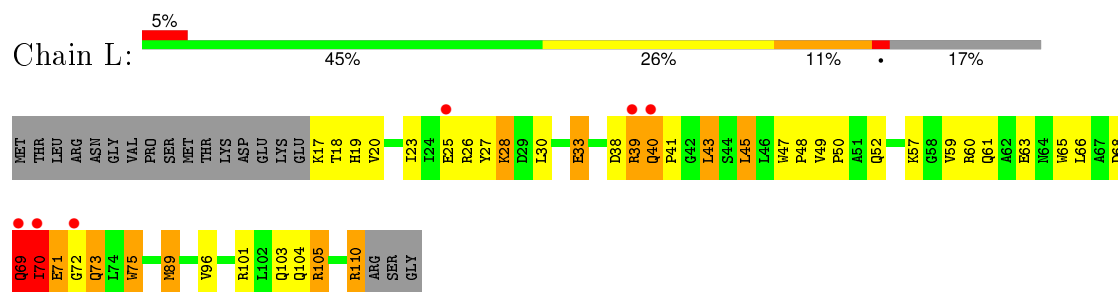
- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



- Molecule 2: Uncharacterized protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 2   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 163.51Å 185.89Å 56.11Å<br>90.00° 90.00° 90.00°              | Depositor        |
| Resolution (Å)  | 48.03 – 2.41<br>48.03 – 2.41                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.9 (48.03-2.41)<br>96.4 (48.03-2.41)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.56 (at 2.42Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.6.1_357)                           | Depositor        |
| R, $R_{free}$   | 0.231 , 0.277<br>0.235 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set   | 3260 reflections (5.33%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 43.3  | Xtriage          |
| Anisotropy  | 0.145   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 58.2   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Outliers  | 0 of 64432 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 11158   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 52.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.43         | 0/1332  | 0.56        | 0/1807         |
| 1   | B     | 0.49         | 0/1332  | 0.58        | 0/1807         |
| 1   | C     | 0.41         | 0/1332  | 0.57        | 0/1807         |
| 1   | D     | 0.55         | 0/1332  | 0.66        | 2/1807 (0.1%)  |
| 2   | E     | 0.45         | 0/770   | 0.66        | 0/1049         |
| 2   | F     | 0.40         | 0/665   | 0.63        | 0/908          |
| 2   | G     | 0.41         | 0/665   | 0.70        | 0/908          |
| 2   | H     | 0.52         | 0/770   | 0.73        | 3/1049 (0.3%)  |
| 2   | I     | 0.44         | 0/770   | 0.62        | 0/1049         |
| 2   | J     | 0.35         | 0/665   | 0.58        | 1/908 (0.1%)   |
| 2   | K     | 0.58         | 0/665   | 0.74        | 1/908 (0.1%)   |
| 2   | L     | 0.79         | 0/770   | 0.77        | 0/1049         |
| All | All   | 0.50         | 0/11068 | 0.64        | 7/15056 (0.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2   | K     | 0                   | 1                   |

There are no bond length outliers.

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | H     | 41  | PRO  | CA-N-CD | -7.00 | 101.69      | 111.50   |
| 2   | H     | 40  | GLN  | C-N-CD  | 5.86  | 140.71      | 128.40   |
| 2   | K     | 42  | GLY  | N-CA-C  | -5.58 | 99.14       | 113.10   |
| 2   | H     | 42  | GLY  | N-CA-C  | 5.49  | 126.81      | 113.10   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 61  | ARG  | NE-CZ-NH2 | -5.40 | 117.60      | 120.30   |
| 2   | J     | 102 | LEU  | CA-CB-CG  | 5.29  | 127.47      | 115.30   |
| 1   | D     | 110 | LEU  | CA-CB-CG  | -5.03 | 103.73      | 115.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | K     | 41  | PRO  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1298  | 0        | 1249     | 57      | 0            |
| 1   | B     | 1298  | 0        | 1249     | 48      | 0            |
| 1   | C     | 1298  | 0        | 1249     | 87      | 0            |
| 1   | D     | 1298  | 0        | 1249     | 51      | 0            |
| 2   | E     | 751   | 0        | 758      | 76      | 0            |
| 2   | F     | 648   | 0        | 650      | 74      | 0            |
| 2   | G     | 648   | 0        | 650      | 93      | 0            |
| 2   | H     | 751   | 0        | 758      | 67      | 0            |
| 2   | I     | 751   | 0        | 758      | 100     | 1            |
| 2   | J     | 648   | 0        | 650      | 91      | 0            |
| 2   | K     | 648   | 0        | 650      | 37      | 0            |
| 2   | L     | 751   | 0        | 758      | 74      | 0            |
| 3   | A     | 21    | 0        | 27       | 1       | 0            |
| 3   | B     | 21    | 0        | 27       | 3       | 0            |
| 3   | C     | 21    | 0        | 27       | 4       | 0            |
| 3   | D     | 21    | 0        | 27       | 0       | 0            |
| 4   | A     | 25    | 0        | 0        | 21      | 0            |
| 4   | B     | 39    | 0        | 0        | 20      | 0            |
| 4   | C     | 20    | 0        | 0        | 22      | 1            |
| 4   | D     | 52    | 0        | 0        | 14      | 0            |
| 4   | E     | 29    | 0        | 0        | 26      | 0            |
| 4   | F     | 14    | 0        | 0        | 10      | 0            |
| 4   | G     | 16    | 0        | 0        | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | H     | 11    | 0        | 0        | 10      | 0            |
| 4   | I     | 12    | 0        | 0        | 21      | 0            |
| 4   | J     | 5     | 0        | 0        | 5       | 0            |
| 4   | K     | 30    | 0        | 0        | 2       | 0            |
| 4   | L     | 33    | 0        | 0        | 17      | 0            |
| All | All   | 11158 | 0        | 10736    | 780     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (780) 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) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:36:PRO:CB    | 2:H:41:PRO:HB2   | 1.36                     | 1.54              |
| 2:H:36:PRO:HB3   | 2:H:41:PRO:CB    | 1.35                     | 1.52              |
| 2:J:30:LEU:HA    | 4:J:205:HOH:O    | 1.16                     | 1.33              |
| 2:I:63:GLU:HA    | 4:I:206:HOH:O    | 1.18                     | 1.31              |
| 2:L:39:ARG:HD3   | 2:L:39:ARG:O     | 1.36                     | 1.24              |
| 2:F:44:SER:HA    | 4:F:201:HOH:O    | 1.43                     | 1.17              |
| 2:G:34:ILE:HG13  | 2:G:43:LEU:HD12  | 1.23                     | 1.15              |
| 2:G:36:PRO:HB3   | 2:G:41:PRO:HB2   | 1.24                     | 1.15              |
| 2:J:101:ARG:HH12 | 2:J:105:ARG:HB2  | 1.07                     | 1.14              |
| 1:C:49:ASN:ND2   | 4:C:318:HOH:O    | 1.81                     | 1.14              |
| 2:E:105:ARG:HH11 | 2:E:105:ARG:HG3  | 1.00                     | 1.13              |
| 2:E:33:GLU:HA    | 4:E:202:HOH:O    | 1.48                     | 1.12              |
| 2:H:36:PRO:CA    | 2:H:41:PRO:HB2   | 1.80                     | 1.12              |
| 1:A:81:GLN:NE2   | 4:A:311:HOH:O    | 1.82                     | 1.11              |
| 2:J:101:ARG:HH22 | 2:J:105:ARG:HD3  | 0.95                     | 1.10              |
| 2:H:36:PRO:CB    | 2:H:41:PRO:CB    | 2.08                     | 1.09              |
| 2:H:38:ASP:OD1   | 4:H:203:HOH:O    | 1.70                     | 1.09              |
| 2:L:17:LYS:N     | 4:L:220:HOH:O    | 1.85                     | 1.09              |
| 2:E:100:THR:C    | 4:E:209:HOH:O    | 1.88                     | 1.08              |
| 2:E:26:ARG:CG    | 4:E:221:HOH:O    | 2.00                     | 1.08              |
| 2:E:101:ARG:N    | 4:E:209:HOH:O    | 1.87                     | 1.08              |
| 2:E:36:PRO:HA    | 2:E:41:PRO:HB2   | 1.36                     | 1.07              |
| 2:G:39:ARG:N     | 4:G:202:HOH:O    | 1.85                     | 1.07              |
| 2:F:105:ARG:HG2  | 2:F:105:ARG:HH11 | 1.17                     | 1.07              |
| 2:G:105:ARG:HB3  | 2:G:105:ARG:HH11 | 1.20                     | 1.06              |
| 1:A:92:ILE:HG23  | 4:A:321:HOH:O    | 1.53                     | 1.05              |
| 1:C:88:TRP:HB2   | 4:C:313:HOH:O    | 1.56                     | 1.05              |
| 2:E:39:ARG:HG3   | 2:E:107:VAL:HB   | 1.39                     | 1.05              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:26:ARG:NH1   | 4:H:210:HOH:O    | 1.87                     | 1.04              |
| 2:I:105:ARG:HB2  | 4:I:210:HOH:O    | 1.57                     | 1.04              |
| 2:F:34:ILE:H     | 2:F:43:LEU:HD12  | 1.22                     | 1.04              |
| 2:G:34:ILE:H     | 2:G:43:LEU:HB3   | 1.23                     | 1.04              |
| 2:G:39:ARG:HE    | 2:G:108:ALA:HA   | 1.19                     | 1.03              |
| 2:K:105:ARG:HH11 | 2:K:105:ARG:CB   | 1.70                     | 1.03              |
| 2:J:105:ARG:HH11 | 2:J:105:ARG:HG2  | 0.90                     | 1.03              |
| 2:E:36:PRO:HB3   | 2:E:41:PRO:HG2   | 1.38                     | 1.03              |
| 2:H:105:ARG:HG3  | 4:H:203:HOH:O    | 1.58                     | 1.03              |
| 2:I:105:ARG:HH11 | 2:I:105:ARG:HB2  | 1.21                     | 1.03              |
| 4:B:308:HOH:O    | 2:H:18:THR:HB    | 1.56                     | 1.03              |
| 2:I:105:ARG:N    | 4:I:210:HOH:O    | 1.83                     | 1.02              |
| 2:E:26:ARG:N     | 4:E:221:HOH:O    | 1.92                     | 1.02              |
| 2:J:87:THR:HG22  | 2:J:89:MET:H     | 1.21                     | 1.02              |
| 2:E:26:ARG:HG2   | 4:E:221:HOH:O    | 1.57                     | 1.02              |
| 2:K:105:ARG:HH11 | 2:K:105:ARG:HB3  | 1.20                     | 1.02              |
| 1:A:66:ARG:NH2   | 4:A:322:HOH:O    | 1.90                     | 1.01              |
| 2:J:32:VAL:O     | 2:J:43:LEU:HD11  | 1.59                     | 1.01              |
| 1:A:92:ILE:N     | 4:A:321:HOH:O    | 1.84                     | 1.00              |
| 2:G:32:VAL:O     | 2:G:43:LEU:HD22  | 1.62                     | 1.00              |
| 2:J:105:ARG:NH1  | 2:J:105:ARG:HG2  | 1.70                     | 0.99              |
| 1:A:92:ILE:CB    | 4:A:321:HOH:O    | 2.09                     | 0.99              |
| 2:G:39:ARG:NE    | 2:G:108:ALA:HA   | 1.78                     | 0.98              |
| 2:L:73:GLN:HA    | 2:L:73:GLN:OE1   | 1.62                     | 0.98              |
| 2:I:105:ARG:CB   | 4:I:210:HOH:O    | 2.08                     | 0.98              |
| 2:E:100:THR:HG22 | 4:E:209:HOH:O    | 1.63                     | 0.97              |
| 2:L:40:GLN:HG3   | 2:L:41:PRO:HD2   | 1.45                     | 0.97              |
| 2:I:62:ALA:O     | 4:I:206:HOH:O    | 1.81                     | 0.97              |
| 1:A:89:GLU:O     | 4:A:321:HOH:O    | 1.82                     | 0.96              |
| 1:D:145:GLU:OE2  | 4:D:338:HOH:O    | 1.84                     | 0.96              |
| 2:G:106:LEU:HG   | 2:H:106:LEU:HD21 | 1.45                     | 0.96              |
| 1:C:24:GLN:OE1   | 4:C:317:HOH:O    | 1.84                     | 0.96              |
| 2:L:52:GLN:NE2   | 4:L:210:HOH:O    | 1.96                     | 0.96              |
| 2:J:32:VAL:HG23  | 2:J:45:LEU:HB3   | 1.47                     | 0.95              |
| 2:E:43:LEU:O     | 4:E:202:HOH:O    | 1.84                     | 0.95              |
| 2:K:105:ARG:CG   | 2:K:105:ARG:HH11 | 1.81                     | 0.94              |
| 2:I:71:GLU:HG3   | 2:J:107:VAL:HG22 | 1.46                     | 0.94              |
| 2:E:105:ARG:NH1  | 2:E:105:ARG:HG3  | 1.76                     | 0.94              |
| 2:J:29:ASP:O     | 4:J:205:HOH:O    | 1.84                     | 0.94              |
| 2:J:101:ARG:NH2  | 2:J:105:ARG:HD3  | 1.81                     | 0.94              |
| 1:D:24:GLN:OE1   | 4:D:305:HOH:O    | 1.85                     | 0.94              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:80:THR:HG22  | 1:D:125:LEU:HD21 | 1.50                     | 0.93              |
| 1:C:45:GLN:O     | 4:C:314:HOH:O    | 1.86                     | 0.93              |
| 2:J:39:ARG:HG2   | 2:J:108:ALA:HA   | 1.50                     | 0.93              |
| 2:L:57:LYS:HD3   | 4:L:223:HOH:O    | 1.67                     | 0.93              |
| 1:B:13:SER:O     | 4:B:319:HOH:O    | 1.84                     | 0.93              |
| 2:F:83:ASP:CB    | 4:F:213:HOH:O    | 2.15                     | 0.93              |
| 2:F:83:ASP:HB2   | 4:F:213:HOH:O    | 1.69                     | 0.93              |
| 2:J:55:ILE:HG13  | 2:J:97:ALA:HB2   | 1.52                     | 0.92              |
| 2:L:57:LYS:CG    | 4:L:223:HOH:O    | 2.16                     | 0.92              |
| 2:F:43:LEU:O     | 4:F:201:HOH:O    | 1.85                     | 0.92              |
| 2:G:34:ILE:HG13  | 2:G:43:LEU:CD1   | 1.99                     | 0.92              |
| 2:J:34:ILE:H     | 2:J:43:LEU:HD22  | 1.35                     | 0.91              |
| 2:G:40:GLN:OE1   | 4:G:215:HOH:O    | 1.87                     | 0.91              |
| 2:E:56:ASP:OD1   | 4:E:227:HOH:O    | 1.87                     | 0.91              |
| 2:F:43:LEU:HD22  | 2:F:44:SER:N     | 1.84                     | 0.91              |
| 1:B:33:SER:OG    | 4:B:315:HOH:O    | 1.89                     | 0.91              |
| 1:C:141:ASN:ND2  | 4:C:316:HOH:O    | 1.98                     | 0.91              |
| 2:G:105:ARG:CB   | 2:G:105:ARG:HH11 | 1.84                     | 0.91              |
| 2:E:104:GLN:OE1  | 4:E:210:HOH:O    | 1.89                     | 0.90              |
| 2:G:105:ARG:HB3  | 2:G:105:ARG:NH1  | 1.86                     | 0.90              |
| 2:G:46:LEU:O     | 4:G:216:HOH:O    | 1.89                     | 0.90              |
| 2:F:83:ASP:OD2   | 4:F:213:HOH:O    | 1.90                     | 0.89              |
| 2:H:36:PRO:HB3   | 2:H:41:PRO:CG    | 2.01                     | 0.89              |
| 2:G:34:ILE:CG1   | 2:G:43:LEU:HD12  | 2.02                     | 0.88              |
| 1:D:117:PRO:O    | 4:D:324:HOH:O    | 1.91                     | 0.88              |
| 2:H:26:ARG:CZ    | 4:H:210:HOH:O    | 2.19                     | 0.88              |
| 1:C:141:ASN:OD1  | 4:C:316:HOH:O    | 1.89                     | 0.88              |
| 1:A:39:LEU:O     | 4:A:324:HOH:O    | 1.90                     | 0.88              |
| 2:E:105:ARG:CG   | 2:E:105:ARG:HH11 | 1.86                     | 0.87              |
| 2:G:34:ILE:H     | 2:G:43:LEU:CB    | 1.88                     | 0.87              |
| 2:H:38:ASP:OD2   | 4:H:203:HOH:O    | 1.93                     | 0.87              |
| 1:B:152:TRP:HZ3  | 2:G:83:ASP:OD2   | 1.58                     | 0.86              |
| 2:H:26:ARG:NH2   | 4:H:210:HOH:O    | 2.09                     | 0.86              |
| 2:H:36:PRO:CA    | 2:H:41:PRO:CB    | 2.48                     | 0.85              |
| 2:F:105:ARG:HH11 | 2:F:105:ARG:CG   | 1.87                     | 0.85              |
| 2:G:34:ILE:HB    | 2:G:43:LEU:HB2   | 1.59                     | 0.85              |
| 1:D:48:GLU:HG3   | 4:D:311:HOH:O    | 1.76                     | 0.85              |
| 1:D:48:GLU:OE2   | 4:D:311:HOH:O    | 1.93                     | 0.85              |
| 2:J:101:ARG:NH1  | 2:J:105:ARG:HB2  | 1.91                     | 0.84              |
| 2:H:33:GLU:H     | 2:H:52:GLN:NE2   | 1.75                     | 0.84              |
| 2:H:25:GLU:O     | 2:H:28:LYS:HE3   | 1.77                     | 0.84              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:B:164:GLY:N    | 4:B:323:HOH:O   | 2.09                     | 0.84              |
| 2:I:55:ILE:CG2   | 4:I:204:HOH:O   | 2.25                     | 0.84              |
| 2:I:52:GLN:NE2   | 4:I:204:HOH:O   | 2.11                     | 0.84              |
| 1:B:71:ARG:NH2   | 4:B:335:HOH:O   | 1.82                     | 0.84              |
| 2:L:61:GLN:NE2   | 4:L:208:HOH:O   | 2.10                     | 0.84              |
| 2:F:36:PRO:HB3   | 2:F:41:PRO:HB2  | 1.58                     | 0.83              |
| 1:A:71:ARG:HH11  | 1:A:71:ARG:CG   | 1.91                     | 0.83              |
| 1:A:71:ARG:HH11  | 1:A:71:ARG:HG2  | 1.43                     | 0.83              |
| 1:A:78:HIS:CD2   | 1:A:86:ILE:HB   | 2.12                     | 0.83              |
| 2:L:70:ILE:HG23  | 2:L:71:GLU:N    | 1.92                     | 0.83              |
| 2:K:105:ARG:HB3  | 2:K:105:ARG:NH1 | 1.94                     | 0.83              |
| 2:L:66:LEU:O     | 2:L:69:GLN:HG2  | 1.79                     | 0.82              |
| 2:L:69:GLN:HA    | 2:L:70:ILE:O    | 1.80                     | 0.82              |
| 2:I:34:ILE:O     | 2:I:42:GLY:HA2  | 1.78                     | 0.82              |
| 1:B:48:GLU:OE2   | 4:B:335:HOH:O   | 1.98                     | 0.82              |
| 1:A:92:ILE:CG1   | 4:A:321:HOH:O   | 2.26                     | 0.81              |
| 1:A:96:ARG:HD3   | 1:A:96:ARG:C    | 1.99                     | 0.81              |
| 1:C:141:ASN:CG   | 4:C:316:HOH:O   | 2.19                     | 0.81              |
| 1:A:96:ARG:HD3   | 1:A:96:ARG:O    | 1.80                     | 0.81              |
| 2:G:73:GLN:O     | 4:G:211:HOH:O   | 1.97                     | 0.81              |
| 2:L:39:ARG:HD3   | 2:L:39:ARG:C    | 2.01                     | 0.81              |
| 2:J:36:PRO:HA    | 2:J:41:PRO:HB2  | 1.60                     | 0.81              |
| 2:L:60:ARG:NH2   | 4:L:230:HOH:O   | 2.13                     | 0.80              |
| 2:J:105:ARG:HH11 | 2:J:105:ARG:CG  | 1.83                     | 0.80              |
| 2:I:66:LEU:HD12  | 4:I:206:HOH:O   | 1.80                     | 0.80              |
| 2:L:69:GLN:CA    | 2:L:70:ILE:O    | 2.29                     | 0.80              |
| 1:C:24:GLN:HE22  | 1:D:25:LYS:NZ   | 1.79                     | 0.80              |
| 2:K:34:ILE:HD12  | 2:K:43:LEU:HD23 | 1.63                     | 0.80              |
| 2:G:43:LEU:HD21  | 2:G:45:LEU:HB3  | 1.63                     | 0.80              |
| 2:I:33:GLU:H     | 2:I:52:GLN:HE21 | 1.27                     | 0.79              |
| 2:G:36:PRO:CB    | 2:G:41:PRO:HB2  | 2.10                     | 0.79              |
| 2:L:70:ILE:HG23  | 2:L:71:GLU:H    | 1.47                     | 0.79              |
| 2:E:20:VAL:C     | 4:E:205:HOH:O   | 2.21                     | 0.79              |
| 2:I:36:PRO:HA    | 2:I:41:PRO:HB2  | 1.65                     | 0.79              |
| 2:G:32:VAL:O     | 2:G:43:LEU:CD2  | 2.30                     | 0.79              |
| 2:G:99:LEU:O     | 2:H:74:LEU:HD23 | 1.83                     | 0.78              |
| 1:C:46:ASP:OD1   | 4:C:319:HOH:O   | 2.01                     | 0.78              |
| 2:F:85:LEU:HD13  | 2:F:94:PHE:HB2  | 1.66                     | 0.78              |
| 1:B:152:TRP:CZ3  | 2:G:83:ASP:OD2  | 2.35                     | 0.78              |
| 2:E:39:ARG:O     | 2:E:41:PRO:HG3  | 1.83                     | 0.78              |
| 1:B:16:LYS:HE2   | 1:B:165:LEU:O   | 1.84                     | 0.77              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:41:PRO:O    | 4:B:310:HOH:O    | 2.02                     | 0.77              |
| 2:I:18:THR:HG22 | 2:I:19:HIS:N     | 1.99                     | 0.77              |
| 2:L:48:PRO:O    | 4:L:205:HOH:O    | 2.03                     | 0.77              |
| 1:B:73:ASP:O    | 4:B:311:HOH:O    | 2.01                     | 0.77              |
| 1:D:167:PHE:CA  | 4:D:344:HOH:O    | 2.31                     | 0.77              |
| 2:H:36:PRO:HB3  | 2:H:41:PRO:HB2   | 0.77                     | 0.77              |
| 2:L:33:GLU:H    | 2:L:52:GLN:HE22  | 1.33                     | 0.77              |
| 2:K:73:GLN:HE22 | 2:L:103:GLN:HE22 | 1.29                     | 0.77              |
| 2:E:20:VAL:O    | 4:E:205:HOH:O    | 2.01                     | 0.77              |
| 2:K:38:ASP:OD2  | 2:K:105:ARG:HG3  | 1.85                     | 0.76              |
| 1:C:9:GLU:OE1   | 4:C:309:HOH:O    | 2.02                     | 0.76              |
| 1:C:102:PHE:HD1 | 1:C:102:PHE:O    | 1.67                     | 0.76              |
| 2:L:68:ASP:OD1  | 4:L:215:HOH:O    | 2.01                     | 0.76              |
| 2:G:39:ARG:CA   | 4:G:202:HOH:O    | 2.24                     | 0.76              |
| 2:G:59:VAL:HG23 | 2:G:97:ALA:HB1   | 1.68                     | 0.76              |
| 2:E:33:GLU:H    | 2:E:52:GLN:HE21  | 1.31                     | 0.76              |
| 1:D:167:PHE:CB  | 4:D:344:HOH:O    | 2.33                     | 0.76              |
| 2:I:57:LYS:HD2  | 2:I:85:LEU:HD21  | 1.65                     | 0.76              |
| 2:E:36:PRO:HA   | 2:E:41:PRO:CB    | 2.14                     | 0.76              |
| 2:I:105:ARG:CB  | 2:I:105:ARG:HH11 | 1.96                     | 0.75              |
| 2:G:39:ARG:C    | 4:G:202:HOH:O    | 2.24                     | 0.75              |
| 2:J:34:ILE:N    | 2:J:43:LEU:HD22  | 2.02                     | 0.75              |
| 2:F:33:GLU:OE2  | 4:F:201:HOH:O    | 2.04                     | 0.75              |
| 2:H:36:PRO:CB   | 2:H:41:PRO:HB3   | 2.13                     | 0.75              |
| 2:I:101:ARG:NH1 | 4:I:210:HOH:O    | 2.19                     | 0.75              |
| 2:F:43:LEU:O    | 2:F:43:LEU:HD13  | 1.87                     | 0.75              |
| 2:F:105:ARG:HG2 | 2:F:105:ARG:NH1  | 1.94                     | 0.75              |
| 2:J:30:LEU:CA   | 4:J:205:HOH:O    | 1.95                     | 0.75              |
| 2:J:34:ILE:HB   | 2:J:43:LEU:HB3   | 1.68                     | 0.74              |
| 2:H:59:VAL:HG23 | 2:H:97:ALA:HB1   | 1.68                     | 0.74              |
| 1:D:4:VAL:HG23  | 4:L:205:HOH:O    | 1.87                     | 0.74              |
| 2:G:38:ASP:HA   | 4:G:209:HOH:O    | 1.85                     | 0.74              |
| 2:I:52:GLN:CD   | 4:I:204:HOH:O    | 2.25                     | 0.74              |
| 2:J:102:LEU:O   | 2:J:106:LEU:HB2  | 1.88                     | 0.74              |
| 4:B:308:HOH:O   | 2:H:18:THR:CB    | 2.21                     | 0.74              |
| 2:J:33:GLU:HA   | 2:J:43:LEU:HD21  | 1.70                     | 0.74              |
| 2:E:36:PRO:CB   | 2:E:41:PRO:HG2   | 2.18                     | 0.73              |
| 2:H:36:PRO:HA   | 2:H:41:PRO:HB2   | 1.67                     | 0.73              |
| 1:A:33:SER:OG   | 4:A:305:HOH:O    | 2.06                     | 0.73              |
| 2:I:23:ILE:O    | 2:I:26:ARG:O     | 2.06                     | 0.73              |
| 2:E:26:ARG:CA   | 4:E:221:HOH:O    | 2.34                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:36:PRO:CA    | 2:J:41:PRO:HB2   | 2.19                     | 0.73              |
| 1:D:167:PHE:N    | 4:D:344:HOH:O    | 2.22                     | 0.72              |
| 1:C:132:VAL:O    | 4:C:307:HOH:O    | 2.05                     | 0.72              |
| 2:L:18:THR:HG22  | 2:L:19:HIS:N     | 2.04                     | 0.72              |
| 2:I:74:LEU:HB2   | 2:J:103:GLN:HG3  | 1.71                     | 0.72              |
| 2:J:33:GLU:HA    | 2:J:43:LEU:CD2   | 2.19                     | 0.72              |
| 2:I:18:THR:HG22  | 2:I:19:HIS:H     | 1.54                     | 0.72              |
| 2:G:73:GLN:HE21  | 2:H:43:LEU:HD11  | 1.55                     | 0.72              |
| 2:I:26:ARG:O     | 2:I:27:TYR:HB2   | 1.90                     | 0.72              |
| 2:H:104:GLN:OE1  | 4:H:205:HOH:O    | 2.08                     | 0.72              |
| 1:C:88:TRP:O     | 4:C:313:HOH:O    | 2.07                     | 0.71              |
| 2:F:43:LEU:HD21  | 2:F:45:LEU:HB2   | 1.71                     | 0.71              |
| 2:J:43:LEU:HD12  | 2:J:45:LEU:HB2   | 1.70                     | 0.71              |
| 2:F:66:LEU:O     | 4:F:214:HOH:O    | 2.06                     | 0.71              |
| 1:A:51:PHE:CB    | 4:A:324:HOH:O    | 2.37                     | 0.71              |
| 2:G:107:VAL:HG22 | 2:H:71:GLU:HG3   | 1.71                     | 0.71              |
| 2:E:68:ASP:OD1   | 4:E:223:HOH:O    | 2.09                     | 0.71              |
| 2:L:57:LYS:HG3   | 4:L:228:HOH:O    | 1.90                     | 0.71              |
| 2:F:43:LEU:C     | 2:F:43:LEU:HD13  | 2.11                     | 0.71              |
| 1:D:45:GLN:HA    | 1:D:45:GLN:NE2   | 2.06                     | 0.70              |
| 1:C:25:LYS:HZ2   | 1:D:24:GLN:HE22  | 1.36                     | 0.70              |
| 2:I:41:PRO:CB    | 2:I:104:GLN:HE21 | 2.05                     | 0.70              |
| 2:G:60:ARG:NH1   | 4:G:214:HOH:O    | 2.10                     | 0.70              |
| 1:A:139:GLU:OE2  | 2:E:18:THR:HG21  | 1.91                     | 0.70              |
| 2:H:36:PRO:HA    | 2:H:41:PRO:CB    | 2.20                     | 0.70              |
| 1:A:92:ILE:CA    | 4:A:321:HOH:O    | 2.19                     | 0.70              |
| 2:H:38:ASP:CG    | 4:H:203:HOH:O    | 2.08                     | 0.70              |
| 1:D:40:LEU:HD22  | 1:D:44:SER:HB3   | 1.74                     | 0.70              |
| 2:G:36:PRO:HB3   | 2:G:41:PRO:CB    | 2.14                     | 0.70              |
| 2:G:105:ARG:CG   | 2:G:105:ARG:HH11 | 2.04                     | 0.69              |
| 2:L:68:ASP:O     | 2:L:69:GLN:C     | 2.30                     | 0.69              |
| 2:J:37:ALA:H     | 2:J:41:PRO:CB    | 2.06                     | 0.69              |
| 2:E:101:ARG:HH12 | 2:E:105:ARG:HB2  | 1.57                     | 0.69              |
| 2:I:63:GLU:CA    | 4:I:206:HOH:O    | 1.99                     | 0.69              |
| 4:G:215:HOH:O    | 2:H:71:GLU:O     | 2.10                     | 0.69              |
| 1:C:25:LYS:NZ    | 4:C:306:HOH:O    | 2.26                     | 0.69              |
| 1:C:45:GLN:HB3   | 4:C:314:HOH:O    | 1.91                     | 0.69              |
| 1:B:48:GLU:CD    | 4:B:335:HOH:O    | 2.31                     | 0.69              |
| 2:J:37:ALA:H     | 2:J:41:PRO:HB3   | 1.58                     | 0.69              |
| 2:I:70:ILE:HD12  | 2:I:70:ILE:H     | 1.56                     | 0.69              |
| 2:G:95:GLU:CD    | 2:H:82:ARG:HH12  | 1.95                     | 0.69              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:G:43:LEU:C    | 2:G:43:LEU:HD23  | 2.14                     | 0.68              |
| 2:E:41:PRO:CB   | 2:E:104:GLN:HE21 | 2.06                     | 0.68              |
| 1:A:81:GLN:CD   | 4:A:311:HOH:O    | 2.23                     | 0.68              |
| 2:J:32:VAL:C    | 2:J:43:LEU:HD11  | 2.13                     | 0.68              |
| 2:J:52:GLN:O    | 2:J:55:ILE:HG22  | 1.92                     | 0.68              |
| 2:E:106:LEU:O   | 4:E:212:HOH:O    | 2.10                     | 0.68              |
| 1:C:25:LYS:NZ   | 1:D:24:GLN:HE22  | 1.91                     | 0.68              |
| 2:J:63:GLU:HA   | 2:J:66:LEU:HB2   | 1.76                     | 0.68              |
| 1:D:167:PHE:HB2 | 4:D:344:HOH:O    | 1.93                     | 0.68              |
| 2:L:39:ARG:CD   | 2:L:39:ARG:O     | 2.29                     | 0.67              |
| 2:K:105:ARG:CG  | 2:K:105:ARG:NH1  | 2.46                     | 0.67              |
| 1:C:137:ARG:CZ  | 1:C:137:ARG:HB2  | 2.23                     | 0.67              |
| 2:I:41:PRO:HB2  | 2:I:104:GLN:HE21 | 1.59                     | 0.67              |
| 1:D:136:ASN:ND2 | 1:D:139:GLU:H    | 1.91                     | 0.67              |
| 1:C:156:ASP:O   | 1:C:160:GLN:HG2  | 1.95                     | 0.67              |
| 2:J:32:VAL:CG2  | 2:J:45:LEU:HB3   | 2.24                     | 0.67              |
| 1:A:92:ILE:CG2  | 4:A:321:HOH:O    | 2.12                     | 0.66              |
| 2:J:34:ILE:H    | 2:J:43:LEU:CD2   | 2.07                     | 0.66              |
| 1:B:9:GLU:HB3   | 1:B:22:ILE:HD13  | 1.76                     | 0.66              |
| 2:G:70:ILE:O    | 2:G:70:ILE:HG23  | 1.95                     | 0.66              |
| 1:C:58:ALA:O    | 1:C:62:GLU:HG2   | 1.95                     | 0.66              |
| 1:C:45:GLN:CA   | 4:C:314:HOH:O    | 2.43                     | 0.66              |
| 1:D:149:PRO:HG2 | 2:L:45:LEU:HG    | 1.78                     | 0.66              |
| 1:B:20:SER:O    | 4:B:333:HOH:O    | 2.13                     | 0.66              |
| 2:K:34:ILE:CD1  | 2:K:43:LEU:HD23  | 2.25                     | 0.66              |
| 2:F:33:GLU:HA   | 2:F:43:LEU:CD1   | 2.26                     | 0.66              |
| 2:L:38:ASP:C    | 2:L:40:GLN:H     | 1.99                     | 0.65              |
| 2:I:52:GLN:OE1  | 4:I:204:HOH:O    | 2.14                     | 0.65              |
| 2:I:102:LEU:O   | 2:I:106:LEU:HB2  | 1.96                     | 0.65              |
| 2:K:105:ARG:NH1 | 2:K:105:ARG:HG2  | 2.11                     | 0.65              |
| 1:A:25:LYS:NZ   | 4:A:307:HOH:O    | 1.93                     | 0.65              |
| 1:B:45:GLN:HE21 | 1:B:45:GLN:H     | 1.44                     | 0.65              |
| 2:F:34:ILE:H    | 2:F:43:LEU:CD1   | 2.05                     | 0.65              |
| 2:G:43:LEU:HD21 | 2:G:45:LEU:CB    | 2.27                     | 0.65              |
| 2:J:87:THR:HB   | 2:J:90:GLN:HG2   | 1.79                     | 0.65              |
| 1:D:45:GLN:HE21 | 1:D:45:GLN:HA    | 1.61                     | 0.65              |
| 1:B:139:GLU:OE1 | 4:B:308:HOH:O    | 2.14                     | 0.65              |
| 1:A:51:PHE:HB3  | 4:A:324:HOH:O    | 1.97                     | 0.65              |
| 1:A:149:PRO:HG2 | 2:E:45:LEU:HG    | 1.79                     | 0.65              |
| 2:E:39:ARG:O    | 2:E:41:PRO:CG    | 2.45                     | 0.64              |
| 1:D:45:GLN:C    | 1:D:47:TYR:H     | 2.00                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:48:GLU:OE1   | 4:B:335:HOH:O    | 2.13                     | 0.64              |
| 2:K:29:ASP:OD2   | 4:K:213:HOH:O    | 2.15                     | 0.64              |
| 1:D:45:GLN:O     | 1:D:47:TYR:N     | 2.31                     | 0.64              |
| 1:C:33:SER:OG    | 4:C:305:HOH:O    | 2.15                     | 0.64              |
| 1:A:155:LYS:NZ   | 4:F:213:HOH:O    | 2.28                     | 0.64              |
| 2:K:73:GLN:NE2   | 2:L:103:GLN:HE22 | 1.95                     | 0.64              |
| 1:B:31:GLY:HA3   | 2:H:23:ILE:HD13  | 1.80                     | 0.64              |
| 2:L:69:GLN:HA    | 2:L:70:ILE:C     | 2.15                     | 0.63              |
| 2:F:85:LEU:CD1   | 2:F:94:PHE:HB2   | 2.28                     | 0.63              |
| 2:G:39:ARG:O     | 2:G:41:PRO:HB3   | 1.98                     | 0.63              |
| 1:C:134:ALA:CB   | 1:C:140:ALA:HB2  | 2.28                     | 0.63              |
| 2:L:18:THR:CG2   | 2:L:19:HIS:N     | 2.61                     | 0.63              |
| 2:L:33:GLU:HG2   | 4:L:210:HOH:O    | 1.99                     | 0.63              |
| 2:I:101:ARG:HD2  | 2:I:101:ARG:O    | 1.98                     | 0.63              |
| 2:L:70:ILE:CG2   | 2:L:71:GLU:N     | 2.61                     | 0.63              |
| 2:I:22:ALA:O     | 4:I:205:HOH:O    | 2.16                     | 0.62              |
| 2:J:38:ASP:OD2   | 2:J:105:ARG:HG3  | 2.00                     | 0.62              |
| 2:E:69:GLN:C     | 2:E:71:GLU:H     | 2.02                     | 0.62              |
| 2:F:43:LEU:HD23  | 2:F:45:LEU:HD13  | 1.81                     | 0.62              |
| 2:L:57:LYS:CD    | 4:L:223:HOH:O    | 2.24                     | 0.62              |
| 2:G:107:VAL:HG22 | 2:H:71:GLU:HB2   | 1.81                     | 0.62              |
| 1:C:152:TRP:HZ3  | 2:J:83:ASP:OD2   | 1.83                     | 0.62              |
| 1:A:160:GLN:NE2  | 4:A:303:HOH:O    | 2.32                     | 0.62              |
| 2:L:38:ASP:OD2   | 2:L:105:ARG:HD3  | 1.99                     | 0.61              |
| 2:E:61:GLN:NE2   | 4:E:211:HOH:O    | 2.33                     | 0.61              |
| 2:J:39:ARG:HD3   | 2:J:39:ARG:N     | 2.15                     | 0.61              |
| 2:L:26:ARG:O     | 2:L:27:TYR:HB2   | 2.00                     | 0.61              |
| 2:F:43:LEU:CD2   | 2:F:45:LEU:HD13  | 2.30                     | 0.61              |
| 2:L:73:GLN:CA    | 2:L:73:GLN:OE1   | 2.45                     | 0.61              |
| 2:L:18:THR:HG22  | 2:L:20:VAL:H     | 1.64                     | 0.61              |
| 1:B:42:LYS:HG3   | 1:B:123:GLY:HA3  | 1.83                     | 0.61              |
| 2:F:87:THR:HG22  | 2:F:89:MET:N     | 2.15                     | 0.61              |
| 1:B:149:PRO:HG2  | 2:H:45:LEU:HG    | 1.81                     | 0.61              |
| 1:C:69:TYR:HD2   | 1:C:101:PHE:CD2  | 2.18                     | 0.61              |
| 2:F:33:GLU:HA    | 2:F:43:LEU:HD11  | 1.83                     | 0.61              |
| 2:E:43:LEU:HD11  | 2:F:73:GLN:NE2   | 2.16                     | 0.61              |
| 2:I:69:GLN:HB3   | 2:I:70:ILE:HD12  | 1.83                     | 0.60              |
| 2:G:34:ILE:CB    | 2:G:43:LEU:HB2   | 2.28                     | 0.60              |
| 2:J:39:ARG:HG2   | 2:J:108:ALA:CA   | 2.27                     | 0.60              |
| 1:D:48:GLU:CG    | 4:D:311:HOH:O    | 2.42                     | 0.60              |
| 2:G:37:ALA:O     | 4:G:209:HOH:O    | 2.16                     | 0.60              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:I:43:LEU:HD11 | 2:J:73:GLN:OE1   | 2.02                     | 0.60              |
| 2:I:41:PRO:HB2  | 2:I:104:GLN:NE2  | 2.16                     | 0.60              |
| 1:C:152:TRP:CZ3 | 2:J:83:ASP:OD2   | 2.55                     | 0.60              |
| 2:I:99:LEU:O    | 2:J:74:LEU:HD23  | 2.02                     | 0.60              |
| 2:I:38:ASP:HA   | 4:I:203:HOH:O    | 2.01                     | 0.60              |
| 2:G:34:ILE:N    | 2:G:43:LEU:HB3   | 2.05                     | 0.60              |
| 2:E:101:ARG:HD3 | 4:E:210:HOH:O    | 2.00                     | 0.60              |
| 2:H:41:PRO:HA   | 2:H:104:GLN:HE21 | 1.67                     | 0.59              |
| 2:G:73:GLN:NE2  | 2:H:43:LEU:HD11  | 2.16                     | 0.59              |
| 2:I:106:LEU:O   | 2:I:106:LEU:HD23 | 2.03                     | 0.59              |
| 2:L:49:VAL:HG22 | 2:L:89:MET:HG2   | 1.83                     | 0.59              |
| 1:C:10:LEU:HD13 | 1:C:22:ILE:HG22  | 1.84                     | 0.59              |
| 2:F:87:THR:HG22 | 2:F:89:MET:H     | 1.66                     | 0.59              |
| 2:J:34:ILE:N    | 2:J:43:LEU:HD13  | 2.17                     | 0.59              |
| 2:G:104:GLN:OE1 | 4:G:205:HOH:O    | 2.16                     | 0.59              |
| 1:B:61:ARG:HD2  | 4:B:302:HOH:O    | 2.02                     | 0.59              |
| 2:G:68:ASP:O    | 2:G:68:ASP:OD1   | 2.20                     | 0.59              |
| 2:E:41:PRO:HB3  | 2:E:104:GLN:HE21 | 1.67                     | 0.59              |
| 1:C:45:GLN:CB   | 4:C:314:HOH:O    | 2.50                     | 0.59              |
| 1:C:67:ALA:HB3  | 1:C:69:TYR:HE1   | 1.68                     | 0.59              |
| 1:C:45:GLN:O    | 1:C:47:TYR:N     | 2.36                     | 0.59              |
| 1:B:160:GLN:O   | 4:B:323:HOH:O    | 2.17                     | 0.59              |
| 1:C:58:ALA:HB2  | 4:C:310:HOH:O    | 2.02                     | 0.59              |
| 2:G:39:ARG:HE   | 2:G:108:ALA:CA   | 2.06                     | 0.59              |
| 1:A:78:HIS:HD2  | 1:A:86:ILE:CG2   | 2.16                     | 0.59              |
| 2:F:89:MET:HA   | 2:F:89:MET:HE3   | 1.84                     | 0.59              |
| 2:G:85:LEU:HD13 | 2:G:94:PHE:HB2   | 1.85                     | 0.59              |
| 2:F:36:PRO:CB   | 2:F:41:PRO:HB2   | 2.33                     | 0.58              |
| 2:I:43:LEU:HD11 | 2:J:73:GLN:CD    | 2.24                     | 0.58              |
| 1:C:77:SER:HA   | 1:C:80:THR:HG23  | 1.84                     | 0.58              |
| 2:I:36:PRO:HB3  | 2:I:41:PRO:HG2   | 1.85                     | 0.58              |
| 1:D:145:GLU:HG3 | 4:D:338:HOH:O    | 2.03                     | 0.58              |
| 2:J:85:LEU:CD1  | 2:J:94:PHE:HB2   | 2.34                     | 0.58              |
| 2:E:23:ILE:N    | 4:E:205:HOH:O    | 1.91                     | 0.58              |
| 2:L:57:LYS:HG3  | 4:L:223:HOH:O    | 1.95                     | 0.58              |
| 2:I:62:ALA:O    | 2:I:66:LEU:HG    | 2.04                     | 0.58              |
| 2:E:70:ILE:O    | 2:E:71:GLU:O     | 2.20                     | 0.58              |
| 1:A:74:PRO:HG2  | 1:A:93:TYR:CD1   | 2.38                     | 0.58              |
| 2:I:70:ILE:HD12 | 2:I:70:ILE:N     | 2.19                     | 0.58              |
| 2:G:43:LEU:HD23 | 2:G:45:LEU:N     | 2.18                     | 0.58              |
| 2:I:87:THR:HB   | 2:I:88:PRO:HD2   | 1.86                     | 0.57              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:L:17:LYS:HE3   | 2:L:25:GLU:OE1  | 2.03                     | 0.57              |
| 1:B:152:TRP:HZ3  | 2:G:83:ASP:CG   | 2.07                     | 0.57              |
| 2:I:55:ILE:HG21  | 4:I:204:HOH:O   | 1.98                     | 0.57              |
| 2:I:26:ARG:O     | 2:I:27:TYR:CB   | 2.52                     | 0.57              |
| 2:F:34:ILE:N     | 2:F:43:LEU:HD12 | 2.05                     | 0.57              |
| 1:C:24:GLN:HE22  | 1:D:25:LYS:HZ2  | 1.50                     | 0.57              |
| 1:C:149:PRO:HG2  | 2:I:45:LEU:HG   | 1.86                     | 0.57              |
| 2:K:38:ASP:OD2   | 2:K:105:ARG:CG  | 2.51                     | 0.57              |
| 1:C:25:LYS:NZ    | 1:D:24:GLN:NE2  | 2.52                     | 0.57              |
| 2:E:23:ILE:HB    | 4:E:205:HOH:O   | 2.05                     | 0.57              |
| 1:C:133:GLU:HG2  | 4:C:303:HOH:O   | 2.05                     | 0.57              |
| 2:L:70:ILE:C     | 2:L:71:GLU:HG2  | 2.24                     | 0.57              |
| 2:L:110:ARG:NH2  | 4:L:229:HOH:O   | 2.37                     | 0.57              |
| 1:D:63:HIS:HE1   | 1:D:104:GLU:OE1 | 1.88                     | 0.57              |
| 2:G:34:ILE:CD1   | 2:G:43:LEU:HD12 | 2.35                     | 0.56              |
| 1:B:6:GLY:HA3    | 1:B:26:MET:SD   | 2.44                     | 0.56              |
| 1:C:42:LYS:HA    | 1:C:123:GLY:O   | 2.05                     | 0.56              |
| 2:E:30:LEU:HB3   | 2:E:47:TRP:O    | 2.05                     | 0.56              |
| 2:J:101:ARG:HH12 | 2:J:105:ARG:CB  | 1.98                     | 0.56              |
| 2:J:101:ARG:HH22 | 2:J:105:ARG:CD  | 1.90                     | 0.56              |
| 2:G:101:ARG:HH12 | 2:G:105:ARG:HD3 | 1.69                     | 0.56              |
| 2:I:102:LEU:O    | 2:I:106:LEU:CB  | 2.53                     | 0.56              |
| 1:B:36:LEU:C     | 1:B:36:LEU:HD23 | 2.26                     | 0.56              |
| 2:I:34:ILE:CD1   | 2:I:97:ALA:HA   | 2.35                     | 0.56              |
| 2:F:30:LEU:HD12  | 2:F:47:TRP:O    | 2.05                     | 0.56              |
| 2:E:26:ARG:CB    | 4:E:221:HOH:O   | 2.38                     | 0.56              |
| 1:C:152:TRP:HZ3  | 2:J:83:ASP:CG   | 2.09                     | 0.56              |
| 1:A:50:ALA:O     | 1:A:52:ILE:HD12 | 2.05                     | 0.56              |
| 1:A:119:HIS:ND1  | 4:A:319:HOH:O   | 2.33                     | 0.56              |
| 2:J:49:VAL:HB    | 2:J:50:PRO:HD2  | 1.88                     | 0.56              |
| 2:J:96:VAL:O     | 2:J:100:THR:HB  | 2.05                     | 0.56              |
| 2:L:38:ASP:C     | 2:L:40:GLN:N    | 2.59                     | 0.56              |
| 1:D:36:LEU:C     | 1:D:36:LEU:HD23 | 2.26                     | 0.56              |
| 2:F:43:LEU:HD23  | 2:F:45:LEU:HD22 | 1.87                     | 0.56              |
| 1:D:4:VAL:HG21   | 2:L:49:VAL:HG13 | 1.88                     | 0.56              |
| 1:D:45:GLN:C     | 1:D:47:TYR:N    | 2.59                     | 0.56              |
| 2:G:30:LEU:CD2   | 2:I:80:PHE:HE1  | 2.18                     | 0.56              |
| 4:B:308:HOH:O    | 2:H:21:ASP:OD2  | 2.18                     | 0.55              |
| 2:E:69:GLN:O     | 2:E:71:GLU:N    | 2.39                     | 0.55              |
| 1:A:62:GLU:HB3   | 4:A:322:HOH:O   | 2.05                     | 0.55              |
| 2:J:43:LEU:HD23  | 2:J:43:LEU:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:68:ASP:C     | 2:L:69:GLN:O     | 2.43                     | 0.55              |
| 1:A:16:LYS:HD3   | 1:A:51:PHE:HE1   | 1.72                     | 0.55              |
| 2:L:49:VAL:HB    | 2:L:50:PRO:HD2   | 1.88                     | 0.55              |
| 2:H:54:ALA:HB2   | 2:H:90:GLN:HE21  | 1.71                     | 0.55              |
| 4:G:215:HOH:O    | 2:H:72:GLY:HA2   | 2.06                     | 0.55              |
| 1:B:31:GLY:HA3   | 2:H:23:ILE:CD1   | 2.36                     | 0.55              |
| 2:G:95:GLU:OE1   | 2:H:82:ARG:NH1   | 2.37                     | 0.55              |
| 2:I:108:ALA:O    | 2:I:109:ALA:HB2  | 2.07                     | 0.55              |
| 1:C:3:LEU:HD11   | 2:I:27:TYR:CE1   | 2.42                     | 0.55              |
| 1:C:6:GLY:HA3    | 1:C:26:MET:SD    | 2.47                     | 0.55              |
| 2:I:110:ARG:H    | 2:I:110:ARG:CZ   | 2.19                     | 0.55              |
| 1:C:94:GLN:O     | 1:C:99:HIS:NE2   | 2.41                     | 0.55              |
| 1:C:48:GLU:HG2   | 1:C:65:ASP:HB3   | 1.89                     | 0.54              |
| 2:G:107:VAL:HG22 | 2:H:71:GLU:CG    | 2.36                     | 0.54              |
| 2:L:59:VAL:O     | 2:L:63:GLU:HG3   | 2.08                     | 0.54              |
| 2:I:41:PRO:CB    | 2:I:104:GLN:NE2  | 2.70                     | 0.54              |
| 1:C:98:GLN:O     | 1:C:101:PHE:HB3  | 2.07                     | 0.54              |
| 2:I:18:THR:CG2   | 2:I:19:HIS:N     | 2.68                     | 0.54              |
| 2:J:70:ILE:O     | 2:J:70:ILE:HG23  | 2.08                     | 0.54              |
| 2:I:18:THR:CG2   | 2:I:19:HIS:H     | 2.21                     | 0.54              |
| 1:B:80:THR:HG22  | 1:B:125:LEU:HD21 | 1.88                     | 0.54              |
| 2:G:70:ILE:O     | 2:G:70:ILE:CG2   | 2.56                     | 0.54              |
| 1:A:155:LYS:HD2  | 1:A:155:LYS:C    | 2.27                     | 0.54              |
| 2:I:75:TRP:CD2   | 2:J:96:VAL:HG22  | 2.43                     | 0.54              |
| 1:D:4:VAL:HG21   | 2:L:49:VAL:CG1   | 2.39                     | 0.53              |
| 2:J:67:ALA:O     | 2:J:68:ASP:C     | 2.45                     | 0.53              |
| 2:H:75:TRP:CD1   | 2:H:76:THR:N     | 2.76                     | 0.53              |
| 1:A:78:HIS:CD2   | 1:A:86:ILE:CB    | 2.90                     | 0.53              |
| 1:C:152:TRP:HZ3  | 2:J:83:ASP:OD1   | 1.91                     | 0.53              |
| 2:E:91:LYS:O     | 2:E:95:GLU:HG3   | 2.08                     | 0.53              |
| 1:C:136:ASN:ND2  | 1:C:138:ALA:HB3  | 2.23                     | 0.53              |
| 2:F:44:SER:CA    | 4:F:201:HOH:O    | 2.24                     | 0.53              |
| 2:F:43:LEU:CD2   | 2:F:45:LEU:N     | 2.71                     | 0.53              |
| 2:J:34:ILE:HB    | 2:J:43:LEU:CB    | 2.37                     | 0.53              |
| 2:G:85:LEU:CD1   | 2:G:94:PHE:HB2   | 2.38                     | 0.53              |
| 2:I:33:GLU:H     | 2:I:52:GLN:NE2   | 2.01                     | 0.53              |
| 1:C:86:ILE:HD11  | 1:C:92:ILE:HG21  | 1.91                     | 0.53              |
| 1:C:86:ILE:O     | 1:C:86:ILE:HG23  | 2.08                     | 0.53              |
| 2:G:89:MET:SD    | 2:J:89:MET:HE2   | 2.49                     | 0.53              |
| 2:K:69:GLN:NE2   | 2:K:69:GLN:HA    | 2.23                     | 0.53              |
| 2:I:34:ILE:HD11  | 2:I:97:ALA:HA    | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:47:TRP:CD1   | 2:L:48:PRO:HD2   | 2.44                     | 0.53              |
| 2:G:39:ARG:NH1   | 2:G:110:ARG:HD2  | 2.23                     | 0.53              |
| 2:E:37:ALA:HB3   | 2:E:104:GLN:HB3  | 1.91                     | 0.53              |
| 2:G:107:VAL:C    | 2:G:109:ALA:H    | 2.13                     | 0.52              |
| 1:A:31:GLY:HA3   | 2:E:23:ILE:HG13  | 1.91                     | 0.52              |
| 2:G:107:VAL:O    | 2:G:109:ALA:N    | 2.42                     | 0.52              |
| 4:B:308:HOH:O    | 2:H:21:ASP:CG    | 2.48                     | 0.52              |
| 2:L:18:THR:HG22  | 2:L:20:VAL:N     | 2.25                     | 0.52              |
| 1:B:86:ILE:O     | 1:B:86:ILE:HG23  | 2.10                     | 0.52              |
| 1:A:152:TRP:HZ3  | 2:F:83:ASP:OD2   | 1.92                     | 0.52              |
| 2:K:87:THR:HG23  | 2:K:88:PRO:HD2   | 1.91                     | 0.52              |
| 2:G:40:GLN:NE2   | 2:G:110:ARG:HH22 | 2.08                     | 0.52              |
| 2:I:36:PRO:CB    | 2:I:41:PRO:HG2   | 2.38                     | 0.52              |
| 1:C:27:ALA:HB2   | 1:C:35:ILE:HD13  | 1.91                     | 0.52              |
| 2:F:87:THR:HG23  | 2:F:88:PRO:HD2   | 1.91                     | 0.52              |
| 1:C:95:THR:O     | 1:C:99:HIS:CD2   | 2.62                     | 0.52              |
| 1:A:71:ARG:CG    | 1:A:71:ARG:NH1   | 2.60                     | 0.52              |
| 2:J:49:VAL:HB    | 2:J:50:PRO:CD    | 2.39                     | 0.51              |
| 1:D:114:LEU:HD23 | 1:D:114:LEU:N    | 2.24                     | 0.51              |
| 2:E:103:GLN:HE22 | 2:F:73:GLN:NE2   | 2.08                     | 0.51              |
| 2:I:36:PRO:HA    | 2:I:41:PRO:CB    | 2.39                     | 0.51              |
| 2:H:33:GLU:H     | 2:H:52:GLN:HE22  | 1.55                     | 0.51              |
| 2:F:87:THR:HB    | 2:F:90:GLN:HG2   | 1.91                     | 0.51              |
| 2:J:46:LEU:HB3   | 4:J:204:HOH:O    | 2.09                     | 0.51              |
| 2:E:83:ASP:CB    | 2:K:50:PRO:HG2   | 2.41                     | 0.51              |
| 2:K:95:GLU:OE1   | 2:L:75:TRP:HZ3   | 1.93                     | 0.51              |
| 2:K:42:GLY:O     | 2:K:43:LEU:HB3   | 2.11                     | 0.51              |
| 2:H:110:ARG:H    | 2:H:110:ARG:HD3  | 1.76                     | 0.51              |
| 2:E:41:PRO:HB3   | 2:E:104:GLN:NE2  | 2.26                     | 0.51              |
| 1:B:38:GLY:HA2   | 1:B:51:PHE:O     | 2.10                     | 0.51              |
| 2:F:39:ARG:NH1   | 2:F:110:ARG:HG3  | 2.25                     | 0.51              |
| 1:B:61:ARG:NH2   | 1:B:65:ASP:OD2   | 2.44                     | 0.51              |
| 2:E:38:ASP:HB2   | 2:E:108:ALA:HB2  | 1.92                     | 0.51              |
| 2:G:39:ARG:NH1   | 2:G:110:ARG:HB2  | 2.26                     | 0.50              |
| 2:L:68:ASP:O     | 2:L:69:GLN:O     | 2.29                     | 0.50              |
| 2:K:59:VAL:O     | 2:K:63:GLU:HG3   | 2.11                     | 0.50              |
| 1:C:58:ALA:CB    | 4:C:310:HOH:O    | 2.59                     | 0.50              |
| 1:C:24:GLN:HE22  | 1:D:25:LYS:HZ3   | 1.56                     | 0.50              |
| 1:A:78:HIS:CE1   | 1:A:82:SER:HB3   | 2.45                     | 0.50              |
| 2:I:99:LEU:HD11  | 2:J:78:PHE:CG    | 2.47                     | 0.50              |
| 2:I:105:ARG:HB2  | 2:I:105:ARG:NH1  | 2.06                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:43:LEU:HD22  | 2:F:45:LEU:N     | 2.26                     | 0.50              |
| 1:A:92:ILE:HD13  | 4:A:321:HOH:O    | 2.11                     | 0.50              |
| 2:H:41:PRO:HD2   | 2:H:41:PRO:O     | 2.11                     | 0.50              |
| 2:G:39:ARG:O     | 2:G:41:PRO:CB    | 2.60                     | 0.50              |
| 2:J:39:ARG:HG3   | 2:J:110:ARG:CZ   | 2.42                     | 0.50              |
| 1:C:63:HIS:HD1   | 1:C:63:HIS:C     | 2.15                     | 0.50              |
| 1:D:159:LEU:HD12 | 1:D:159:LEU:O    | 2.12                     | 0.50              |
| 2:I:55:ILE:HG22  | 4:I:204:HOH:O    | 2.02                     | 0.50              |
| 2:I:95:GLU:O     | 2:I:99:LEU:HB2   | 2.10                     | 0.50              |
| 2:E:68:ASP:CG    | 4:E:223:HOH:O    | 2.49                     | 0.50              |
| 1:C:69:TYR:HB3   | 1:C:101:PHE:HE2  | 1.76                     | 0.50              |
| 2:I:68:ASP:O     | 2:I:69:GLN:O     | 2.30                     | 0.50              |
| 2:E:23:ILE:CB    | 4:E:205:HOH:O    | 2.60                     | 0.50              |
| 1:C:120:GLY:HA3  | 1:C:124:GLU:OE1  | 2.12                     | 0.50              |
| 2:G:58:GLY:HA2   | 2:G:94:PHE:CE2   | 2.47                     | 0.49              |
| 1:C:35:ILE:HG13  | 1:C:36:LEU:N     | 2.27                     | 0.49              |
| 2:K:95:GLU:HB3   | 2:L:75:TRP:HZ3   | 1.77                     | 0.49              |
| 2:J:37:ALA:H     | 2:J:41:PRO:HB2   | 1.77                     | 0.49              |
| 1:A:25:LYS:O     | 1:A:25:LYS:HD2   | 2.12                     | 0.49              |
| 1:A:50:ALA:HB3   | 1:A:52:ILE:HD11  | 1.93                     | 0.49              |
| 1:C:138:ALA:O    | 1:C:142:ARG:HG3  | 2.12                     | 0.49              |
| 2:E:38:ASP:HB2   | 2:E:108:ALA:CB   | 2.42                     | 0.49              |
| 2:I:17:LYS:HG3   | 2:I:17:LYS:O     | 2.10                     | 0.49              |
| 1:C:83:VAL:HG12  | 1:C:119:HIS:HD2  | 1.78                     | 0.49              |
| 2:J:34:ILE:H     | 2:J:43:LEU:HD13  | 1.78                     | 0.49              |
| 2:J:106:LEU:C    | 2:J:106:LEU:HD23 | 2.33                     | 0.49              |
| 2:L:33:GLU:N     | 2:L:52:GLN:HE22  | 2.08                     | 0.49              |
| 2:E:25:GLU:O     | 2:E:28:LYS:HG3   | 2.12                     | 0.49              |
| 2:H:37:ALA:HB3   | 2:H:104:GLN:HB3  | 1.93                     | 0.49              |
| 2:J:39:ARG:O     | 2:J:40:GLN:C     | 2.50                     | 0.49              |
| 2:J:52:GLN:HB3   | 2:J:53:PRO:HD3   | 1.95                     | 0.49              |
| 2:I:36:PRO:CA    | 2:I:41:PRO:HG2   | 2.43                     | 0.49              |
| 2:G:67:ALA:O     | 2:G:68:ASP:C     | 2.51                     | 0.49              |
| 2:G:43:LEU:C     | 2:G:43:LEU:CD2   | 2.82                     | 0.49              |
| 2:L:69:GLN:CA    | 2:L:70:ILE:C     | 2.80                     | 0.49              |
| 2:L:71:GLU:HB3   | 4:L:219:HOH:O    | 2.12                     | 0.49              |
| 2:H:109:ALA:O    | 2:H:110:ARG:C    | 2.52                     | 0.49              |
| 2:F:45:LEU:HG    | 2:K:46:LEU:CD2   | 2.43                     | 0.48              |
| 2:E:102:LEU:O    | 2:E:106:LEU:HD12 | 2.13                     | 0.48              |
| 1:D:136:ASN:C    | 1:D:136:ASN:HD22 | 2.16                     | 0.48              |
| 2:G:39:ARG:HG3   | 2:G:108:ALA:CA   | 2.43                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:41:PRO:HB3   | 2:I:104:GLN:HG2  | 1.96                     | 0.48              |
| 2:G:107:VAL:HG22 | 2:H:71:GLU:CB    | 2.43                     | 0.48              |
| 1:C:102:PHE:CD1  | 1:C:102:PHE:C    | 2.87                     | 0.48              |
| 1:D:45:GLN:HE21  | 1:D:45:GLN:CA    | 2.22                     | 0.48              |
| 1:D:96:ARG:O     | 1:D:96:ARG:HD2   | 2.13                     | 0.48              |
| 2:F:32:VAL:O     | 2:F:43:LEU:HD11  | 2.13                     | 0.48              |
| 2:L:68:ASP:O     | 2:L:70:ILE:O     | 2.30                     | 0.48              |
| 1:A:152:TRP:HZ3  | 2:F:83:ASP:CG    | 2.16                     | 0.48              |
| 2:G:43:LEU:CD2   | 2:G:45:LEU:CB    | 2.92                     | 0.48              |
| 1:B:148:LEU:N    | 1:B:149:PRO:CD   | 2.76                     | 0.48              |
| 2:L:40:GLN:HB3   | 2:L:104:GLN:HG2  | 1.96                     | 0.48              |
| 1:C:102:PHE:C    | 1:C:102:PHE:HD1  | 2.17                     | 0.48              |
| 1:D:152:TRP:HZ3  | 2:K:83:ASP:CG    | 2.17                     | 0.48              |
| 2:J:63:GLU:OE2   | 2:J:101:ARG:NE   | 2.35                     | 0.47              |
| 2:I:85:LEU:N     | 2:I:85:LEU:HD23  | 2.29                     | 0.47              |
| 2:H:68:ASP:O     | 2:H:69:GLN:C     | 2.52                     | 0.47              |
| 1:B:24:GLN:NE2   | 4:B:333:HOH:O    | 2.44                     | 0.47              |
| 1:D:10:LEU:HD13  | 1:D:22:ILE:HG22  | 1.95                     | 0.47              |
| 2:I:105:ARG:HH11 | 2:I:105:ARG:CG   | 2.26                     | 0.47              |
| 2:I:39:ARG:O     | 2:I:41:PRO:N     | 2.47                     | 0.47              |
| 1:C:67:ALA:HB3   | 1:C:69:TYR:CE1   | 2.47                     | 0.47              |
| 2:I:66:LEU:CG    | 4:I:206:HOH:O    | 2.62                     | 0.47              |
| 2:F:38:ASP:OD2   | 2:F:105:ARG:HG3  | 2.14                     | 0.47              |
| 2:H:25:GLU:O     | 2:H:28:LYS:HG2   | 2.14                     | 0.47              |
| 1:C:3:LEU:N      | 1:C:3:LEU:HD12   | 2.30                     | 0.47              |
| 1:D:149:PRO:O    | 1:D:152:TRP:HD1  | 1.97                     | 0.47              |
| 2:H:19:HIS:NE2   | 2:H:23:ILE:HD11  | 2.29                     | 0.47              |
| 1:B:81:GLN:NE2   | 4:B:307:HOH:O    | 2.48                     | 0.47              |
| 2:I:49:VAL:HG22  | 2:I:89:MET:HG2   | 1.96                     | 0.47              |
| 1:C:90:PRO:HB3   | 1:C:102:PHE:HE2  | 1.79                     | 0.47              |
| 1:C:51:PHE:CG    | 1:C:166:ALA:HB2  | 2.50                     | 0.47              |
| 1:D:167:PHE:C    | 4:D:344:HOH:O    | 2.53                     | 0.47              |
| 2:E:69:GLN:C     | 2:E:71:GLU:N     | 2.67                     | 0.47              |
| 2:F:39:ARG:HH11  | 2:F:110:ARG:HG3  | 1.80                     | 0.47              |
| 1:C:116:MET:HE3  | 1:C:128:LEU:HD13 | 1.97                     | 0.47              |
| 2:L:61:GLN:NE2   | 4:L:221:HOH:O    | 2.47                     | 0.46              |
| 2:G:37:ALA:C     | 4:G:209:HOH:O    | 2.52                     | 0.46              |
| 2:I:66:LEU:CD1   | 4:I:206:HOH:O    | 2.51                     | 0.46              |
| 2:J:39:ARG:NH1   | 2:J:110:ARG:HD2  | 2.31                     | 0.46              |
| 2:J:36:PRO:HA    | 2:J:41:PRO:O     | 2.15                     | 0.46              |
| 2:G:55:ILE:HG23  | 2:G:97:ALA:HB2   | 1.98                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:56:ASP:OD1   | 4:K:229:HOH:O    | 2.20                     | 0.46              |
| 2:G:89:MET:CE    | 2:J:89:MET:HE2   | 2.44                     | 0.46              |
| 2:E:19:HIS:O     | 4:E:205:HOH:O    | 2.21                     | 0.46              |
| 1:C:58:ALA:N     | 4:C:310:HOH:O    | 2.36                     | 0.46              |
| 2:L:19:HIS:CE1   | 2:L:23:ILE:HD13  | 2.50                     | 0.46              |
| 1:C:42:LYS:HB2   | 1:C:123:GLY:HA3  | 1.98                     | 0.46              |
| 1:D:94:GLN:NE2   | 4:D:307:HOH:O    | 2.48                     | 0.46              |
| 2:I:101:ARG:HH12 | 2:I:105:ARG:NH1  | 2.14                     | 0.46              |
| 2:I:71:GLU:HG2   | 2:I:71:GLU:H     | 1.40                     | 0.46              |
| 1:C:35:ILE:HD12  | 1:C:130:LEU:HG   | 1.97                     | 0.46              |
| 2:K:95:GLU:OE1   | 2:L:75:TRP:CZ3   | 2.68                     | 0.46              |
| 1:B:88:TRP:CE2   | 3:B:201:OHN:H5C2 | 2.51                     | 0.46              |
| 2:I:70:ILE:CD1   | 2:I:70:ILE:H     | 2.27                     | 0.46              |
| 2:L:39:ARG:NH1   | 2:L:39:ARG:O     | 2.30                     | 0.46              |
| 2:E:26:ARG:O     | 2:E:27:TYR:HB2   | 2.15                     | 0.46              |
| 2:K:87:THR:HB    | 2:K:90:GLN:HG3   | 1.96                     | 0.46              |
| 2:K:70:ILE:HG23  | 2:K:70:ILE:O     | 2.15                     | 0.46              |
| 1:A:9:GLU:HB3    | 1:A:22:ILE:HD13  | 1.97                     | 0.46              |
| 2:I:63:GLU:HG3   | 2:I:101:ARG:NE   | 2.31                     | 0.46              |
| 2:L:39:ARG:C     | 2:L:39:ARG:CD    | 2.72                     | 0.46              |
| 2:E:101:ARG:HH22 | 2:E:105:ARG:NH1  | 2.14                     | 0.46              |
| 2:J:91:LYS:O     | 2:J:95:GLU:HG3   | 2.15                     | 0.46              |
| 2:F:39:ARG:HG3   | 2:F:108:ALA:HA   | 1.97                     | 0.46              |
| 2:H:38:ASP:OD2   | 2:H:105:ARG:HG3  | 2.15                     | 0.46              |
| 2:G:106:LEU:HD11 | 2:H:102:LEU:HD22 | 1.96                     | 0.46              |
| 1:C:89:GLU:OE2   | 4:C:316:HOH:O    | 2.21                     | 0.46              |
| 2:I:52:GLN:N     | 2:I:53:PRO:CD    | 2.79                     | 0.46              |
| 1:D:16:LYS:O     | 1:D:20:SER:HB2   | 2.15                     | 0.46              |
| 2:G:103:GLN:OE1  | 2:H:72:GLY:O     | 2.33                     | 0.46              |
| 2:E:41:PRO:O     | 2:E:42:GLY:C     | 2.54                     | 0.46              |
| 1:B:83:VAL:HG21  | 2:G:81:GLY:HA2   | 1.97                     | 0.46              |
| 2:K:34:ILE:HD12  | 2:K:43:LEU:CD2   | 2.41                     | 0.46              |
| 2:L:30:LEU:HB3   | 2:L:47:TRP:O     | 2.16                     | 0.46              |
| 2:J:85:LEU:HD11  | 2:J:94:PHE:HB2   | 1.96                     | 0.46              |
| 2:E:17:LYS:CE    | 2:E:25:GLU:HG3   | 2.45                     | 0.46              |
| 2:I:54:ALA:HB2   | 2:I:90:GLN:HE21  | 1.81                     | 0.46              |
| 2:K:87:THR:HB    | 2:K:90:GLN:CG    | 2.46                     | 0.45              |
| 1:B:88:TRP:CZ2   | 3:B:201:OHN:H5C2 | 2.51                     | 0.45              |
| 2:K:87:THR:CG2   | 2:K:88:PRO:HD2   | 2.46                     | 0.45              |
| 2:H:33:GLU:H     | 2:H:52:GLN:HE21  | 1.60                     | 0.45              |
| 3:B:201:OHN:H172 | 3:B:201:OHN:H202 | 1.70                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:75:TRP:CG    | 2:L:96:VAL:HG13  | 2.51                     | 0.45              |
| 2:F:70:ILE:O     | 2:F:70:ILE:HG23  | 2.16                     | 0.45              |
| 1:A:78:HIS:CD2   | 1:A:86:ILE:CG2   | 2.98                     | 0.45              |
| 2:J:43:LEU:CD1   | 2:J:45:LEU:HB2   | 2.42                     | 0.45              |
| 1:C:73:ASP:OD2   | 3:C:201:OHN:H101 | 2.17                     | 0.45              |
| 2:E:107:VAL:C    | 2:E:109:ALA:H    | 2.20                     | 0.45              |
| 2:J:33:GLU:OE2   | 2:J:43:LEU:HD21  | 2.17                     | 0.45              |
| 2:F:39:ARG:CG    | 2:F:108:ALA:HA   | 2.47                     | 0.45              |
| 2:K:57:LYS:HE3   | 2:K:61:GLN:OE1   | 2.16                     | 0.45              |
| 2:L:69:GLN:C     | 2:L:70:ILE:O     | 2.55                     | 0.45              |
| 2:I:74:LEU:HG    | 2:J:99:LEU:HD22  | 1.97                     | 0.45              |
| 2:F:29:ASP:C     | 2:F:31:MET:H     | 2.19                     | 0.45              |
| 2:J:38:ASP:C     | 2:J:39:ARG:HD3   | 2.37                     | 0.45              |
| 1:B:45:GLN:NE2   | 1:B:45:GLN:H     | 2.11                     | 0.45              |
| 1:A:136:ASN:HD21 | 1:A:138:ALA:HB3  | 1.81                     | 0.45              |
| 2:I:59:VAL:HG22  | 2:I:101:ARG:HB2  | 1.99                     | 0.45              |
| 2:H:32:VAL:HG22  | 2:H:45:LEU:O     | 2.17                     | 0.45              |
| 2:I:91:LYS:O     | 2:I:95:GLU:HG3   | 2.17                     | 0.45              |
| 1:C:136:ASN:HD22 | 1:C:138:ALA:H    | 1.64                     | 0.45              |
| 1:A:78:HIS:NE2   | 1:A:86:ILE:HB    | 2.31                     | 0.44              |
| 1:A:12:ARG:O     | 1:D:12:ARG:HG2   | 2.17                     | 0.44              |
| 2:I:66:LEU:C     | 2:I:68:ASP:H     | 2.20                     | 0.44              |
| 2:I:34:ILE:HG21  | 2:I:100:THR:HG22 | 1.98                     | 0.44              |
| 2:F:39:ARG:NE    | 2:F:108:ALA:CB   | 2.80                     | 0.44              |
| 1:C:116:MET:CE   | 1:C:128:LEU:HD13 | 2.47                     | 0.44              |
| 2:I:37:ALA:H     | 2:I:41:PRO:CG    | 2.30                     | 0.44              |
| 2:F:39:ARG:CD    | 2:F:108:ALA:HA   | 2.46                     | 0.44              |
| 2:F:101:ARG:HD2  | 2:F:104:GLN:OE1  | 2.18                     | 0.44              |
| 1:B:26:MET:HE3   | 1:B:154:LEU:CD1  | 2.48                     | 0.44              |
| 2:E:49:VAL:HB    | 2:E:50:PRO:HD2   | 2.00                     | 0.44              |
| 2:K:95:GLU:HB3   | 2:L:75:TRP:CZ3   | 2.51                     | 0.44              |
| 1:A:10:LEU:HD13  | 1:A:22:ILE:HG22  | 1.99                     | 0.44              |
| 2:F:35:PRO:HA    | 2:F:36:PRO:HD3   | 1.81                     | 0.44              |
| 2:F:43:LEU:CD2   | 2:F:45:LEU:HD22  | 2.47                     | 0.44              |
| 2:J:95:GLU:O     | 2:J:99:LEU:HB2   | 2.18                     | 0.44              |
| 2:H:40:GLN:HG3   | 2:H:107:VAL:HG12 | 2.00                     | 0.44              |
| 2:J:33:GLU:HA    | 2:J:43:LEU:HD22  | 1.99                     | 0.44              |
| 1:A:152:TRP:CZ3  | 2:F:83:ASP:OD2   | 2.70                     | 0.44              |
| 1:C:9:GLU:HB3    | 1:C:22:ILE:HD13  | 1.99                     | 0.44              |
| 2:J:37:ALA:HB3   | 2:J:104:GLN:HB3  | 1.99                     | 0.44              |
| 2:I:66:LEU:HB2   | 4:I:206:HOH:O    | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:43:LEU:CD2   | 2:G:45:LEU:N     | 2.80                     | 0.44              |
| 1:C:51:PHE:CD2   | 1:C:166:ALA:HB2  | 2.52                     | 0.44              |
| 2:G:73:GLN:HB3   | 4:H:208:HOH:O    | 2.18                     | 0.43              |
| 2:F:39:ARG:HG3   | 2:F:108:ALA:N    | 2.31                     | 0.43              |
| 1:C:152:TRP:HB2  | 2:J:80:PHE:CZ    | 2.53                     | 0.43              |
| 2:G:33:GLU:HA    | 2:G:43:LEU:HD22  | 2.00                     | 0.43              |
| 1:D:136:ASN:HD21 | 1:D:139:GLU:H    | 1.64                     | 0.43              |
| 1:C:84:LEU:HD21  | 2:J:77:ALA:HA    | 1.99                     | 0.43              |
| 2:E:101:ARG:CA   | 4:E:209:HOH:O    | 2.49                     | 0.43              |
| 2:G:106:LEU:HG   | 2:H:106:LEU:CD2  | 2.31                     | 0.43              |
| 1:C:78:HIS:CD2   | 1:C:86:ILE:HB    | 2.53                     | 0.43              |
| 1:D:114:LEU:HD23 | 1:D:114:LEU:H    | 1.82                     | 0.43              |
| 2:H:86:PRO:HG2   | 2:H:87:THR:H     | 1.84                     | 0.43              |
| 1:A:36:LEU:HD23  | 1:A:37:PHE:N     | 2.33                     | 0.43              |
| 1:B:35:ILE:O     | 1:B:54:GLY:HA3   | 2.19                     | 0.43              |
| 2:G:91:LYS:O     | 2:G:94:PHE:HB3   | 2.19                     | 0.43              |
| 2:I:109:ALA:O    | 2:I:110:ARG:C    | 2.57                     | 0.43              |
| 2:I:110:ARG:NH1  | 2:I:110:ARG:H    | 2.17                     | 0.43              |
| 2:G:68:ASP:C     | 2:G:68:ASP:OD1   | 2.57                     | 0.43              |
| 2:G:96:VAL:HG22  | 2:H:75:TRP:CD2   | 2.54                     | 0.43              |
| 2:F:43:LEU:C     | 2:F:43:LEU:HD22  | 2.36                     | 0.43              |
| 2:F:45:LEU:HD12  | 2:F:45:LEU:HA    | 1.60                     | 0.43              |
| 2:F:39:ARG:HG2   | 2:F:108:ALA:HB2  | 2.01                     | 0.43              |
| 2:F:78:PHE:CZ    | 2:F:95:GLU:HG2   | 2.54                     | 0.43              |
| 2:L:66:LEU:HD13  | 2:L:105:ARG:HG3  | 1.99                     | 0.43              |
| 2:E:71:GLU:OE2   | 4:E:218:HOH:O    | 2.21                     | 0.43              |
| 2:I:99:LEU:HD23  | 2:I:99:LEU:HA    | 1.71                     | 0.43              |
| 2:G:34:ILE:HD13  | 2:G:100:THR:HG21 | 2.01                     | 0.43              |
| 2:G:39:ARG:HG3   | 2:G:108:ALA:N    | 2.34                     | 0.43              |
| 2:I:55:ILE:HB    | 4:I:204:HOH:O    | 2.19                     | 0.43              |
| 2:K:68:ASP:HB2   | 2:K:71:GLU:CG    | 2.48                     | 0.43              |
| 2:G:47:TRP:HA    | 2:G:48:PRO:HD3   | 1.83                     | 0.43              |
| 1:D:48:GLU:HG2   | 1:D:65:ASP:O     | 2.18                     | 0.42              |
| 2:I:39:ARG:O     | 2:I:41:PRO:CD    | 2.66                     | 0.42              |
| 2:E:100:THR:CB   | 4:E:209:HOH:O    | 2.65                     | 0.42              |
| 2:E:41:PRO:CB    | 2:E:104:GLN:NE2  | 2.77                     | 0.42              |
| 2:G:105:ARG:HG2  | 2:G:105:ARG:HH11 | 1.83                     | 0.42              |
| 1:B:152:TRP:HB2  | 2:G:80:PHE:CZ    | 2.55                     | 0.42              |
| 2:L:75:TRP:CD1   | 2:L:75:TRP:C     | 2.88                     | 0.42              |
| 2:I:105:ARG:CA   | 4:I:210:HOH:O    | 2.32                     | 0.42              |
| 2:L:40:GLN:HE21  | 2:L:40:GLN:HB2   | 1.64                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:J:103:GLN:HB3 | 2:J:103:GLN:HE21 | 1.58                     | 0.42              |
| 1:C:69:TYR:CD2  | 1:C:101:PHE:CD2  | 3.03                     | 0.42              |
| 2:E:47:TRP:CZ2  | 2:E:93:ALA:HA    | 2.54                     | 0.42              |
| 1:D:89:GLU:O    | 1:D:92:ILE:HG12  | 2.19                     | 0.42              |
| 2:G:52:GLN:N    | 2:G:53:PRO:CD    | 2.82                     | 0.42              |
| 2:E:33:GLU:H    | 2:E:52:GLN:NE2   | 2.05                     | 0.42              |
| 2:L:25:GLU:O    | 2:L:28:LYS:HB3   | 2.20                     | 0.42              |
| 2:F:39:ARG:HG3  | 2:F:107:VAL:HG12 | 2.02                     | 0.42              |
| 1:C:69:TYR:OH   | 1:C:104:GLU:OE1  | 2.31                     | 0.42              |
| 2:G:30:LEU:HD23 | 2:I:80:PHE:HE1   | 1.83                     | 0.42              |
| 2:J:45:LEU:HD12 | 2:J:47:TRP:HE3   | 1.84                     | 0.42              |
| 2:I:39:ARG:HG3  | 2:I:107:VAL:HG13 | 2.01                     | 0.42              |
| 2:E:66:LEU:C    | 2:E:68:ASP:H     | 2.22                     | 0.42              |
| 1:B:26:MET:HE3  | 1:B:154:LEU:HD13 | 2.01                     | 0.42              |
| 2:E:72:GLY:HA2  | 2:F:40:GLN:OE1   | 2.19                     | 0.42              |
| 1:B:149:PRO:O   | 1:B:152:TRP:HD1  | 2.02                     | 0.42              |
| 2:F:39:ARG:HG3  | 2:F:108:ALA:CA   | 2.50                     | 0.42              |
| 1:C:73:ASP:OD1  | 1:C:74:PRO:HD2   | 2.20                     | 0.42              |
| 1:B:37:PHE:CE2  | 1:B:118:LEU:HD11 | 2.55                     | 0.42              |
| 1:B:46:ASP:OD2  | 1:B:49:ASN:HB2   | 2.19                     | 0.42              |
| 2:L:101:ARG:HD2 | 2:L:101:ARG:HA   | 1.81                     | 0.42              |
| 1:D:116:MET:HA  | 1:D:117:PRO:HD3  | 1.95                     | 0.42              |
| 2:K:57:LYS:O    | 2:K:61:GLN:HB2   | 2.20                     | 0.42              |
| 2:H:105:ARG:NH2 | 4:H:201:HOH:O    | 2.06                     | 0.42              |
| 1:A:62:GLU:HB3  | 1:A:66:ARG:HH21  | 1.85                     | 0.42              |
| 2:J:107:VAL:C   | 2:J:109:ALA:H    | 2.23                     | 0.42              |
| 1:D:152:TRP:CZ3 | 2:K:83:ASP:OD2   | 2.73                     | 0.42              |
| 1:B:153:MET:O   | 1:B:154:LEU:C    | 2.59                     | 0.42              |
| 1:C:52:ILE:HD11 | 3:C:201:OHN:H162 | 2.02                     | 0.42              |
| 2:E:101:ARG:HD2 | 2:E:101:ARG:HA   | 1.80                     | 0.41              |
| 2:E:39:ARG:O    | 2:E:41:PRO:CD    | 2.67                     | 0.41              |
| 1:C:88:TRP:CZ3  | 1:C:131:SER:HB2  | 2.55                     | 0.41              |
| 2:L:40:GLN:CG   | 2:L:41:PRO:HD2   | 2.33                     | 0.41              |
| 2:J:107:VAL:O   | 2:J:109:ALA:N    | 2.52                     | 0.41              |
| 2:J:55:ILE:O    | 2:J:59:VAL:HG23  | 2.20                     | 0.41              |
| 2:K:42:GLY:O    | 2:K:43:LEU:CB    | 2.68                     | 0.41              |
| 2:J:29:ASP:C    | 4:J:205:HOH:O    | 2.43                     | 0.41              |
| 1:C:103:GLU:HG2 | 1:C:104:GLU:N    | 2.35                     | 0.41              |
| 1:C:48:GLU:OE2  | 1:C:65:ASP:O     | 2.37                     | 0.41              |
| 2:H:57:LYS:O    | 2:H:61:GLN:HB2   | 2.20                     | 0.41              |
| 1:A:84:LEU:CD2  | 2:F:77:ALA:HA    | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:43:LEU:HD22  | 2:F:44:SER:CA    | 2.50                     | 0.41              |
| 2:E:71:GLU:HG3   | 2:F:107:VAL:HG22 | 2.03                     | 0.41              |
| 2:E:101:ARG:NH1  | 2:E:105:ARG:HB2  | 2.32                     | 0.41              |
| 1:A:92:ILE:HG12  | 4:A:321:HOH:O    | 2.08                     | 0.41              |
| 1:C:10:LEU:HD13  | 1:C:22:ILE:CG2   | 2.51                     | 0.41              |
| 1:C:126:GLY:HA2  | 3:C:201:OHN:H212 | 2.01                     | 0.41              |
| 1:A:76:VAL:HG13  | 3:A:201:OHN:H201 | 2.02                     | 0.41              |
| 2:I:69:GLN:HB3   | 2:I:70:ILE:H     | 1.48                     | 0.41              |
| 2:F:65:TRP:CE3   | 2:F:74:LEU:HD13  | 2.56                     | 0.41              |
| 2:E:94:PHE:CD1   | 2:E:94:PHE:C     | 2.94                     | 0.41              |
| 2:K:52:GLN:N     | 2:K:53:PRO:CD    | 2.84                     | 0.41              |
| 1:A:51:PHE:HB2   | 4:A:324:HOH:O    | 2.13                     | 0.41              |
| 2:I:34:ILE:HD12  | 2:I:97:ALA:HA    | 2.03                     | 0.41              |
| 1:A:74:PRO:HG2   | 1:A:93:TYR:CE1   | 2.55                     | 0.41              |
| 2:F:69:GLN:NE2   | 4:F:207:HOH:O    | 2.53                     | 0.41              |
| 2:H:98:PHE:CD1   | 2:H:98:PHE:C     | 2.94                     | 0.41              |
| 2:H:36:PRO:HA    | 2:H:41:PRO:CA    | 2.51                     | 0.41              |
| 2:G:39:ARG:CG    | 2:G:108:ALA:HB2  | 2.50                     | 0.41              |
| 2:G:39:ARG:CZ    | 2:G:110:ARG:HB2  | 2.51                     | 0.41              |
| 2:E:41:PRO:O     | 2:E:43:LEU:N     | 2.54                     | 0.41              |
| 2:J:45:LEU:HA    | 2:J:45:LEU:HD22  | 1.85                     | 0.41              |
| 2:H:45:LEU:HD12  | 2:H:45:LEU:HA    | 1.85                     | 0.41              |
| 2:E:69:GLN:HB3   | 2:E:70:ILE:H     | 1.48                     | 0.41              |
| 2:F:39:ARG:HE    | 2:F:108:ALA:CB   | 2.33                     | 0.41              |
| 1:A:10:LEU:HD22  | 1:A:26:MET:CE    | 2.51                     | 0.41              |
| 2:F:69:GLN:O     | 2:F:70:ILE:C     | 2.59                     | 0.41              |
| 1:A:36:LEU:HD12  | 1:A:56:TYR:CD2   | 2.56                     | 0.41              |
| 1:B:99:HIS:CE1   | 4:B:337:HOH:O    | 2.74                     | 0.41              |
| 1:B:141:ASN:O    | 1:B:145:GLU:HB2  | 2.20                     | 0.41              |
| 2:I:34:ILE:CD1   | 2:I:55:ILE:HG23  | 2.51                     | 0.41              |
| 2:I:78:PHE:CG    | 2:J:99:LEU:HD11  | 2.56                     | 0.41              |
| 2:F:39:ARG:NE    | 2:F:108:ALA:HA   | 2.36                     | 0.41              |
| 2:F:42:GLY:O     | 2:F:43:LEU:HB3   | 2.20                     | 0.40              |
| 2:F:43:LEU:HD21  | 2:F:45:LEU:N     | 2.36                     | 0.40              |
| 1:B:17:LEU:C     | 1:B:17:LEU:HD23  | 2.42                     | 0.40              |
| 2:G:39:ARG:O     | 2:G:41:PRO:N     | 2.54                     | 0.40              |
| 3:C:201:OHN:H152 | 3:C:201:OHN:H182 | 1.31                     | 0.40              |
| 2:F:34:ILE:HA    | 2:F:35:PRO:HD2   | 1.84                     | 0.40              |
| 2:J:105:ARG:NH1  | 2:J:105:ARG:CG   | 2.54                     | 0.40              |
| 2:H:102:LEU:HA   | 2:H:102:LEU:HD23 | 1.92                     | 0.40              |
| 2:I:92:THR:HA    | 2:I:95:GLU:HG3   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:16:LYS:HE2   | 1:D:165:LEU:O    | 2.21                     | 0.40              |
| 2:F:74:LEU:HD21  | 2:F:102:LEU:HD11 | 2.02                     | 0.40              |
| 1:C:29:ASP:OD1   | 4:C:302:HOH:O    | 2.21                     | 0.40              |
| 2:L:43:LEU:HD23  | 2:L:43:LEU:HA    | 1.92                     | 0.40              |
| 2:G:107:VAL:HA   | 2:H:71:GLU:HG3   | 2.03                     | 0.40              |
| 2:L:65:TRP:O     | 4:L:219:HOH:O    | 2.22                     | 0.40              |
| 1:B:73:ASP:HA    | 1:B:74:PRO:HD3   | 1.90                     | 0.40              |
| 2:I:106:LEU:HD23 | 2:I:106:LEU:C    | 2.41                     | 0.40              |
| 1:D:133:GLU:HG3  | 4:D:301:HOH:O    | 2.22                     | 0.40              |
| 2:J:34:ILE:H     | 2:J:43:LEU:CG    | 2.34                     | 0.40              |
| 2:L:38:ASP:OD2   | 2:L:105:ARG:HG2  | 2.22                     | 0.40              |
| 2:I:99:LEU:CD1   | 2:J:78:PHE:CG    | 3.05                     | 0.40              |
| 1:C:63:HIS:ND1   | 1:C:63:HIS:C     | 2.75                     | 0.40              |
| 1:A:136:ASN:ND2  | 1:A:138:ALA:HB3  | 2.37                     | 0.40              |

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

| Atom-1       | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|--------------|----------------------|--------------------------|-------------------|
| 2:I:36:PRO:O | 4:C:318:HOH:O[1_554] | 1.92                     | 0.28              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 164/184 (89%) | 158 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | B     | 164/184 (89%) | 157 (96%) | 6 (4%)  | 1 (1%)   | 30          | 41  |
| 1   | C     | 164/184 (89%) | 154 (94%) | 9 (6%)  | 1 (1%)   | 30          | 41  |
| 1   | D     | 164/184 (89%) | 158 (96%) | 4 (2%)  | 2 (1%)   | 16          | 22  |
| 2   | E     | 92/113 (81%)  | 75 (82%)  | 9 (10%) | 8 (9%)   | 1           | 0   |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 2   | F     | 80/113 (71%)    | 66 (82%)   | 9 (11%)  | 5 (6%)   | 2           | 0 |
| 2   | G     | 80/113 (71%)    | 64 (80%)   | 10 (12%) | 6 (8%)   | 1           | 0 |
| 2   | H     | 92/113 (81%)    | 75 (82%)   | 12 (13%) | 5 (5%)   | 2           | 1 |
| 2   | I     | 92/113 (81%)    | 73 (79%)   | 13 (14%) | 6 (6%)   | 1           | 0 |
| 2   | J     | 80/113 (71%)    | 55 (69%)   | 18 (22%) | 7 (9%)   | 1           | 0 |
| 2   | K     | 80/113 (71%)    | 75 (94%)   | 2 (2%)   | 3 (4%)   | 4           | 3 |
| 2   | L     | 92/113 (81%)    | 85 (92%)   | 4 (4%)   | 3 (3%)   | 5           | 3 |
| All | All   | 1344/1640 (82%) | 1195 (89%) | 102 (8%) | 47 (4%)  | 4           | 3 |

All (47) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 46  | ASP  |
| 1   | D     | 47  | TYR  |
| 2   | E     | 41  | PRO  |
| 2   | E     | 42  | GLY  |
| 2   | E     | 69  | GLN  |
| 2   | E     | 70  | ILE  |
| 2   | E     | 71  | GLU  |
| 2   | F     | 41  | PRO  |
| 2   | F     | 67  | ALA  |
| 2   | F     | 70  | ILE  |
| 2   | G     | 41  | PRO  |
| 2   | H     | 41  | PRO  |
| 2   | H     | 69  | GLN  |
| 2   | I     | 69  | GLN  |
| 2   | I     | 109 | ALA  |
| 2   | J     | 41  | PRO  |
| 2   | J     | 67  | ALA  |
| 2   | J     | 108 | ALA  |
| 2   | L     | 70  | ILE  |
| 1   | D     | 46  | ASP  |
| 2   | E     | 40  | GLN  |
| 2   | F     | 108 | ALA  |
| 2   | G     | 38  | ASP  |
| 2   | G     | 108 | ALA  |
| 2   | H     | 38  | ASP  |
| 2   | K     | 43  | LEU  |
| 2   | K     | 69  | GLN  |
| 2   | G     | 67  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 68  | ASP  |
| 2   | L     | 69  | GLN  |
| 2   | L     | 72  | GLY  |
| 1   | B     | 43  | ASP  |
| 2   | E     | 67  | ALA  |
| 2   | E     | 72  | GLY  |
| 2   | G     | 107 | VAL  |
| 2   | I     | 67  | ALA  |
| 2   | I     | 104 | GLN  |
| 2   | J     | 40  | GLN  |
| 2   | J     | 104 | GLN  |
| 2   | G     | 40  | GLN  |
| 2   | I     | 40  | GLN  |
| 2   | I     | 41  | PRO  |
| 2   | J     | 69  | GLN  |
| 2   | K     | 70  | ILE  |
| 2   | F     | 40  | GLN  |
| 2   | H     | 86  | PRO  |
| 2   | H     | 72  | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 132/151 (87%) | 119 (90%) | 13 (10%) | 10          | 14 |
| 1   | B     | 132/151 (87%) | 120 (91%) | 12 (9%)  | 12          | 16 |
| 1   | C     | 132/151 (87%) | 117 (89%) | 15 (11%) | 7           | 9  |
| 1   | D     | 132/151 (87%) | 122 (92%) | 10 (8%)  | 16          | 25 |
| 2   | E     | 78/95 (82%)   | 67 (86%)  | 11 (14%) | 4           | 5  |
| 2   | F     | 67/95 (70%)   | 59 (88%)  | 8 (12%)  | 6           | 8  |
| 2   | G     | 67/95 (70%)   | 61 (91%)  | 6 (9%)   | 12          | 17 |
| 2   | H     | 78/95 (82%)   | 70 (90%)  | 8 (10%)  | 9           | 12 |
| 2   | I     | 78/95 (82%)   | 63 (81%)  | 15 (19%) | 2           | 2  |

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| Mol | Chain | Analysed        | Rotameric | Outliers  | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|-------------|----|
| 2   | J     | 67/95 (70%)     | 55 (82%)  | 12 (18%)  | 2           | 2  |
| 2   | K     | 67/95 (70%)     | 61 (91%)  | 6 (9%)    | 12          | 17 |
| 2   | L     | 78/95 (82%)     | 64 (82%)  | 14 (18%)  | 2           | 2  |
| All | All   | 1108/1364 (81%) | 978 (88%) | 130 (12%) | 7           | 8  |

All (130) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 20  | SER  |
| 1   | A     | 26  | MET  |
| 1   | A     | 56  | TYR  |
| 1   | A     | 71  | ARG  |
| 1   | A     | 80  | THR  |
| 1   | A     | 92  | ILE  |
| 1   | A     | 95  | THR  |
| 1   | A     | 96  | ARG  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 135 | GLU  |
| 1   | A     | 152 | TRP  |
| 1   | A     | 155 | LYS  |
| 1   | A     | 156 | ASP  |
| 1   | B     | 4   | VAL  |
| 1   | B     | 16  | LYS  |
| 1   | B     | 43  | ASP  |
| 1   | B     | 45  | GLN  |
| 1   | B     | 91  | SER  |
| 1   | B     | 99  | HIS  |
| 1   | B     | 103 | GLU  |
| 1   | B     | 128 | LEU  |
| 1   | B     | 152 | TRP  |
| 1   | B     | 156 | ASP  |
| 1   | B     | 160 | GLN  |
| 1   | B     | 167 | PHE  |
| 1   | C     | 13  | SER  |
| 1   | C     | 14  | SER  |
| 1   | C     | 28  | SER  |
| 1   | C     | 35  | ILE  |
| 1   | C     | 46  | ASP  |
| 1   | C     | 48  | GLU  |
| 1   | C     | 80  | THR  |
| 1   | C     | 96  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 102 | PHE  |
| 1   | C     | 103 | GLU  |
| 1   | C     | 114 | LEU  |
| 1   | C     | 122 | ARG  |
| 1   | C     | 128 | LEU  |
| 1   | C     | 131 | SER  |
| 1   | C     | 152 | TRP  |
| 1   | D     | 12  | ARG  |
| 1   | D     | 20  | SER  |
| 1   | D     | 44  | SER  |
| 1   | D     | 122 | ARG  |
| 1   | D     | 128 | LEU  |
| 1   | D     | 136 | ASN  |
| 1   | D     | 137 | ARG  |
| 1   | D     | 152 | TRP  |
| 1   | D     | 155 | LYS  |
| 1   | D     | 167 | PHE  |
| 2   | E     | 18  | THR  |
| 2   | E     | 25  | GLU  |
| 2   | E     | 28  | LYS  |
| 2   | E     | 38  | ASP  |
| 2   | E     | 39  | ARG  |
| 2   | E     | 45  | LEU  |
| 2   | E     | 69  | GLN  |
| 2   | E     | 73  | GLN  |
| 2   | E     | 105 | ARG  |
| 2   | E     | 107 | VAL  |
| 2   | E     | 110 | ARG  |
| 2   | F     | 30  | LEU  |
| 2   | F     | 38  | ASP  |
| 2   | F     | 43  | LEU  |
| 2   | F     | 45  | LEU  |
| 2   | F     | 57  | LYS  |
| 2   | F     | 68  | ASP  |
| 2   | F     | 89  | MET  |
| 2   | F     | 105 | ARG  |
| 2   | G     | 38  | ASP  |
| 2   | G     | 69  | GLN  |
| 2   | G     | 70  | ILE  |
| 2   | G     | 99  | LEU  |
| 2   | G     | 105 | ARG  |
| 2   | G     | 106 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 33  | GLU  |
| 2   | H     | 45  | LEU  |
| 2   | H     | 47  | TRP  |
| 2   | H     | 71  | GLU  |
| 2   | H     | 75  | TRP  |
| 2   | H     | 76  | THR  |
| 2   | H     | 80  | PHE  |
| 2   | H     | 110 | ARG  |
| 2   | I     | 17  | LYS  |
| 2   | I     | 25  | GLU  |
| 2   | I     | 26  | ARG  |
| 2   | I     | 28  | LYS  |
| 2   | I     | 31  | MET  |
| 2   | I     | 33  | GLU  |
| 2   | I     | 38  | ASP  |
| 2   | I     | 39  | ARG  |
| 2   | I     | 44  | SER  |
| 2   | I     | 45  | LEU  |
| 2   | I     | 71  | GLU  |
| 2   | I     | 100 | THR  |
| 2   | I     | 105 | ARG  |
| 2   | I     | 107 | VAL  |
| 2   | I     | 110 | ARG  |
| 2   | J     | 32  | VAL  |
| 2   | J     | 38  | ASP  |
| 2   | J     | 39  | ARG  |
| 2   | J     | 43  | LEU  |
| 2   | J     | 45  | LEU  |
| 2   | J     | 55  | ILE  |
| 2   | J     | 57  | LYS  |
| 2   | J     | 68  | ASP  |
| 2   | J     | 69  | GLN  |
| 2   | J     | 100 | THR  |
| 2   | J     | 103 | GLN  |
| 2   | J     | 105 | ARG  |
| 2   | K     | 39  | ARG  |
| 2   | K     | 57  | LYS  |
| 2   | K     | 68  | ASP  |
| 2   | K     | 85  | LEU  |
| 2   | K     | 105 | ARG  |
| 2   | K     | 110 | ARG  |
| 2   | L     | 28  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 33  | GLU  |
| 2   | L     | 39  | ARG  |
| 2   | L     | 40  | GLN  |
| 2   | L     | 43  | LEU  |
| 2   | L     | 45  | LEU  |
| 2   | L     | 69  | GLN  |
| 2   | L     | 70  | ILE  |
| 2   | L     | 71  | GLU  |
| 2   | L     | 73  | GLN  |
| 2   | L     | 75  | TRP  |
| 2   | L     | 89  | MET  |
| 2   | L     | 105 | ARG  |
| 2   | L     | 110 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 78  | HIS  |
| 1   | A     | 99  | HIS  |
| 1   | A     | 136 | ASN  |
| 1   | B     | 24  | GLN  |
| 1   | B     | 45  | GLN  |
| 1   | B     | 136 | ASN  |
| 1   | C     | 24  | GLN  |
| 1   | C     | 119 | HIS  |
| 1   | C     | 136 | ASN  |
| 1   | D     | 24  | GLN  |
| 1   | D     | 45  | GLN  |
| 1   | D     | 63  | HIS  |
| 1   | D     | 136 | ASN  |
| 2   | E     | 52  | GLN  |
| 2   | E     | 73  | GLN  |
| 2   | F     | 73  | GLN  |
| 2   | G     | 40  | GLN  |
| 2   | G     | 73  | GLN  |
| 2   | H     | 52  | GLN  |
| 2   | H     | 90  | GLN  |
| 2   | H     | 104 | GLN  |
| 2   | I     | 52  | GLN  |
| 2   | I     | 90  | GLN  |
| 2   | J     | 73  | GLN  |
| 2   | J     | 103 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 69  | GLN  |
| 2   | K     | 73  | GLN  |
| 2   | L     | 40  | GLN  |
| 2   | L     | 52  | GLN  |
| 2   | L     | 90  | 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](#)

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 3   | OHN  | A     | 201 | -    | 21,21,21     | 1.53 | 3 (14%)     | 20,25,25    | 1.58 | 3 (15%)     |
| 3   | OHN  | B     | 201 | -    | 21,21,21     | 1.54 | 2 (9%)      | 20,25,25    | 1.73 | 3 (15%)     |
| 3   | OHN  | C     | 201 | -    | 21,21,21     | 1.57 | 2 (9%)      | 20,25,25    | 1.37 | 3 (15%)     |
| 3   | OHN  | D     | 201 | -    | 21,21,21     | 1.41 | 2 (9%)      | 20,25,25    | 1.30 | 2 (10%)     |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means



no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 3   | OHN  | A     | 201 | -    | -       | 0/17/27/27 | 0/1/1/1 |
| 3   | OHN  | B     | 201 | -    | -       | 0/17/27/27 | 0/1/1/1 |
| 3   | OHN  | C     | 201 | -    | -       | 0/17/27/27 | 0/1/1/1 |
| 3   | OHN  | D     | 201 | -    | -       | 0/17/27/27 | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 3   | D     | 201 | OHN  | OAP-C4 | -2.90 | 1.38        | 1.46     |
| 3   | B     | 201 | OHN  | OAP-C4 | -2.71 | 1.39        | 1.46     |
| 3   | C     | 201 | OHN  | OAP-C4 | -2.62 | 1.39        | 1.46     |
| 3   | A     | 201 | OHN  | C1-C2  | -2.32 | 1.46        | 1.52     |
| 3   | A     | 201 | OHN  | OAP-C4 | -2.31 | 1.40        | 1.46     |
| 3   | D     | 201 | OHN  | C8-N7  | 5.19  | 1.44        | 1.34     |
| 3   | A     | 201 | OHN  | C8-N7  | 5.74  | 1.45        | 1.34     |
| 3   | B     | 201 | OHN  | C8-N7  | 5.79  | 1.45        | 1.34     |
| 3   | C     | 201 | OHN  | C8-N7  | 5.87  | 1.45        | 1.34     |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | B     | 201 | OHN  | O9-C8-C10   | -3.24 | 117.12      | 121.48   |
| 3   | D     | 201 | OHN  | C14-C13-C11 | -2.95 | 107.96      | 115.12   |
| 3   | A     | 201 | OHN  | C14-C13-C11 | -2.79 | 108.33      | 115.12   |
| 3   | A     | 201 | OHN  | C4-OAP-C2   | -2.75 | 108.12      | 110.62   |
| 3   | C     | 201 | OHN  | O9-C8-C10   | -2.26 | 118.44      | 121.48   |
| 3   | C     | 201 | OHN  | C10-C8-N7   | 2.40  | 119.24      | 115.93   |
| 3   | D     | 201 | OHN  | OAP-C2-O6   | 2.90  | 124.64      | 121.44   |
| 3   | B     | 201 | OHN  | C10-C8-N7   | 3.69  | 121.02      | 115.93   |
| 3   | C     | 201 | OHN  | OAP-C2-O6   | 3.72  | 125.54      | 121.44   |
| 3   | A     | 201 | OHN  | OAP-C2-O6   | 4.44  | 126.34      | 121.44   |
| 3   | B     | 201 | OHN  | OAP-C2-O6   | 4.48  | 126.38      | 121.44   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | A     | 201 | OHN  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 201 | OHN  | 3       | 0            |
| 3   | C     | 201 | OHN  | 4       | 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 166/184 (90%)   | 0.09   | 4 (2%) 62 61  | 22, 47, 77, 104       | 0     |
| 1   | B     | 166/184 (90%)   | -0.07  | 0 100 100     | 21, 39, 70, 102       | 0     |
| 1   | C     | 166/184 (90%)   | 0.35   | 11 (6%) 22 21 | 26, 54, 97, 134       | 0     |
| 1   | D     | 166/184 (90%)   | -0.05  | 4 (2%) 62 61  | 17, 34, 69, 161       | 0     |
| 2   | E     | 94/113 (83%)    | 0.23   | 5 (5%) 30 29  | 25, 45, 95, 130       | 0     |
| 2   | F     | 82/113 (72%)    | 0.40   | 8 (9%) 10 8   | 27, 46, 109, 157      | 0     |
| 2   | G     | 82/113 (72%)    | 0.60   | 9 (10%) 7 7   | 35, 55, 106, 144      | 0     |
| 2   | H     | 94/113 (83%)    | 0.50   | 9 (9%) 10 9   | 32, 58, 108, 174      | 0     |
| 2   | I     | 94/113 (83%)    | 0.84   | 11 (11%) 6 6  | 32, 60, 104, 182      | 0     |
| 2   | J     | 82/113 (72%)    | 1.24   | 13 (15%) 3 2  | 43, 73, 120, 181      | 0     |
| 2   | K     | 82/113 (72%)    | 0.01   | 1 (1%) 81 81  | 19, 31, 64, 189       | 0     |
| 2   | L     | 94/113 (83%)    | 0.10   | 6 (6%) 23 22  | 22, 36, 89, 179       | 0     |
| All | All   | 1368/1640 (83%) | 0.29   | 81 (5%) 26 25 | 17, 46, 99, 189       | 0     |

All (81) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | I     | 70  | ILE  | 10.6 |
| 2   | H     | 70  | ILE  | 10.2 |
| 2   | J     | 40  | GLN  | 10.2 |
| 2   | J     | 44  | SER  | 9.8  |
| 2   | J     | 110 | ARG  | 9.1  |
| 2   | G     | 43  | LEU  | 7.8  |
| 2   | I     | 40  | GLN  | 6.7  |
| 2   | L     | 70  | ILE  | 6.4  |
| 2   | K     | 69  | GLN  | 6.3  |
| 2   | H     | 72  | GLY  | 6.3  |
| 2   | F     | 44  | SER  | 6.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | I     | 72  | GLY  | 5.9  |
| 2   | G     | 69  | GLN  | 5.7  |
| 2   | H     | 69  | GLN  | 5.4  |
| 1   | C     | 49  | ASN  | 5.1  |
| 2   | J     | 69  | GLN  | 5.1  |
| 2   | F     | 40  | GLN  | 5.0  |
| 2   | E     | 70  | ILE  | 4.9  |
| 2   | J     | 70  | ILE  | 4.8  |
| 2   | F     | 43  | LEU  | 4.8  |
| 1   | D     | 48  | GLU  | 4.6  |
| 2   | E     | 40  | GLN  | 4.5  |
| 2   | J     | 43  | LEU  | 4.4  |
| 1   | C     | 96  | ARG  | 4.3  |
| 2   | I     | 42  | GLY  | 4.3  |
| 2   | J     | 30  | LEU  | 4.3  |
| 2   | J     | 39  | ARG  | 4.2  |
| 2   | G     | 40  | GLN  | 4.0  |
| 2   | I     | 69  | GLN  | 3.9  |
| 2   | F     | 110 | ARG  | 3.8  |
| 2   | L     | 69  | GLN  | 3.7  |
| 2   | F     | 68  | ASP  | 3.7  |
| 2   | L     | 40  | GLN  | 3.6  |
| 2   | I     | 77  | ALA  | 3.6  |
| 2   | H     | 39  | ARG  | 3.5  |
| 2   | G     | 39  | ARG  | 3.5  |
| 1   | D     | 49  | ASN  | 3.5  |
| 2   | E     | 72  | GLY  | 3.5  |
| 1   | D     | 96  | ARG  | 3.3  |
| 2   | F     | 70  | ILE  | 3.2  |
| 2   | G     | 70  | ILE  | 3.2  |
| 2   | I     | 102 | LEU  | 3.2  |
| 2   | H     | 71  | GLU  | 3.1  |
| 2   | E     | 69  | GLN  | 3.0  |
| 2   | L     | 39  | ARG  | 3.0  |
| 1   | C     | 69  | TYR  | 3.0  |
| 2   | L     | 72  | GLY  | 3.0  |
| 1   | C     | 97  | LYS  | 2.9  |
| 1   | C     | 43  | ASP  | 2.8  |
| 2   | H     | 41  | PRO  | 2.8  |
| 1   | A     | 92  | ILE  | 2.8  |
| 1   | C     | 48  | GLU  | 2.8  |
| 1   | C     | 71  | ARG  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 105 | ARG  | 2.6  |
| 1   | C     | 66  | ARG  | 2.6  |
| 2   | H     | 80  | PHE  | 2.5  |
| 2   | G     | 110 | ARG  | 2.5  |
| 2   | I     | 107 | VAL  | 2.5  |
| 2   | J     | 60  | ARG  | 2.5  |
| 2   | H     | 37  | ALA  | 2.4  |
| 1   | D     | 43  | ASP  | 2.4  |
| 2   | J     | 34  | ILE  | 2.4  |
| 1   | A     | 70  | ALA  | 2.4  |
| 1   | A     | 47  | TYR  | 2.4  |
| 2   | I     | 67  | ALA  | 2.4  |
| 1   | C     | 93  | TYR  | 2.3  |
| 1   | A     | 96  | ARG  | 2.3  |
| 2   | J     | 107 | VAL  | 2.3  |
| 2   | E     | 37  | ALA  | 2.3  |
| 1   | C     | 98  | GLN  | 2.3  |
| 2   | L     | 25  | GLU  | 2.3  |
| 2   | I     | 39  | ARG  | 2.3  |
| 2   | F     | 69  | GLN  | 2.2  |
| 2   | G     | 44  | SER  | 2.2  |
| 1   | C     | 103 | GLU  | 2.2  |
| 2   | J     | 38  | ASP  | 2.2  |
| 2   | G     | 71  | GLU  | 2.1  |
| 2   | J     | 51  | ALA  | 2.0  |
| 2   | F     | 41  | PRO  | 2.0  |
| 2   | G     | 30  | LEU  | 2.0  |
| 2   | I     | 25  | GLU  | 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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 3   | OHN  | B     | 201 | 21/21 | 0.96 | 0.17 | 1.52 | 29,37,41,45                | 0     |
| 3   | OHN  | C     | 201 | 21/21 | 0.93 | 0.23 | 1.19 | 46,54,59,62                | 0     |
| 3   | OHN  | D     | 201 | 21/21 | 0.97 | 0.15 | 0.52 | 19,28,32,35                | 0     |
| 3   | OHN  | A     | 201 | 21/21 | 0.95 | 0.17 | 0.41 | 29,38,42,45                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.