



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:04 am GMT

PDB ID : 1K5D  
Title : Crystal structure of Ran-GPPNHP-RanBP1-RanGAP complex  
Authors : Seewald, M.J.; Koerner, C.; Wittinghofer, A.; Vetter, I.R.  
Deposited on : 2001-10-10  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

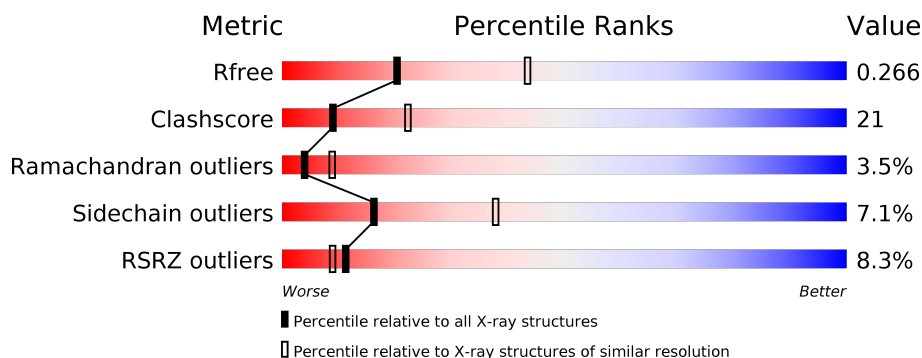
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 111664                      | 2449 (2.70-2.70)                                      |
| Clashscore            | 122126                      | 2756 (2.70-2.70)                                      |
| Ramachandran outliers | 120053                      | 2716 (2.70-2.70)                                      |
| Sidechain outliers    | 120020                      | 2716 (2.70-2.70)                                      |
| RSRZ outliers         | 108989                      | 2376 (2.70-2.70)                                      |

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     | 216    | <div> <div>11%</div> <div> <div></div> <div>55%</div> <div>31%</div> <div>9%</div> <div>5%</div> </div> </div>  |
| 1   | D     | 216    | <div> <div>10%</div> <div> <div></div> <div>56%</div> <div>30%</div> <div>8%</div> <div>5%</div> </div> </div>  |
| 1   | G     | 216    | <div> <div>11%</div> <div> <div></div> <div>59%</div> <div>27%</div> <div>8%</div> <div>5%</div> </div> </div>  |
| 1   | J     | 216    | <div> <div>9%</div> <div> <div></div> <div>56%</div> <div>31%</div> <div>8%</div> <div>5%</div> </div> </div>   |
| 2   | B     | 201    | <div> <div>12%</div> <div> <div></div> <div>34%</div> <div>30%</div> <div>7%</div> <div>27%</div> </div> </div> |
| 2   | E     | 201    | <div> <div>21%</div> <div> <div></div> <div>33%</div> <div>32%</div> <div>7%</div> <div>27%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2   | H     | 201    | <div><div></div><div>12%</div><div>35%</div><div>30%</div><div>7%</div><div>27%</div></div> |
| 2   | K     | 201    | <div><div></div><div>10%</div><div>35%</div><div>31%</div><div>6%</div><div>27%</div></div> |
| 3   | C     | 386    | <div><div></div><div>%</div><div>60%</div><div>26%</div><div>•</div><div>11%</div></div>    |
| 3   | F     | 386    | <div><div></div><div>4%</div><div>64%</div><div>23%</div><div>•</div><div>11%</div></div>   |
| 3   | I     | 386    | <div><div></div><div>%</div><div>62%</div><div>25%</div><div>•</div><div>11%</div></div>    |
| 3   | L     | 386    | <div><div></div><div>3%</div><div>62%</div><div>24%</div><div>•</div><div>11%</div></div>   |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22738 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 GTP-binding nuclear protein RAN.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1652  | 1067 | 284 | 295 | 6 |         |         |       |
| 1   | D     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1652  | 1067 | 284 | 295 | 6 |         |         |       |
| 1   | G     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1652  | 1067 | 284 | 295 | 6 |         |         |       |
| 1   | J     | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1652  | 1067 | 284 | 295 | 6 |         |         |       |

- Molecule 2 is a protein called Ran-specific GTPase-activating protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1216  | 769 | 214 | 226 | 7 |         |         |       |
| 2   | E     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1216  | 769 | 214 | 226 | 7 |         |         |       |
| 2   | H     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1216  | 769 | 214 | 226 | 7 |         |         |       |
| 2   | K     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1216  | 769 | 214 | 226 | 7 |         |         |       |

- Molecule 3 is a protein called Ran GTPase activating protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 344      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2698  | 1699 | 469 | 522 | 8 |         |         |       |
| 3   | F     | 344      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2698  | 1699 | 469 | 522 | 8 |         |         |       |
| 3   | I     | 344      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2698  | 1699 | 469 | 522 | 8 |         |         |       |
| 3   | L     | 344      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2698  | 1699 | 469 | 522 | 8 |         |         |       |

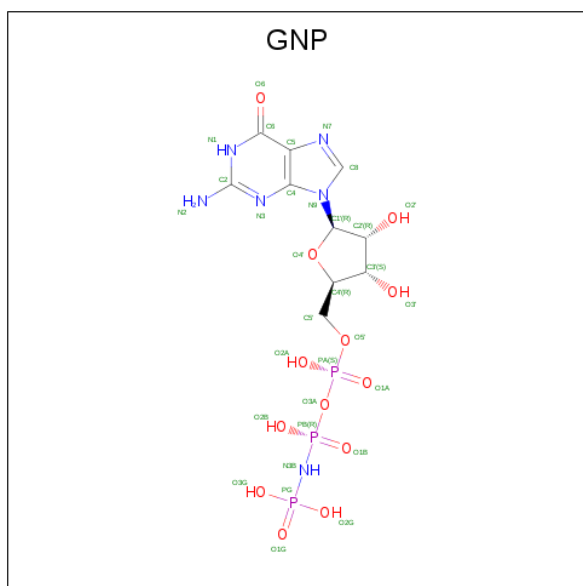
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 2       | ALA      | SER    | SEE REMARK 999 | UNP P41391 |
| F     | 2       | ALA      | SER    | SEE REMARK 999 | UNP P41391 |
| I     | 2       | ALA      | SER    | SEE REMARK 999 | UNP P41391 |
| L     | 2       | ALA      | SER    | SEE REMARK 999 | UNP P41391 |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | J     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms                         | ZeroOcc | AltConf |
|-----|-------|----------|-------------------------------|---------|---------|
| 5   | A     | 1        | Total C N O P<br>32 10 6 13 3 | 0       | 0       |
| 5   | D     | 1        | Total C N O P<br>32 10 6 13 3 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5   | G     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 10 | 6 | 13 | 3 |         |         |
| 5   | J     | 1        | Total | C  | N | O  | P | 0       | 0       |
|     |       |          | 32    | 10 | 6 | 13 | 3 |         |         |

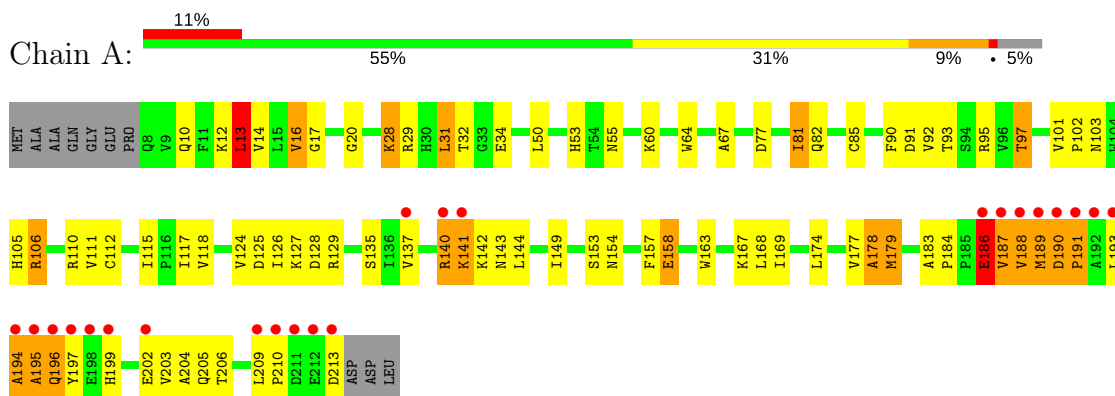
- Molecule 6 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 6   | A     | 24       | Total | O  | 0       | 0       |
|     |       |          | 24    | 24 |         |         |
| 6   | B     | 3        | Total | O  | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 6   | C     | 71       | Total | O  | 0       | 0       |
|     |       |          | 71    | 71 |         |         |
| 6   | D     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |
| 6   | E     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 6   | F     | 47       | Total | O  | 0       | 0       |
|     |       |          | 47    | 47 |         |         |
| 6   | G     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 6   | H     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 6   | I     | 53       | Total | O  | 0       | 0       |
|     |       |          | 53    | 53 |         |         |
| 6   | J     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 6   | K     | 4        | Total | O  | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 6   | L     | 48       | Total | O  | 0       | 0       |
|     |       |          | 48    | 48 |         |         |

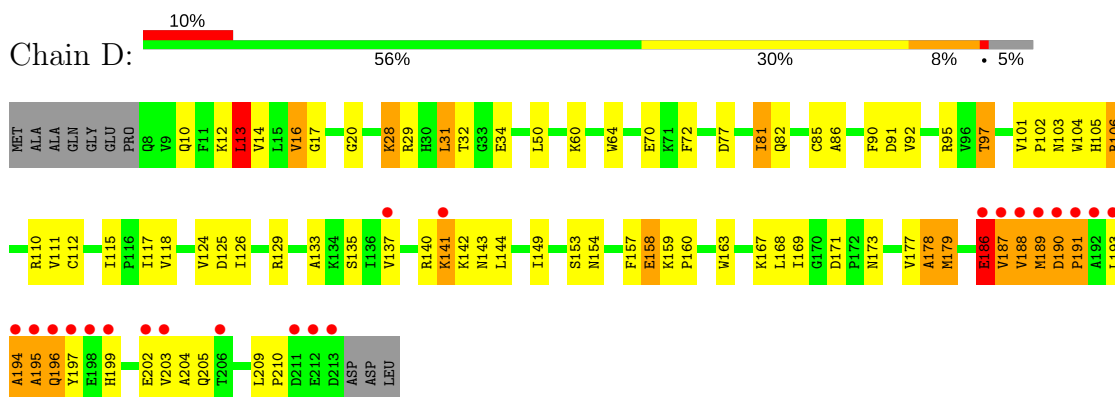
### 3 Residue-property plots [i](#)

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

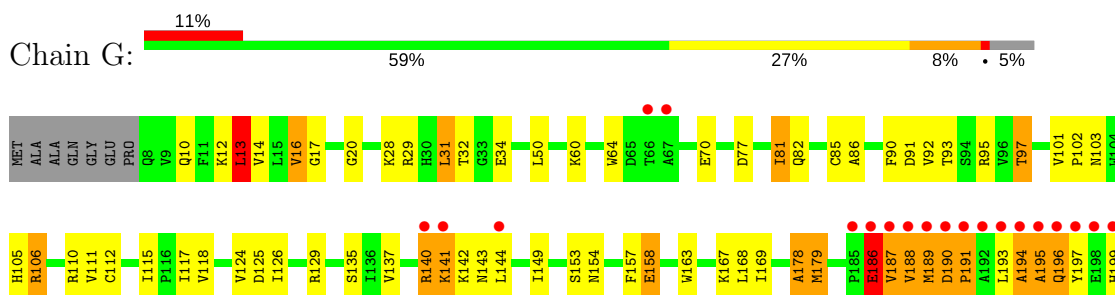
#### • Molecule 1: GTP-binding nuclear protein RAN

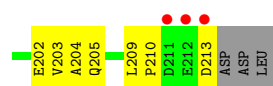


#### • Molecule 1: GTP-binding nuclear protein RAN

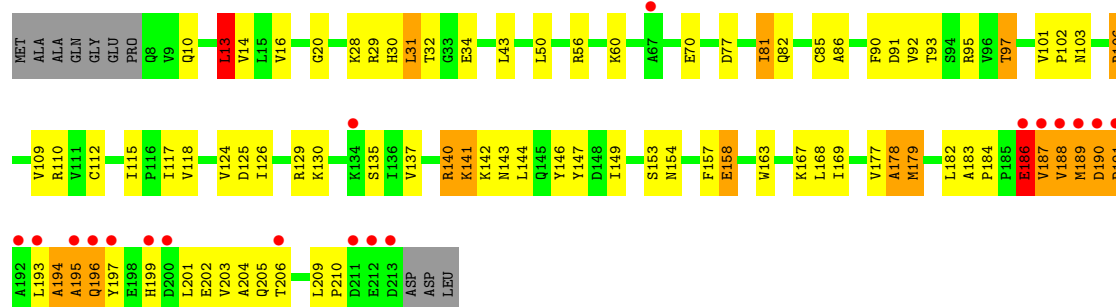


#### • Molecule 1: GTP-binding nuclear protein RAN

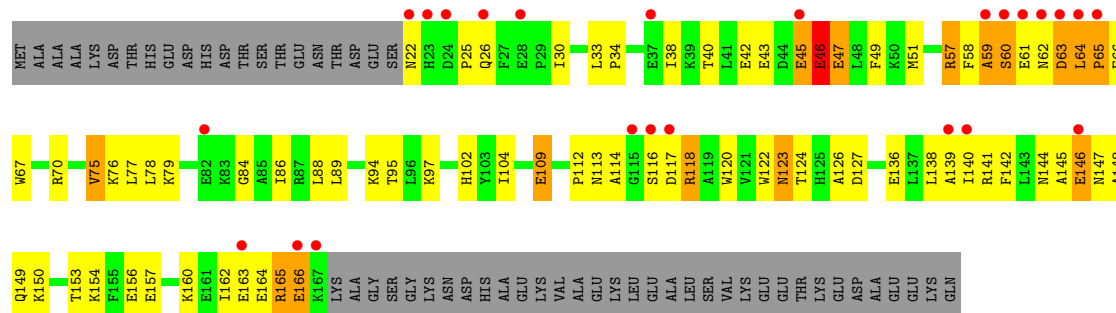




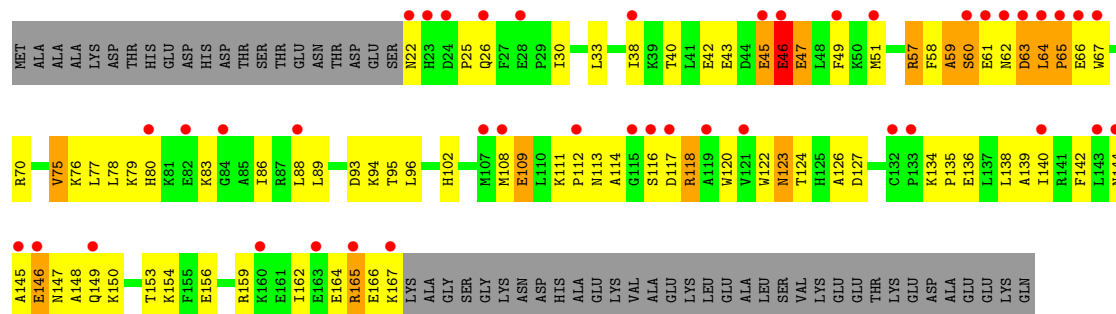
- Molecule 1: GTP-binding nuclear protein RAN



- Molecule 2: Ran-specific GTPase-activating protein



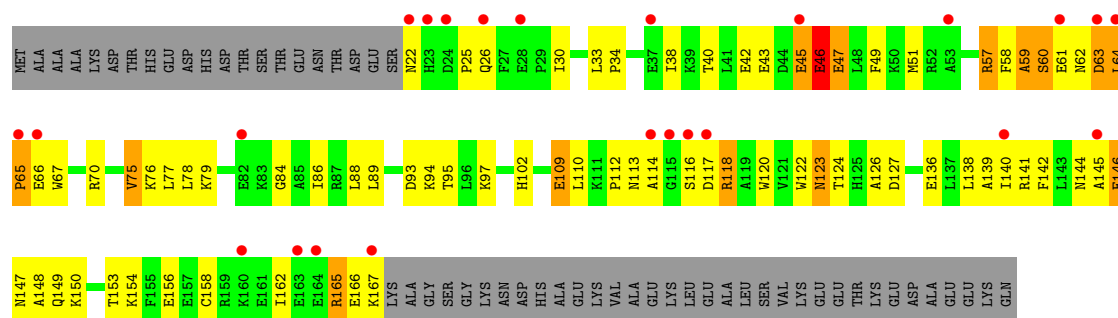
- Molecule 2: Ran-specific GTPase-activating protein



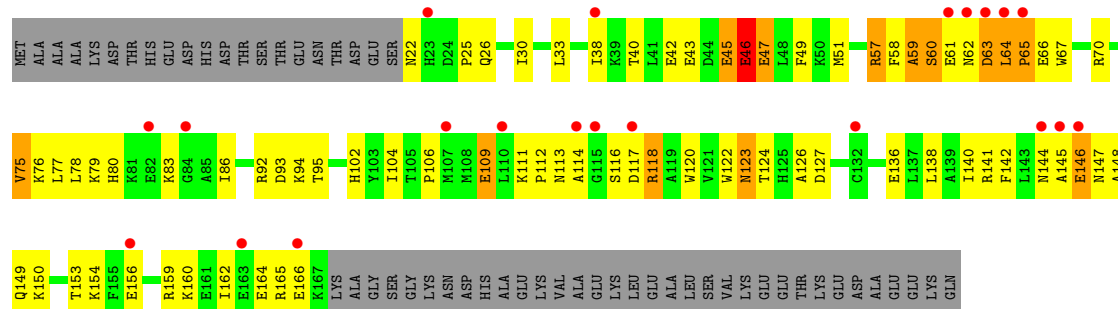
- Molecule 2: Ran-specific GTPase-activating protein



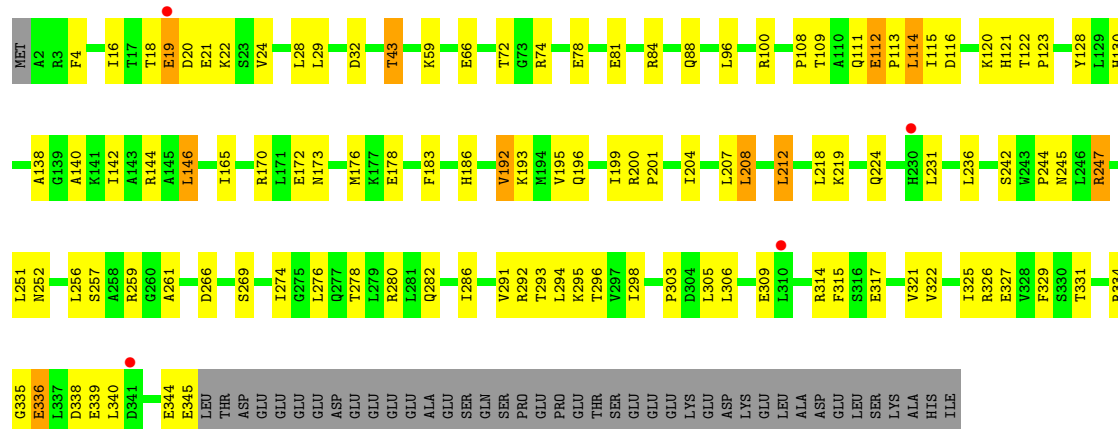




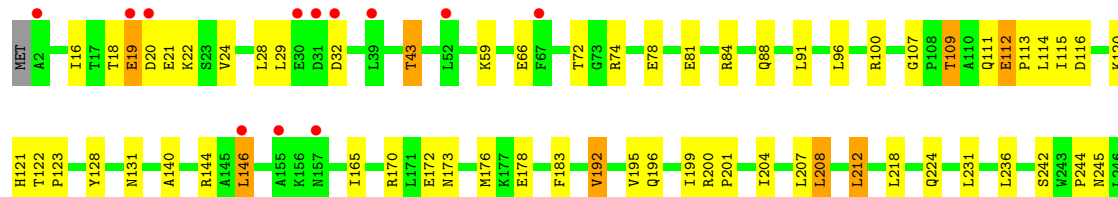
• Molecule 2: Ran-specific GTPase-activating protein

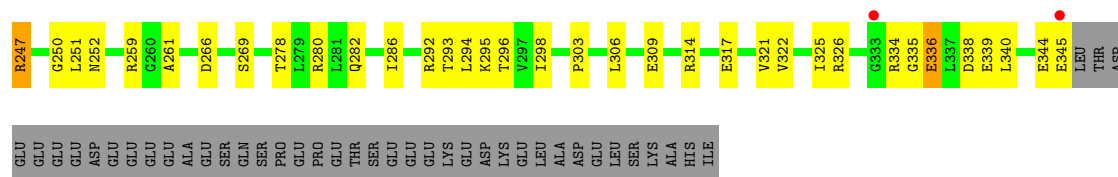


• Molecule 3: Ran GTPase activating protein 1



• Molecule 3: Ran GTPase activating protein 1





### • Molecule 3: Ran GTPase activating protein 1



### • Molecule 3: Ran GTPase activating protein 1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 101.55Å 103.11Å 120.18Å<br>71.59° 80.55° 67.78°             | Depositor        |
| Resolution (Å)                                                          | 20.00 – 2.70<br>20.07 – 2.41                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 98.0 (20.00-2.70)<br>96.3 (20.07-2.41)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.22 (at 2.41Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.237 , 0.267<br>0.237 , 0.266                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 15265 reflections (9.59%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 51.9                                                        | Xtriage          |
| Anisotropy                                                              | 0.183                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 55.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 22738                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 58.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.41         | 0/1693  | 0.65        | 1/2296 (0.0%)  |
| 1   | D     | 0.41         | 0/1693  | 0.64        | 1/2296 (0.0%)  |
| 1   | G     | 0.42         | 0/1693  | 0.64        | 1/2296 (0.0%)  |
| 1   | J     | 0.43         | 0/1693  | 0.65        | 1/2296 (0.0%)  |
| 2   | B     | 0.36         | 0/1242  | 0.62        | 0/1666         |
| 2   | E     | 0.34         | 0/1242  | 0.61        | 0/1666         |
| 2   | H     | 0.36         | 0/1242  | 0.63        | 0/1666         |
| 2   | K     | 0.36         | 0/1242  | 0.62        | 0/1666         |
| 3   | C     | 0.41         | 0/2737  | 0.66        | 0/3697         |
| 3   | F     | 0.39         | 0/2737  | 0.65        | 0/3697         |
| 3   | I     | 0.39         | 0/2737  | 0.66        | 0/3697         |
| 3   | L     | 0.39         | 0/2737  | 0.66        | 0/3697         |
| All | All   | 0.39         | 0/22688 | 0.64        | 4/30636 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | G     | 13  | LEU  | CA-CB-CG | 5.55 | 128.07      | 115.30   |
| 1   | J     | 13  | LEU  | CA-CB-CG | 5.54 | 128.03      | 115.30   |
| 1   | A     | 13  | LEU  | CA-CB-CG | 5.28 | 127.43      | 115.30   |
| 1   | D     | 13  | LEU  | CA-CB-CG | 5.26 | 127.41      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1652  | 0        | 1659     | 76      | 0            |
| 1   | D     | 1652  | 0        | 1659     | 77      | 0            |
| 1   | G     | 1652  | 0        | 1659     | 71      | 0            |
| 1   | J     | 1652  | 0        | 1659     | 89      | 0            |
| 2   | B     | 1216  | 0        | 1208     | 80      | 0            |
| 2   | E     | 1216  | 0        | 1208     | 85      | 0            |
| 2   | H     | 1216  | 0        | 1208     | 79      | 0            |
| 2   | K     | 1216  | 0        | 1208     | 88      | 0            |
| 3   | C     | 2698  | 0        | 2733     | 103     | 0            |
| 3   | F     | 2698  | 0        | 2733     | 85      | 0            |
| 3   | I     | 2698  | 0        | 2733     | 98      | 0            |
| 3   | L     | 2698  | 0        | 2733     | 93      | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | G     | 1     | 0        | 0        | 0       | 0            |
| 4   | J     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 32    | 0        | 13       | 2       | 0            |
| 5   | D     | 32    | 0        | 13       | 3       | 0            |
| 5   | G     | 32    | 0        | 13       | 3       | 0            |
| 5   | J     | 32    | 0        | 13       | 6       | 0            |
| 6   | A     | 24    | 0        | 0        | 4       | 0            |
| 6   | B     | 3     | 0        | 0        | 0       | 0            |
| 6   | C     | 71    | 0        | 0        | 17      | 0            |
| 6   | D     | 29    | 0        | 0        | 5       | 0            |
| 6   | E     | 2     | 0        | 0        | 0       | 0            |
| 6   | F     | 47    | 0        | 0        | 7       | 0            |
| 6   | G     | 25    | 0        | 0        | 4       | 0            |
| 6   | H     | 5     | 0        | 0        | 0       | 0            |
| 6   | I     | 53    | 0        | 0        | 8       | 0            |
| 6   | J     | 31    | 0        | 0        | 6       | 0            |
| 6   | K     | 4     | 0        | 0        | 1       | 0            |
| 6   | L     | 48    | 0        | 0        | 5       | 0            |
| All | All   | 22738 | 0        | 22452    | 964     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (964) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:165:ILE:HA   | 6:C:445:HOH:O    | 1.52                     | 1.09              |
| 5:J:4250:GNP:PG  | 6:J:4252:HOH:O   | 2.14                     | 1.03              |
| 1:A:91:ASP:H     | 1:A:97:THR:HG21  | 1.22                     | 1.01              |
| 1:G:91:ASP:H     | 1:G:97:THR:HG21  | 1.21                     | 1.00              |
| 1:J:91:ASP:H     | 1:J:97:THR:HG21  | 1.23                     | 0.99              |
| 1:D:91:ASP:H     | 1:D:97:THR:HG21  | 1.24                     | 0.98              |
| 2:H:86:ILE:HB    | 2:H:162:ILE:HD11 | 1.49                     | 0.94              |
| 2:E:86:ILE:HB    | 2:E:162:ILE:HD11 | 1.46                     | 0.93              |
| 2:E:42:GLU:O     | 2:E:45:GLU:HB3   | 1.69                     | 0.93              |
| 2:B:42:GLU:O     | 2:B:45:GLU:HB3   | 1.70                     | 0.91              |
| 2:H:42:GLU:O     | 2:H:45:GLU:HB3   | 1.68                     | 0.91              |
| 2:K:42:GLU:O     | 2:K:45:GLU:HB3   | 1.71                     | 0.91              |
| 1:J:158:GLU:HG2  | 2:K:94:LYS:HB3   | 1.52                     | 0.90              |
| 1:D:158:GLU:HG2  | 2:E:94:LYS:HB3   | 1.55                     | 0.88              |
| 1:J:206:THR:O    | 2:K:114:ALA:HB2  | 1.74                     | 0.88              |
| 1:A:90:PHE:HB2   | 1:A:97:THR:HG23  | 1.57                     | 0.86              |
| 2:B:86:ILE:HB    | 2:B:162:ILE:HD11 | 1.58                     | 0.85              |
| 1:A:158:GLU:HG2  | 2:B:94:LYS:HB3   | 1.59                     | 0.84              |
| 5:J:4250:GNP:O2G | 6:J:4252:HOH:O   | 1.93                     | 0.83              |
| 1:J:209:LEU:HD23 | 2:K:113:ASN:ND2  | 1.93                     | 0.83              |
| 3:C:317:GLU:HG2  | 3:C:340:LEU:HB2  | 1.61                     | 0.83              |
| 1:J:90:PHE:HB2   | 1:J:97:THR:HG23  | 1.62                     | 0.81              |
| 1:G:90:PHE:HB2   | 1:G:97:THR:HG23  | 1.61                     | 0.80              |
| 3:C:176:MET:HE3  | 3:C:207:LEU:HB2  | 1.63                     | 0.80              |
| 1:G:91:ASP:H     | 1:G:97:THR:CG2   | 1.95                     | 0.80              |
| 3:I:317:GLU:HG2  | 3:I:340:LEU:HB2  | 1.62                     | 0.80              |
| 3:I:176:MET:HE3  | 3:I:207:LEU:HB2  | 1.63                     | 0.80              |
| 1:D:90:PHE:HB2   | 1:D:97:THR:HG23  | 1.62                     | 0.79              |
| 3:F:317:GLU:HG2  | 3:F:340:LEU:HB2  | 1.64                     | 0.79              |
| 2:H:124:THR:HG22 | 2:H:126:ALA:H    | 1.47                     | 0.79              |
| 3:L:176:MET:HE3  | 3:L:207:LEU:HB2  | 1.64                     | 0.79              |
| 3:C:173:ASN:HD21 | 3:C:200:ARG:H    | 1.31                     | 0.78              |
| 1:J:205:GLN:O    | 2:K:114:ALA:N    | 2.15                     | 0.78              |
| 2:B:124:THR:HG22 | 2:B:126:ALA:H    | 1.49                     | 0.78              |
| 1:D:143:ASN:ND2  | 2:E:25:PRO:HB3   | 1.99                     | 0.78              |
| 1:G:158:GLU:HG2  | 2:H:94:LYS:HB3   | 1.64                     | 0.77              |
| 1:J:205:GLN:HB2  | 2:K:112:PRO:O    | 1.84                     | 0.77              |
| 2:K:124:THR:HG22 | 2:K:126:ALA:H    | 1.49                     | 0.77              |
| 3:L:317:GLU:HG2  | 3:L:340:LEU:HB2  | 1.65                     | 0.77              |
| 1:G:91:ASP:N     | 1:G:97:THR:HG21  | 1.98                     | 0.77              |
| 1:J:91:ASP:N     | 1:J:97:THR:HG21  | 1.99                     | 0.76              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:C:173:ASN:ND2  | 3:C:200:ARG:H     | 1.83                     | 0.76              |
| 6:G:3266:HOH:O   | 3:I:72:THR:HG21   | 1.84                     | 0.76              |
| 3:I:72:THR:HG23  | 6:I:431:HOH:O     | 1.84                     | 0.76              |
| 1:J:91:ASP:H     | 1:J:97:THR:CG2    | 1.98                     | 0.76              |
| 1:A:91:ASP:N     | 1:A:97:THR:HG21   | 2.00                     | 0.76              |
| 3:F:173:ASN:HD21 | 3:F:200:ARG:H     | 1.33                     | 0.76              |
| 1:J:143:ASN:HA   | 2:K:22:ASN:ND2    | 1.99                     | 0.75              |
| 2:E:124:THR:HG22 | 2:E:126:ALA:H     | 1.51                     | 0.75              |
| 3:F:173:ASN:ND2  | 3:F:200:ARG:H     | 1.84                     | 0.75              |
| 3:F:176:MET:HE3  | 3:F:207:LEU:HB2   | 1.67                     | 0.75              |
| 1:A:91:ASP:H     | 1:A:97:THR:CG2    | 2.00                     | 0.75              |
| 1:D:91:ASP:H     | 1:D:97:THR:CG2    | 1.99                     | 0.75              |
| 1:A:186:GLU:CD   | 1:A:187:VAL:H     | 1.90                     | 0.74              |
| 3:L:259:ARG:NH1  | 3:L:259:ARG:HB3   | 2.02                     | 0.74              |
| 1:J:186:GLU:CD   | 1:J:187:VAL:H     | 1.91                     | 0.74              |
| 3:C:193:LYS:HB2  | 6:C:445:HOH:O     | 1.85                     | 0.74              |
| 3:I:173:ASN:ND2  | 3:I:200:ARG:H     | 1.85                     | 0.74              |
| 3:F:259:ARG:HB3  | 3:F:259:ARG:NH1   | 2.02                     | 0.74              |
| 3:I:259:ARG:NH1  | 3:I:259:ARG:HB3   | 2.02                     | 0.74              |
| 3:C:259:ARG:HB3  | 3:C:259:ARG:NH1   | 2.02                     | 0.74              |
| 1:D:91:ASP:N     | 1:D:97:THR:HG21   | 2.00                     | 0.74              |
| 1:G:20:GLY:H     | 5:G:3250:GNP:HNB3 | 1.34                     | 0.73              |
| 1:G:186:GLU:CD   | 1:G:187:VAL:H     | 1.90                     | 0.73              |
| 3:L:173:ASN:ND2  | 3:L:200:ARG:H     | 1.87                     | 0.73              |
| 3:C:176:MET:CE   | 3:C:207:LEU:HB2   | 2.19                     | 0.73              |
| 1:D:186:GLU:CD   | 1:D:187:VAL:H     | 1.92                     | 0.73              |
| 3:I:173:ASN:HD21 | 3:I:200:ARG:H     | 1.36                     | 0.72              |
| 1:A:20:GLY:H     | 5:A:1250:GNP:HNB3 | 1.38                     | 0.71              |
| 2:E:46:GLU:HB2   | 2:E:79:LYS:O      | 1.91                     | 0.71              |
| 3:L:43:THR:HG22  | 3:L:74:ARG:HE     | 1.56                     | 0.71              |
| 1:D:70:GLU:HA    | 6:F:406:HOH:O     | 1.90                     | 0.70              |
| 1:A:209:LEU:HD23 | 2:B:113:ASN:ND2   | 2.06                     | 0.70              |
| 1:J:143:ASN:ND2  | 2:K:25:PRO:HB3    | 2.06                     | 0.70              |
| 1:D:20:GLY:H     | 5:D:2250:GNP:HNB3 | 1.40                     | 0.70              |
| 3:F:112:GLU:HB2  | 6:F:425:HOH:O     | 1.92                     | 0.70              |
| 2:H:46:GLU:HB2   | 2:H:79:LYS:O      | 1.92                     | 0.70              |
| 1:J:29:ARG:HD3   | 1:J:154:ASN:OD1   | 1.92                     | 0.70              |
| 3:I:43:THR:HG22  | 3:I:74:ARG:HE     | 1.57                     | 0.70              |
| 2:K:46:GLU:HB2   | 2:K:79:LYS:O      | 1.92                     | 0.70              |
| 2:K:59:ALA:O     | 2:K:60:SER:HB2    | 1.93                     | 0.69              |
| 2:H:146:GLU:O    | 2:H:150:LYS:HG3   | 1.93                     | 0.69              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:146:GLU:O    | 2:E:150:LYS:HG3   | 1.91                     | 0.69              |
| 2:H:59:ALA:O     | 2:H:60:SER:HB2    | 1.92                     | 0.69              |
| 1:J:20:GLY:H     | 5:J:4250:GNP:HNB3 | 1.41                     | 0.69              |
| 2:B:146:GLU:O    | 2:B:150:LYS:HG3   | 1.93                     | 0.69              |
| 3:L:32:ASP:HA    | 3:L:59:LYS:HE2    | 1.74                     | 0.69              |
| 2:E:59:ALA:O     | 2:E:60:SER:HB2    | 1.92                     | 0.68              |
| 3:F:20:ASP:O     | 3:F:22:LYS:N      | 2.26                     | 0.68              |
| 1:J:189:MET:O    | 1:J:190:ASP:HB2   | 1.91                     | 0.68              |
| 1:A:189:MET:O    | 1:A:190:ASP:HB2   | 1.91                     | 0.68              |
| 2:B:46:GLU:HB2   | 2:B:79:LYS:O      | 1.94                     | 0.68              |
| 1:D:189:MET:O    | 1:D:190:ASP:HB2   | 1.92                     | 0.68              |
| 5:D:2250:GNP:PG  | 6:D:2252:HOH:O    | 2.51                     | 0.68              |
| 2:E:75:VAL:HG21  | 2:E:140:ILE:HD11  | 1.76                     | 0.68              |
| 3:F:170:ARG:NH1  | 6:F:426:HOH:O     | 2.22                     | 0.68              |
| 1:G:143:ASN:ND2  | 2:H:25:PRO:HB3    | 2.08                     | 0.68              |
| 1:G:189:MET:O    | 1:G:190:ASP:HB2   | 1.92                     | 0.68              |
| 3:L:173:ASN:HD21 | 3:L:200:ARG:H     | 1.42                     | 0.68              |
| 3:I:176:MET:CE   | 3:I:207:LEU:HB2   | 2.23                     | 0.68              |
| 2:K:146:GLU:O    | 2:K:150:LYS:HG3   | 1.94                     | 0.68              |
| 2:B:59:ALA:O     | 2:B:60:SER:HB2    | 1.93                     | 0.67              |
| 1:D:29:ARG:HD3   | 1:D:154:ASN:OD1   | 1.94                     | 0.67              |
| 2:B:75:VAL:HG21  | 2:B:140:ILE:HD11  | 1.77                     | 0.67              |
| 3:F:43:THR:HG22  | 3:F:74:ARG:HE     | 1.59                     | 0.67              |
| 2:K:75:VAL:HG21  | 2:K:140:ILE:HD11  | 1.75                     | 0.67              |
| 1:G:29:ARG:HD3   | 1:G:154:ASN:OD1   | 1.94                     | 0.67              |
| 3:F:204:ILE:HG23 | 3:F:208:LEU:CD2   | 2.25                     | 0.67              |
| 3:F:32:ASP:HA    | 3:F:59:LYS:HE2    | 1.77                     | 0.67              |
| 1:G:169:ILE:HD12 | 2:H:33:LEU:HD12   | 1.75                     | 0.67              |
| 3:L:204:ILE:HG23 | 3:L:208:LEU:CD2   | 2.25                     | 0.67              |
| 3:L:176:MET:CE   | 3:L:207:LEU:HB2   | 2.25                     | 0.66              |
| 3:C:20:ASP:O     | 3:C:22:LYS:N      | 2.28                     | 0.66              |
| 1:D:32:THR:HG22  | 1:D:34:GLU:H      | 1.59                     | 0.66              |
| 3:L:20:ASP:O     | 3:L:22:LYS:N      | 2.28                     | 0.66              |
| 2:B:117:ASP:OD2  | 2:B:145:ALA:HB2   | 1.95                     | 0.66              |
| 1:G:32:THR:HG22  | 1:G:34:GLU:H      | 1.61                     | 0.66              |
| 3:I:192:VAL:HG12 | 3:I:218:LEU:HD11  | 1.76                     | 0.66              |
| 2:B:123:ASN:HD22 | 2:B:124:THR:H     | 1.44                     | 0.66              |
| 2:E:62:ASN:O     | 2:E:64:LEU:HD22   | 1.96                     | 0.66              |
| 3:C:327:GLU:HG3  | 1:J:109:VAL:HG21  | 1.76                     | 0.66              |
| 2:E:59:ALA:HB2   | 2:E:65:PRO:HA     | 1.78                     | 0.66              |
| 2:K:59:ALA:HB2   | 2:K:65:PRO:HA     | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:123:ASN:HD22 | 2:E:124:THR:H    | 1.44                     | 0.65              |
| 1:A:13:LEU:HB2   | 1:A:85:CYS:SG    | 2.36                     | 0.65              |
| 3:F:192:VAL:HG12 | 3:F:218:LEU:HD11 | 1.76                     | 0.65              |
| 3:L:192:VAL:HG12 | 3:L:218:LEU:HD11 | 1.78                     | 0.65              |
| 3:I:204:ILE:HG23 | 3:I:208:LEU:CD2  | 2.26                     | 0.65              |
| 2:K:117:ASP:OD2  | 2:K:145:ALA:HB2  | 1.96                     | 0.65              |
| 3:C:176:MET:HE1  | 3:C:207:LEU:HD22 | 1.77                     | 0.65              |
| 2:E:122:TRP:HZ3  | 2:E:140:ILE:HG22 | 1.62                     | 0.65              |
| 1:J:32:THR:HG22  | 1:J:34:GLU:H     | 1.61                     | 0.65              |
| 3:C:43:THR:HG22  | 3:C:74:ARG:HE    | 1.61                     | 0.65              |
| 3:I:32:ASP:HA    | 3:I:59:LYS:HE2   | 1.78                     | 0.65              |
| 2:B:123:ASN:ND2  | 2:B:124:THR:H    | 1.95                     | 0.65              |
| 1:D:143:ASN:HA   | 2:E:22:ASN:ND2   | 2.11                     | 0.65              |
| 1:A:92:VAL:HG13  | 1:A:129:ARG:HG3  | 1.79                     | 0.65              |
| 2:E:123:ASN:ND2  | 2:E:124:THR:H    | 1.95                     | 0.65              |
| 2:H:46:GLU:HG3   | 2:H:79:LYS:HB3   | 1.77                     | 0.65              |
| 2:B:49:PHE:HB3   | 2:B:77:LEU:HD12  | 1.79                     | 0.65              |
| 2:K:62:ASN:O     | 2:K:64:LEU:HD22  | 1.97                     | 0.65              |
| 1:A:143:ASN:ND2  | 2:B:25:PRO:HB3   | 2.12                     | 0.65              |
| 2:H:123:ASN:ND2  | 2:H:124:THR:H    | 1.95                     | 0.65              |
| 2:K:46:GLU:HG3   | 2:K:79:LYS:HB3   | 1.79                     | 0.65              |
| 1:A:29:ARG:HD3   | 1:A:154:ASN:OD1  | 1.96                     | 0.65              |
| 1:A:53:HIS:ND1   | 6:A:1269:HOH:O   | 2.28                     | 0.65              |
| 2:B:62:ASN:O     | 2:B:64:LEU:HD22  | 1.97                     | 0.65              |
| 3:F:200:ARG:HB3  | 3:F:201:PRO:CD   | 2.27                     | 0.65              |
| 2:H:75:VAL:HG21  | 2:H:140:ILE:HD11 | 1.78                     | 0.65              |
| 2:H:123:ASN:HD22 | 2:H:124:THR:H    | 1.45                     | 0.64              |
| 3:I:20:ASP:O     | 3:I:22:LYS:N     | 2.31                     | 0.64              |
| 3:C:200:ARG:HB3  | 3:C:201:PRO:CD   | 2.28                     | 0.64              |
| 2:E:117:ASP:OD2  | 2:E:145:ALA:HB2  | 1.96                     | 0.64              |
| 3:I:187:ARG:NH1  | 3:L:272:GLU:HG3  | 2.11                     | 0.64              |
| 3:F:176:MET:CE   | 3:F:207:LEU:HB2  | 2.27                     | 0.64              |
| 2:H:117:ASP:OD2  | 2:H:145:ALA:HB2  | 1.97                     | 0.64              |
| 1:J:193:LEU:HD12 | 1:J:193:LEU:H    | 1.62                     | 0.64              |
| 2:H:59:ALA:HB2   | 2:H:65:PRO:HA    | 1.80                     | 0.64              |
| 2:B:59:ALA:HB2   | 2:B:65:PRO:HA    | 1.79                     | 0.64              |
| 3:C:112:GLU:HB2  | 6:C:388:HOH:O    | 1.98                     | 0.64              |
| 3:F:252:ASN:ND2  | 3:F:282:GLN:H    | 1.95                     | 0.64              |
| 2:B:122:TRP:HZ3  | 2:B:140:ILE:HG22 | 1.62                     | 0.63              |
| 2:B:46:GLU:HG3   | 2:B:79:LYS:HB3   | 1.80                     | 0.63              |
| 3:C:204:ILE:HG23 | 3:C:208:LEU:CD2  | 2.28                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:192:VAL:HG12 | 3:C:218:LEU:HD11 | 1.80                     | 0.63              |
| 2:H:167:LYS:N    | 2:H:167:LYS:HD2  | 2.13                     | 0.63              |
| 3:C:32:ASP:HA    | 3:C:59:LYS:HE2   | 1.79                     | 0.63              |
| 3:I:176:MET:HE1  | 3:I:207:LEU:HD22 | 1.78                     | 0.63              |
| 3:L:112:GLU:HB2  | 6:L:423:HOH:O    | 1.98                     | 0.63              |
| 6:D:2277:HOH:O   | 3:F:109:THR:CG2  | 2.47                     | 0.63              |
| 1:A:169:ILE:HD12 | 2:B:33:LEU:HD12  | 1.81                     | 0.63              |
| 1:D:92:VAL:HG13  | 1:D:129:ARG:HG3  | 1.81                     | 0.63              |
| 3:L:200:ARG:HB3  | 3:L:201:PRO:CD   | 2.28                     | 0.63              |
| 1:A:127:LYS:HB3  | 6:A:1262:HOH:O   | 1.98                     | 0.63              |
| 1:G:13:LEU:HB2   | 1:G:85:CYS:SG    | 2.39                     | 0.63              |
| 1:A:193:LEU:H    | 1:A:193:LEU:HD12 | 1.64                     | 0.63              |
| 1:A:92:VAL:CG1   | 1:A:129:ARG:HG3  | 2.29                     | 0.62              |
| 1:G:126:ILE:HD11 | 5:G:3250:GNP:N2  | 2.14                     | 0.62              |
| 2:K:104:ILE:O    | 2:K:162:ILE:HD13 | 1.99                     | 0.62              |
| 2:E:49:PHE:HB3   | 2:E:77:LEU:HD12  | 1.79                     | 0.62              |
| 2:K:123:ASN:HD22 | 2:K:124:THR:H    | 1.47                     | 0.62              |
| 2:E:46:GLU:HG3   | 2:E:79:LYS:HB3   | 1.80                     | 0.62              |
| 1:G:153:SER:O    | 1:G:154:ASN:HB2  | 1.99                     | 0.62              |
| 2:E:47:GLU:HA    | 2:E:78:LEU:HD23  | 1.82                     | 0.62              |
| 1:A:153:SER:O    | 1:A:154:ASN:HB2  | 1.98                     | 0.62              |
| 3:F:200:ARG:HB3  | 3:F:201:PRO:HD2  | 1.81                     | 0.62              |
| 2:K:136:GLU:HG2  | 2:K:138:LEU:HD21 | 1.80                     | 0.62              |
| 3:L:176:MET:HE1  | 3:L:207:LEU:HD22 | 1.80                     | 0.62              |
| 1:A:32:THR:HG22  | 1:A:34:GLU:H     | 1.65                     | 0.62              |
| 2:B:47:GLU:HA    | 2:B:78:LEU:HD23  | 1.81                     | 0.62              |
| 2:K:47:GLU:HA    | 2:K:78:LEU:HD23  | 1.80                     | 0.62              |
| 1:D:143:ASN:HD21 | 2:E:25:PRO:HB3   | 1.64                     | 0.62              |
| 2:H:62:ASN:O     | 2:H:64:LEU:HD22  | 1.99                     | 0.62              |
| 1:D:189:MET:HB2  | 1:D:193:LEU:HD22 | 1.82                     | 0.62              |
| 1:J:153:SER:O    | 1:J:154:ASN:HB2  | 2.00                     | 0.61              |
| 3:C:200:ARG:HB3  | 3:C:201:PRO:HD2  | 1.82                     | 0.61              |
| 1:D:209:LEU:HD23 | 2:E:113:ASN:ND2  | 2.15                     | 0.61              |
| 1:G:117:ILE:HB   | 1:G:144:LEU:HD22 | 1.83                     | 0.61              |
| 3:C:193:LYS:N    | 6:C:445:HOH:O    | 2.27                     | 0.61              |
| 2:B:136:GLU:HG2  | 2:B:138:LEU:HD21 | 1.81                     | 0.61              |
| 3:I:112:GLU:HB2  | 6:I:425:HOH:O    | 2.00                     | 0.61              |
| 1:J:77:ASP:OD2   | 1:J:110:ARG:NH2  | 2.34                     | 0.61              |
| 1:J:169:ILE:HD12 | 2:K:33:LEU:HD12  | 1.83                     | 0.61              |
| 3:F:111:GLN:O    | 3:F:115:ILE:HG13 | 2.01                     | 0.61              |
| 2:H:136:GLU:HG2  | 2:H:138:LEU:HD21 | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:144:ASN:HB2  | 2:E:146:GLU:HG3  | 1.83                     | 0.61              |
| 2:K:92:ARG:HD2   | 6:K:202:HOH:O    | 2.00                     | 0.61              |
| 1:D:126:ILE:HD11 | 5:D:2250:GNP:N2  | 2.15                     | 0.61              |
| 3:F:176:MET:HE1  | 3:F:207:LEU:HD22 | 1.83                     | 0.61              |
| 1:G:193:LEU:H    | 1:G:193:LEU:HD12 | 1.64                     | 0.61              |
| 2:E:136:GLU:HG2  | 2:E:138:LEU:HD21 | 1.83                     | 0.61              |
| 1:G:92:VAL:HG13  | 1:G:129:ARG:HG3  | 1.82                     | 0.61              |
| 2:H:47:GLU:HA    | 2:H:78:LEU:HD23  | 1.82                     | 0.61              |
| 1:D:92:VAL:CG1   | 1:D:129:ARG:HG3  | 2.30                     | 0.61              |
| 3:L:335:GLY:O    | 3:L:336:GLU:HB2  | 1.99                     | 0.61              |
| 2:K:122:TRP:HZ3  | 2:K:140:ILE:HG22 | 1.65                     | 0.60              |
| 2:K:144:ASN:HB2  | 2:K:146:GLU:HG3  | 1.83                     | 0.60              |
| 1:J:143:ASN:HA   | 2:K:22:ASN:HD22  | 1.64                     | 0.60              |
| 2:B:144:ASN:HB2  | 2:B:146:GLU:HG3  | 1.83                     | 0.60              |
| 1:D:117:ILE:HB   | 1:D:144:LEU:HD22 | 1.82                     | 0.60              |
| 3:I:200:ARG:HB3  | 3:I:201:PRO:CD   | 2.31                     | 0.60              |
| 2:K:49:PHE:HB3   | 2:K:77:LEU:HD12  | 1.83                     | 0.60              |
| 2:H:144:ASN:HB2  | 2:H:146:GLU:HG3  | 1.84                     | 0.60              |
| 1:A:117:ILE:HB   | 1:A:144:LEU:HD22 | 1.84                     | 0.60              |
| 2:H:49:PHE:HB3   | 2:H:77:LEU:HD12  | 1.83                     | 0.60              |
| 3:I:184:GLN:HE22 | 3:L:270:LYS:NZ   | 2.00                     | 0.60              |
| 2:B:43:GLU:C     | 2:B:45:GLU:H     | 2.03                     | 0.60              |
| 1:D:13:LEU:HD12  | 1:D:13:LEU:C     | 2.22                     | 0.60              |
| 2:E:167:LYS:HD2  | 2:E:167:LYS:N    | 2.16                     | 0.60              |
| 3:I:116:ASP:OD2  | 3:I:120:LYS:HE2  | 2.02                     | 0.60              |
| 3:I:200:ARG:HB3  | 3:I:201:PRO:HD2  | 1.83                     | 0.60              |
| 1:D:193:LEU:H    | 1:D:193:LEU:HD12 | 1.66                     | 0.60              |
| 1:G:101:VAL:HB   | 1:G:102:PRO:HD3  | 1.84                     | 0.59              |
| 2:H:122:TRP:HZ3  | 2:H:140:ILE:HG22 | 1.66                     | 0.59              |
| 3:I:252:ASN:ND2  | 3:I:282:GLN:H    | 2.00                     | 0.59              |
| 1:J:101:VAL:HB   | 1:J:102:PRO:HD3  | 1.84                     | 0.59              |
| 1:A:168:LEU:HD22 | 2:B:30:ILE:HD12  | 1.84                     | 0.59              |
| 2:K:123:ASN:ND2  | 2:K:124:THR:H    | 1.99                     | 0.59              |
| 1:D:153:SER:O    | 1:D:154:ASN:HB2  | 2.01                     | 0.59              |
| 3:L:200:ARG:HB3  | 3:L:201:PRO:HD2  | 1.85                     | 0.59              |
| 3:L:252:ASN:ND2  | 3:L:282:GLN:H    | 2.01                     | 0.59              |
| 1:A:189:MET:HB2  | 1:A:193:LEU:HD22 | 1.83                     | 0.59              |
| 2:B:109:GLU:CD   | 2:B:109:GLU:H    | 2.06                     | 0.59              |
| 2:E:43:GLU:C     | 2:E:45:GLU:H     | 2.05                     | 0.59              |
| 2:K:109:GLU:CD   | 2:K:109:GLU:H    | 2.06                     | 0.59              |
| 3:C:140:ALA:O    | 3:C:144:ARG:HG3  | 2.03                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:168:LEU:HD22 | 2:H:30:ILE:HD12  | 1.85                     | 0.59              |
| 2:H:43:GLU:C     | 2:H:45:GLU:H     | 2.04                     | 0.59              |
| 1:J:92:VAL:HG13  | 1:J:129:ARG:HG3  | 1.84                     | 0.59              |
| 2:H:62:ASN:O     | 2:H:63:ASP:HB2   | 2.02                     | 0.58              |
| 3:I:140:ALA:O    | 3:I:144:ARG:HG3  | 2.03                     | 0.58              |
| 2:E:109:GLU:H    | 2:E:109:GLU:CD   | 2.06                     | 0.58              |
| 1:D:169:ILE:HD12 | 2:E:33:LEU:HD12  | 1.85                     | 0.58              |
| 3:F:116:ASP:OD2  | 3:F:120:LYS:HE2  | 2.03                     | 0.58              |
| 3:C:192:VAL:CG1  | 3:C:218:LEU:HD11 | 2.33                     | 0.58              |
| 3:F:335:GLY:O    | 3:F:336:GLU:HB2  | 2.02                     | 0.58              |
| 1:J:189:MET:HB2  | 1:J:193:LEU:HD22 | 1.84                     | 0.58              |
| 1:G:92:VAL:CG1   | 1:G:129:ARG:HG3  | 2.33                     | 0.58              |
| 3:I:111:GLN:O    | 3:I:115:ILE:HG13 | 2.03                     | 0.58              |
| 3:I:192:VAL:CG1  | 3:I:218:LEU:HD11 | 2.33                     | 0.58              |
| 1:A:101:VAL:HB   | 1:A:102:PRO:HD3  | 1.84                     | 0.58              |
| 1:G:189:MET:HB2  | 1:G:193:LEU:HD22 | 1.85                     | 0.58              |
| 3:C:331:THR:HG21 | 1:J:142:LYS:HA   | 1.85                     | 0.58              |
| 1:A:126:ILE:HD11 | 5:A:1250:GNP:N2  | 2.18                     | 0.58              |
| 3:C:219:LYS:NZ   | 6:C:436:HOH:O    | 2.35                     | 0.58              |
| 2:E:75:VAL:HG21  | 2:E:140:ILE:CD1  | 2.33                     | 0.58              |
| 3:L:116:ASP:OD2  | 3:L:120:LYS:HE2  | 2.03                     | 0.58              |
| 1:A:190:ASP:H    | 1:A:193:LEU:HD13 | 1.69                     | 0.58              |
| 2:E:62:ASN:O     | 2:E:63:ASP:HB2   | 2.04                     | 0.58              |
| 1:J:70:GLU:HA    | 6:L:411:HOH:O    | 2.03                     | 0.58              |
| 2:K:59:ALA:HB2   | 2:K:66:GLU:H     | 1.69                     | 0.58              |
| 3:L:18:THR:HG22  | 3:L:21:GLU:OE1   | 2.04                     | 0.58              |
| 2:B:62:ASN:O     | 2:B:63:ASP:HB2   | 2.03                     | 0.58              |
| 2:K:62:ASN:HB3   | 2:K:64:LEU:HD22  | 1.86                     | 0.58              |
| 1:D:77:ASP:OD2   | 1:D:110:ARG:NH2  | 2.36                     | 0.58              |
| 2:H:109:GLU:H    | 2:H:109:GLU:CD   | 2.06                     | 0.58              |
| 1:J:56:ARG:NH1   | 2:K:33:LEU:O     | 2.36                     | 0.58              |
| 2:B:75:VAL:HG21  | 2:B:140:ILE:CD1  | 2.34                     | 0.57              |
| 3:I:344:GLU:HG2  | 3:I:345:GLU:N    | 2.19                     | 0.57              |
| 3:C:112:GLU:CB   | 3:C:113:PRO:HD3  | 2.35                     | 0.57              |
| 1:D:190:ASP:H    | 1:D:193:LEU:HD13 | 1.68                     | 0.57              |
| 1:G:70:GLU:HA    | 6:I:391:HOH:O    | 2.04                     | 0.57              |
| 1:J:92:VAL:CG1   | 1:J:129:ARG:HG3  | 2.34                     | 0.57              |
| 3:F:192:VAL:CG1  | 3:F:218:LEU:HD11 | 2.34                     | 0.57              |
| 3:L:112:GLU:CB   | 3:L:113:PRO:HD3  | 2.34                     | 0.57              |
| 3:C:344:GLU:HG2  | 3:C:345:GLU:N    | 2.20                     | 0.57              |
| 1:J:190:ASP:H    | 1:J:193:LEU:HD13 | 1.69                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:J:4250:GNP:O3G | 6:J:4252:HOH:O   | 2.16                     | 0.57              |
| 2:K:43:GLU:C     | 2:K:45:GLU:H     | 2.05                     | 0.57              |
| 1:A:31:LEU:HB3   | 1:A:50:LEU:CD2   | 2.35                     | 0.57              |
| 3:C:335:GLY:O    | 3:C:336:GLU:HB2  | 2.05                     | 0.57              |
| 1:G:143:ASN:HA   | 2:H:22:ASN:ND2   | 2.20                     | 0.57              |
| 2:K:62:ASN:O     | 2:K:63:ASP:HB2   | 2.04                     | 0.57              |
| 3:L:344:GLU:HG2  | 3:L:345:GLU:N    | 2.19                     | 0.57              |
| 2:K:86:ILE:HB    | 2:K:162:ILE:HD11 | 1.86                     | 0.57              |
| 3:L:192:VAL:CG1  | 3:L:218:LEU:HD11 | 2.35                     | 0.57              |
| 2:B:62:ASN:HB3   | 2:B:64:LEU:HD22  | 1.87                     | 0.57              |
| 2:E:122:TRP:CZ3  | 2:E:140:ILE:HG22 | 2.40                     | 0.57              |
| 2:H:63:ASP:C     | 2:H:64:LEU:HD13  | 2.26                     | 0.57              |
| 3:F:112:GLU:CB   | 3:F:113:PRO:HD3  | 2.35                     | 0.56              |
| 1:G:77:ASP:OD2   | 1:G:110:ARG:NH2  | 2.38                     | 0.56              |
| 1:G:190:ASP:H    | 1:G:193:LEU:HD13 | 1.70                     | 0.56              |
| 3:I:18:THR:HG22  | 3:I:21:GLU:CG    | 2.35                     | 0.56              |
| 2:E:51:MET:HE3   | 2:E:147:ASN:HB3  | 1.87                     | 0.56              |
| 1:J:117:ILE:HB   | 1:J:144:LEU:HD22 | 1.87                     | 0.56              |
| 2:K:75:VAL:HG21  | 2:K:140:ILE:CD1  | 2.36                     | 0.56              |
| 1:A:77:ASP:OD2   | 1:A:110:ARG:NH2  | 2.38                     | 0.56              |
| 3:C:18:THR:HG22  | 3:C:21:GLU:CG    | 2.35                     | 0.56              |
| 3:I:335:GLY:O    | 3:I:336:GLU:HB2  | 2.04                     | 0.56              |
| 3:L:140:ALA:O    | 3:L:144:ARG:HG3  | 2.05                     | 0.56              |
| 3:F:306:LEU:HD21 | 3:F:334:ARG:HD2  | 1.87                     | 0.56              |
| 2:E:86:ILE:CB    | 2:E:162:ILE:HD11 | 2.28                     | 0.56              |
| 3:L:137:GLN:HB2  | 6:L:414:HOH:O    | 2.06                     | 0.56              |
| 1:G:31:LEU:HB3   | 1:G:50:LEU:CD2   | 2.36                     | 0.56              |
| 3:C:165:ILE:HD13 | 6:C:445:HOH:O    | 2.05                     | 0.55              |
| 1:J:168:LEU:HD22 | 2:K:30:ILE:HD12  | 1.87                     | 0.55              |
| 3:F:140:ALA:O    | 3:F:144:ARG:HG3  | 2.06                     | 0.55              |
| 2:B:63:ASP:C     | 2:B:64:LEU:HD13  | 2.27                     | 0.55              |
| 2:E:153:THR:HG23 | 2:E:154:LYS:N    | 2.22                     | 0.55              |
| 2:H:62:ASN:HB3   | 2:H:64:LEU:HD22  | 1.86                     | 0.55              |
| 3:I:199:ILE:CG2  | 3:I:204:ILE:HD12 | 2.36                     | 0.55              |
| 3:F:334:ARG:HG2  | 3:F:334:ARG:HH11 | 1.71                     | 0.55              |
| 1:J:126:ILE:HD11 | 5:J:4250:GNP:N2  | 2.20                     | 0.55              |
| 2:H:144:ASN:CB   | 2:H:146:GLU:HG3  | 2.37                     | 0.55              |
| 3:I:112:GLU:CB   | 3:I:113:PRO:HD3  | 2.35                     | 0.55              |
| 3:L:18:THR:HG22  | 3:L:21:GLU:CG    | 2.37                     | 0.55              |
| 3:C:116:ASP:OD2  | 3:C:120:LYS:HE2  | 2.07                     | 0.55              |
| 1:D:101:VAL:HB   | 1:D:102:PRO:HD3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:344:GLU:HG2  | 3:F:345:GLU:N    | 2.20                     | 0.55              |
| 3:C:252:ASN:ND2  | 3:C:282:GLN:H    | 2.05                     | 0.55              |
| 2:H:153:THR:HG23 | 2:H:154:LYS:N    | 2.22                     | 0.55              |
| 2:B:59:ALA:HB2   | 2:B:66:GLU:H     | 1.72                     | 0.55              |
| 2:E:59:ALA:HB2   | 2:E:66:GLU:H     | 1.72                     | 0.55              |
| 2:B:122:TRP:CZ3  | 2:B:140:ILE:HG22 | 2.40                     | 0.54              |
| 3:F:18:THR:HG22  | 3:F:21:GLU:CG    | 2.37                     | 0.54              |
| 3:C:199:ILE:CG2  | 3:C:204:ILE:HD12 | 2.38                     | 0.54              |
| 3:C:245:ASN:O    | 3:C:247:ARG:HD2  | 2.06                     | 0.54              |
| 3:C:334:ARG:HG2  | 3:C:334:ARG:HH11 | 1.72                     | 0.54              |
| 1:J:31:LEU:HB3   | 1:J:50:LEU:CD2   | 2.37                     | 0.54              |
| 2:B:153:THR:HG23 | 2:B:154:LYS:N    | 2.23                     | 0.54              |
| 2:E:112:PRO:HG3  | 2:E:120:TRP:HZ3  | 1.73                     | 0.54              |
| 3:F:176:MET:CE   | 3:F:207:LEU:HD22 | 2.38                     | 0.54              |
| 1:J:178:ALA:HB3  | 2:K:38:ILE:HD11  | 1.90                     | 0.54              |
| 3:L:245:ASN:O    | 3:L:247:ARG:HD2  | 2.08                     | 0.54              |
| 3:F:112:GLU:HA   | 3:F:112:GLU:OE1  | 2.07                     | 0.54              |
| 1:A:13:LEU:C     | 1:A:13:LEU:HD12  | 2.28                     | 0.54              |
| 1:A:141:LYS:HE3  | 1:A:142:LYS:HD2  | 1.90                     | 0.54              |
| 1:J:13:LEU:HB2   | 1:J:85:CYS:SG    | 2.48                     | 0.54              |
| 2:B:58:PHE:HB2   | 2:B:67:TRP:CZ3   | 2.43                     | 0.54              |
| 2:B:49:PHE:CB    | 2:B:77:LEU:HD12  | 2.38                     | 0.54              |
| 2:B:144:ASN:CB   | 2:B:146:GLU:HG3  | 2.38                     | 0.54              |
| 1:D:141:LYS:HE3  | 1:D:142:LYS:HD2  | 1.90                     | 0.54              |
| 1:D:168:LEU:HD22 | 2:E:30:ILE:HD12  | 1.89                     | 0.54              |
| 3:L:199:ILE:CG2  | 3:L:204:ILE:HD12 | 2.38                     | 0.54              |
| 3:C:183:PHE:HE1  | 3:C:207:LEU:HD11 | 1.72                     | 0.54              |
| 2:E:62:ASN:HB3   | 2:E:64:LEU:HD22  | 1.89                     | 0.54              |
| 1:G:141:LYS:HE3  | 1:G:142:LYS:HD2  | 1.90                     | 0.54              |
| 3:I:334:ARG:HH11 | 3:I:334:ARG:HG2  | 1.73                     | 0.54              |
| 3:F:261:ALA:CB   | 3:F:286:ILE:HG12 | 2.38                     | 0.54              |
| 3:I:259:ARG:HH11 | 3:I:259:ARG:HB3  | 1.72                     | 0.54              |
| 3:C:111:GLN:O    | 3:C:115:ILE:HG13 | 2.07                     | 0.53              |
| 3:F:306:LEU:HD23 | 3:F:334:ARG:HH11 | 1.74                     | 0.53              |
| 1:J:95:ARG:HB2   | 1:J:95:ARG:NH1   | 2.23                     | 0.53              |
| 2:K:153:THR:HG23 | 2:K:154:LYS:N    | 2.22                     | 0.53              |
| 2:E:144:ASN:CB   | 2:E:146:GLU:HG3  | 2.38                     | 0.53              |
| 2:E:49:PHE:CB    | 2:E:77:LEU:HD12  | 2.38                     | 0.53              |
| 1:D:13:LEU:HB2   | 1:D:85:CYS:SG    | 2.47                     | 0.53              |
| 3:F:199:ILE:CG2  | 3:F:204:ILE:HD12 | 2.38                     | 0.53              |
| 2:B:51:MET:HE3   | 2:B:147:ASN:HB3  | 1.89                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:59:ALA:HB2   | 2:H:66:GLU:H     | 1.73                     | 0.53              |
| 6:A:1256:HOH:O   | 3:C:108:PRO:HD3  | 2.08                     | 0.53              |
| 2:K:144:ASN:CB   | 2:K:146:GLU:HG3  | 2.39                     | 0.53              |
| 2:B:104:ILE:O    | 2:B:162:ILE:HD13 | 2.09                     | 0.53              |
| 3:C:18:THR:CG2   | 3:C:21:GLU:HG3   | 2.39                     | 0.53              |
| 3:I:245:ASN:O    | 3:I:247:ARG:HD2  | 2.09                     | 0.53              |
| 3:C:43:THR:HG21  | 3:C:72:THR:O     | 2.09                     | 0.53              |
| 3:F:43:THR:CG2   | 3:F:72:THR:O     | 2.57                     | 0.53              |
| 3:L:112:GLU:OE1  | 3:L:112:GLU:HA   | 2.08                     | 0.53              |
| 2:B:123:ASN:ND2  | 2:B:124:THR:N    | 2.57                     | 0.53              |
| 2:B:57:ARG:HG3   | 2:B:70:ARG:HD3   | 1.91                     | 0.53              |
| 3:I:306:LEU:HD21 | 3:I:334:ARG:HD2  | 1.90                     | 0.53              |
| 3:I:94:PRO:O     | 6:I:417:HOH:O    | 2.19                     | 0.53              |
| 3:F:18:THR:HG22  | 3:F:21:GLU:OE1   | 2.08                     | 0.53              |
| 1:G:190:ASP:N    | 1:G:191:PRO:CD   | 2.72                     | 0.53              |
| 1:G:13:LEU:C     | 1:G:13:LEU:HD12  | 2.30                     | 0.52              |
| 2:H:123:ASN:ND2  | 2:H:124:THR:N    | 2.57                     | 0.52              |
| 2:K:63:ASP:C     | 2:K:64:LEU:HD13  | 2.29                     | 0.52              |
| 3:L:111:GLN:O    | 3:L:115:ILE:HG13 | 2.10                     | 0.52              |
| 3:L:259:ARG:HB3  | 3:L:259:ARG:HH11 | 1.74                     | 0.52              |
| 2:B:164:GLU:O    | 2:B:165:ARG:C    | 2.47                     | 0.52              |
| 1:G:209:LEU:HD23 | 2:H:113:ASN:ND2  | 2.24                     | 0.52              |
| 3:F:245:ASN:O    | 3:F:247:ARG:HD2  | 2.08                     | 0.52              |
| 3:I:176:MET:CE   | 3:I:207:LEU:HD22 | 2.40                     | 0.52              |
| 3:I:266:ASP:O    | 3:I:269:SER:HB3  | 2.10                     | 0.52              |
| 3:F:292:ARG:HG2  | 3:F:321:VAL:HG11 | 1.92                     | 0.52              |
| 1:G:143:ASN:HD21 | 2:H:25:PRO:HB3   | 1.73                     | 0.52              |
| 1:J:13:LEU:HD12  | 1:J:13:LEU:C     | 2.30                     | 0.52              |
| 3:L:306:LEU:HD21 | 3:L:334:ARG:HD2  | 1.91                     | 0.52              |
| 3:L:334:ARG:HG2  | 3:L:334:ARG:HH11 | 1.74                     | 0.52              |
| 2:B:112:PRO:HG3  | 2:B:120:TRP:HZ3  | 1.74                     | 0.52              |
| 3:F:43:THR:HG21  | 3:F:72:THR:O     | 2.10                     | 0.52              |
| 1:J:190:ASP:N    | 1:J:191:PRO:CD   | 2.72                     | 0.52              |
| 3:C:112:GLU:HA   | 3:C:112:GLU:OE1  | 2.09                     | 0.52              |
| 1:J:163:TRP:CZ2  | 1:J:167:LYS:HE3  | 2.44                     | 0.52              |
| 2:K:106:PRO:O    | 2:K:159:ARG:NE   | 2.43                     | 0.52              |
| 1:D:31:LEU:HB3   | 1:D:50:LEU:CD2   | 2.39                     | 0.52              |
| 2:E:63:ASP:C     | 2:E:64:LEU:HD13  | 2.30                     | 0.52              |
| 1:G:188:VAL:C    | 1:G:189:MET:HG2  | 2.30                     | 0.52              |
| 1:J:209:LEU:HD23 | 2:K:113:ASN:HD21 | 1.73                     | 0.52              |
| 3:L:176:MET:CE   | 3:L:207:LEU:HD22 | 2.40                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:103:ASN:OD1  | 1:D:106:ARG:NH2  | 2.43                     | 0.52              |
| 2:E:123:ASN:ND2  | 2:E:124:THR:N    | 2.57                     | 0.52              |
| 2:H:64:LEU:HD13  | 2:H:64:LEU:N     | 2.24                     | 0.52              |
| 3:I:43:THR:HG21  | 3:I:72:THR:O     | 2.10                     | 0.52              |
| 3:L:204:ILE:HG23 | 3:L:208:LEU:HD23 | 1.91                     | 0.52              |
| 2:K:51:MET:HE3   | 2:K:147:ASN:HB3  | 1.92                     | 0.52              |
| 2:K:58:PHE:HB2   | 2:K:67:TRP:CZ3   | 2.44                     | 0.52              |
| 3:F:120:LYS:HD3  | 3:L:318:GLU:HB3  | 1.92                     | 0.52              |
| 3:L:43:THR:CG2   | 3:L:72:THR:O     | 2.58                     | 0.52              |
| 1:A:190:ASP:N    | 1:A:191:PRO:CD   | 2.73                     | 0.51              |
| 3:C:173:ASN:HD21 | 3:C:200:ARG:N    | 2.06                     | 0.51              |
| 1:D:190:ASP:N    | 1:D:191:PRO:CD   | 2.72                     | 0.51              |
| 2:E:58:PHE:HB2   | 2:E:67:TRP:CZ3   | 2.45                     | 0.51              |
| 3:F:178:GLU:HB2  | 6:F:413:HOH:O    | 2.10                     | 0.51              |
| 1:J:140:ARG:O    | 2:K:22:ASN:OD1   | 2.28                     | 0.51              |
| 1:J:141:LYS:HE3  | 1:J:142:LYS:HD2  | 1.91                     | 0.51              |
| 2:B:64:LEU:N     | 2:B:64:LEU:HD13  | 2.26                     | 0.51              |
| 3:C:259:ARG:HB3  | 3:C:259:ARG:HH11 | 1.72                     | 0.51              |
| 3:C:306:LEU:HD23 | 3:C:334:ARG:HH11 | 1.75                     | 0.51              |
| 1:D:199:HIS:O    | 1:D:203:VAL:HG23 | 2.10                     | 0.51              |
| 3:L:306:LEU:HD23 | 3:L:334:ARG:HH11 | 1.75                     | 0.51              |
| 3:L:43:THR:HG21  | 3:L:72:THR:O     | 2.10                     | 0.51              |
| 3:C:306:LEU:HD21 | 3:C:334:ARG:HD2  | 1.93                     | 0.51              |
| 3:F:131:ASN:ND2  | 6:F:414:HOH:O    | 2.43                     | 0.51              |
| 1:G:209:LEU:HD13 | 2:H:67:TRP:CG    | 2.44                     | 0.51              |
| 3:I:43:THR:CG2   | 3:I:72:THR:O     | 2.58                     | 0.51              |
| 2:K:112:PRO:HG3  | 2:K:120:TRP:HZ3  | 1.76                     | 0.51              |
| 1:G:188:VAL:O    | 1:G:189:MET:O    | 2.27                     | 0.51              |
| 2:H:112:PRO:HG3  | 2:H:120:TRP:HZ3  | 1.76                     | 0.51              |
| 2:H:75:VAL:HG21  | 2:H:140:ILE:CD1  | 2.39                     | 0.51              |
| 3:L:292:ARG:HG2  | 3:L:321:VAL:HG11 | 1.92                     | 0.51              |
| 3:I:112:GLU:HA   | 3:I:112:GLU:OE1  | 2.10                     | 0.51              |
| 3:I:306:LEU:HD23 | 3:I:334:ARG:HH11 | 1.74                     | 0.51              |
| 3:C:204:ILE:HG23 | 3:C:208:LEU:HD23 | 1.92                     | 0.51              |
| 3:F:204:ILE:HG23 | 3:F:208:LEU:HD23 | 1.92                     | 0.51              |
| 1:G:190:ASP:OD2  | 1:G:194:ALA:HB2  | 2.10                     | 0.51              |
| 3:L:242:SER:O    | 3:L:244:PRO:HD3  | 2.11                     | 0.51              |
| 3:C:43:THR:CG2   | 3:C:72:THR:O     | 2.58                     | 0.51              |
| 1:D:163:TRP:CZ2  | 1:D:167:LYS:HE3  | 2.45                     | 0.51              |
| 1:J:188:VAL:O    | 1:J:189:MET:O    | 2.29                     | 0.51              |
| 2:K:136:GLU:CG   | 2:K:138:LEU:HD21 | 2.41                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:143:ASN:CA   | 2:K:22:ASN:ND2   | 2.72                     | 0.51              |
| 3:I:18:THR:HG22  | 3:I:21:GLU:OE1   | 2.10                     | 0.51              |
| 3:I:20:ASP:O     | 3:I:21:GLU:HB2   | 2.11                     | 0.51              |
| 3:C:18:THR:HG22  | 3:C:21:GLU:OE1   | 2.11                     | 0.51              |
| 3:C:236:LEU:HD21 | 3:C:251:LEU:HD11 | 1.93                     | 0.51              |
| 3:F:245:ASN:ND2  | 6:F:391:HOH:O    | 2.40                     | 0.51              |
| 1:D:190:ASP:OD2  | 1:D:194:ALA:HB2  | 2.11                     | 0.50              |
| 2:H:51:MET:HE3   | 2:H:147:ASN:HB3  | 1.93                     | 0.50              |
| 6:G:3275:HOH:O   | 3:I:109:THR:CG2  | 2.59                     | 0.50              |
| 3:I:261:ALA:CB   | 3:I:286:ILE:HG12 | 2.41                     | 0.50              |
| 2:K:122:TRP:CZ3  | 2:K:140:ILE:HG22 | 2.45                     | 0.50              |
| 1:J:190:ASP:OD2  | 1:J:194:ALA:HB2  | 2.10                     | 0.50              |
| 3:C:294:LEU:O    | 3:C:298:ILE:HG13 | 2.11                     | 0.50              |
| 3:F:259:ARG:HB3  | 3:F:259:ARG:HH11 | 1.73                     | 0.50              |
| 1:A:188:VAL:C    | 1:A:189:MET:HG2  | 2.32                     | 0.50              |
| 3:C:176:MET:CE   | 3:C:207:LEU:HD22 | 2.40                     | 0.50              |
| 3:C:72:THR:HG23  | 6:C:389:HOH:O    | 2.12                     | 0.50              |
| 1:A:12:LYS:HE3   | 1:A:64:TRP:CE2   | 2.46                     | 0.50              |
| 2:B:78:LEU:O     | 2:B:86:ILE:HA    | 2.11                     | 0.50              |
| 3:C:130:HIS:HE1  | 6:C:435:HOH:O    | 1.94                     | 0.50              |
| 1:G:163:TRP:CZ2  | 1:G:167:LYS:HE3  | 2.47                     | 0.50              |
| 1:G:199:HIS:O    | 1:G:203:VAL:HG23 | 2.11                     | 0.50              |
| 5:J:4250:GNP:O1G | 6:J:4252:HOH:O   | 2.17                     | 0.50              |
| 1:A:209:LEU:HD23 | 2:B:113:ASN:HD21 | 1.76                     | 0.50              |
| 1:D:95:ARG:NH1   | 1:D:95:ARG:HB2   | 2.26                     | 0.50              |
| 1:J:199:HIS:O    | 1:J:203:VAL:HG23 | 2.11                     | 0.50              |
| 2:K:123:ASN:ND2  | 2:K:124:THR:N    | 2.59                     | 0.50              |
| 3:L:20:ASP:O     | 3:L:21:GLU:HB2   | 2.12                     | 0.50              |
| 1:D:188:VAL:O    | 1:D:189:MET:O    | 2.29                     | 0.50              |
| 2:H:78:LEU:O     | 2:H:86:ILE:HA    | 2.11                     | 0.50              |
| 1:J:188:VAL:C    | 1:J:189:MET:HG2  | 2.33                     | 0.50              |
| 3:C:100:ARG:HA   | 3:C:128:TYR:HB2  | 1.94                     | 0.50              |
| 3:C:317:GLU:HB2  | 6:C:441:HOH:O    | 2.10                     | 0.50              |
| 2:H:49:PHE:CB    | 2:H:77:LEU:HD12  | 2.41                     | 0.50              |
| 1:J:32:THR:HG21  | 1:J:34:GLU:OE1   | 2.12                     | 0.50              |
| 1:A:199:HIS:O    | 1:A:203:VAL:HG23 | 2.12                     | 0.49              |
| 2:H:122:TRP:CZ3  | 2:H:140:ILE:HG22 | 2.45                     | 0.49              |
| 2:H:57:ARG:HG3   | 2:H:70:ARG:HD3   | 1.93                     | 0.49              |
| 1:A:143:ASN:HD21 | 2:B:25:PRO:HB3   | 1.75                     | 0.49              |
| 3:C:19:GLU:C     | 3:C:20:ASP:O     | 2.50                     | 0.49              |
| 3:C:326:ARG:NH2  | 6:C:442:HOH:O    | 2.45                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:F:195:VAL:HG22 | 3:F:224:GLN:HB3  | 1.95                     | 0.49              |
| 2:H:38:ILE:HG13  | 2:H:38:ILE:O     | 2.12                     | 0.49              |
| 3:I:295:LYS:HG3  | 3:I:325:ILE:HG13 | 1.94                     | 0.49              |
| 3:L:294:LEU:O    | 3:L:298:ILE:HG13 | 2.12                     | 0.49              |
| 1:D:188:VAL:C    | 1:D:189:MET:HG2  | 2.33                     | 0.49              |
| 1:D:193:LEU:O    | 1:D:196:GLN:NE2  | 2.45                     | 0.49              |
| 1:G:124:VAL:HG22 | 1:G:149:ILE:O    | 2.12                     | 0.49              |
| 3:C:195:VAL:HG22 | 3:C:224:GLN:HB3  | 1.95                     | 0.49              |
| 2:H:136:GLU:CG   | 2:H:138:LEU:HD21 | 2.42                     | 0.49              |
| 3:I:183:PHE:HE1  | 3:I:207:LEU:HD11 | 1.77                     | 0.49              |
| 3:I:292:ARG:HG2  | 3:I:321:VAL:HG11 | 1.94                     | 0.49              |
| 3:L:18:THR:CG2   | 3:L:21:GLU:HG3   | 2.42                     | 0.49              |
| 3:L:309:GLU:HA   | 3:L:338:ASP:OD1  | 2.11                     | 0.49              |
| 1:A:190:ASP:OD2  | 1:A:194:ALA:HB2  | 2.12                     | 0.49              |
| 3:C:128:TYR:CE2  | 3:C:165:ILE:HG13 | 2.47                     | 0.49              |
| 2:E:78:LEU:O     | 2:E:86:ILE:HA    | 2.12                     | 0.49              |
| 3:F:20:ASP:O     | 3:F:21:GLU:HB2   | 2.12                     | 0.49              |
| 3:I:18:THR:CG2   | 3:I:21:GLU:HG3   | 2.41                     | 0.49              |
| 1:J:143:ASN:HD21 | 2:K:25:PRO:HB3   | 1.76                     | 0.49              |
| 2:K:57:ARG:HG3   | 2:K:70:ARG:HD3   | 1.94                     | 0.49              |
| 3:C:242:SER:O    | 3:C:244:PRO:HD3  | 2.12                     | 0.49              |
| 2:K:61:GLU:O     | 2:K:61:GLU:HG3   | 2.12                     | 0.49              |
| 2:K:64:LEU:N     | 2:K:64:LEU:HD13  | 2.28                     | 0.49              |
| 2:B:136:GLU:CG   | 2:B:138:LEU:HD21 | 2.41                     | 0.49              |
| 2:B:61:GLU:HG3   | 2:B:61:GLU:O     | 2.13                     | 0.49              |
| 3:C:20:ASP:O     | 3:C:21:GLU:HB2   | 2.13                     | 0.49              |
| 1:G:95:ARG:HB2   | 1:G:95:ARG:NH1   | 2.28                     | 0.49              |
| 2:H:61:GLU:HG3   | 2:H:61:GLU:O     | 2.13                     | 0.49              |
| 1:A:188:VAL:O    | 1:A:189:MET:O    | 2.29                     | 0.49              |
| 2:E:64:LEU:HD13  | 2:E:64:LEU:N     | 2.28                     | 0.49              |
| 1:G:188:VAL:O    | 1:G:189:MET:HG2  | 2.13                     | 0.49              |
| 1:G:10:GLN:HE21  | 1:G:60:LYS:HD2   | 1.78                     | 0.49              |
| 3:I:326:ARG:NH2  | 6:I:430:HOH:O    | 2.40                     | 0.49              |
| 2:K:49:PHE:CB    | 2:K:77:LEU:HD12  | 2.42                     | 0.49              |
| 1:D:32:THR:HG21  | 1:D:34:GLU:OE1   | 2.12                     | 0.49              |
| 1:G:193:LEU:O    | 1:G:196:GLN:NE2  | 2.46                     | 0.49              |
| 1:G:213:ASP:OD2  | 2:H:141:ARG:NH1  | 2.38                     | 0.49              |
| 2:H:58:PHE:HB2   | 2:H:67:TRP:CZ3   | 2.47                     | 0.49              |
| 2:B:109:GLU:OE1  | 2:B:109:GLU:N    | 2.44                     | 0.49              |
| 2:B:38:ILE:O     | 2:B:38:ILE:HG13  | 2.13                     | 0.49              |
| 3:F:183:PHE:HE1  | 3:F:207:LEU:HD11 | 1.76                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:143:ASN:HA   | 2:B:22:ASN:ND2   | 2.28                     | 0.48              |
| 1:D:13:LEU:HD12  | 1:D:14:VAL:N     | 2.28                     | 0.48              |
| 1:A:202:GLU:C    | 1:A:204:ALA:H    | 2.15                     | 0.48              |
| 2:B:109:GLU:CD   | 2:B:109:GLU:N    | 2.66                     | 0.48              |
| 3:F:18:THR:CG2   | 3:F:21:GLU:HG3   | 2.42                     | 0.48              |
| 3:I:204:ILE:HG23 | 3:I:208:LEU:HD23 | 1.95                     | 0.48              |
| 2:K:78:LEU:O     | 2:K:86:ILE:HA    | 2.13                     | 0.48              |
| 1:A:32:THR:HG21  | 1:A:34:GLU:OE1   | 2.13                     | 0.48              |
| 1:D:125:ASP:OD2  | 1:D:126:ILE:HD12 | 2.14                     | 0.48              |
| 1:G:202:GLU:C    | 1:G:204:ALA:H    | 2.16                     | 0.48              |
| 2:H:58:PHE:HD2   | 2:H:67:TRP:CE2   | 2.32                     | 0.48              |
| 1:A:125:ASP:OD2  | 1:A:126:ILE:HD12 | 2.13                     | 0.48              |
| 2:E:61:GLU:O     | 2:E:61:GLU:HG3   | 2.13                     | 0.48              |
| 1:G:81:ILE:HD13  | 1:G:82:GLN:HG3   | 1.95                     | 0.48              |
| 3:I:199:ILE:HG22 | 3:I:204:ILE:HD12 | 1.96                     | 0.48              |
| 3:L:236:LEU:HD21 | 3:L:251:LEU:HD11 | 1.95                     | 0.48              |
| 1:D:189:MET:CB   | 1:D:193:LEU:HD22 | 2.43                     | 0.48              |
| 1:G:32:THR:HG21  | 1:G:34:GLU:OE1   | 2.13                     | 0.48              |
| 3:I:295:LYS:HG3  | 3:I:325:ILE:CG1  | 2.43                     | 0.48              |
| 3:C:292:ARG:HG2  | 3:C:321:VAL:HG11 | 1.95                     | 0.48              |
| 3:F:173:ASN:HD21 | 3:F:200:ARG:N    | 2.08                     | 0.48              |
| 2:K:109:GLU:N    | 2:K:109:GLU:OE1  | 2.47                     | 0.48              |
| 1:J:201:LEU:HG   | 2:K:111:LYS:HD3  | 1.94                     | 0.48              |
| 1:D:10:GLN:HE21  | 1:D:60:LYS:HD2   | 1.79                     | 0.48              |
| 3:I:259:ARG:CB   | 3:I:259:ARG:HH11 | 2.27                     | 0.48              |
| 3:L:183:PHE:HE1  | 3:L:207:LEU:HD11 | 1.79                     | 0.48              |
| 2:B:58:PHE:HD2   | 2:B:67:TRP:CE2   | 2.31                     | 0.48              |
| 3:C:314:ARG:NH1  | 3:C:344:GLU:OE1  | 2.47                     | 0.48              |
| 3:F:236:LEU:HD21 | 3:F:251:LEU:HD11 | 1.96                     | 0.48              |
| 3:F:242:SER:O    | 3:F:244:PRO:HD3  | 2.14                     | 0.48              |
| 3:I:303:PRO:O    | 3:I:334:ARG:NH2  | 2.47                     | 0.48              |
| 2:K:49:PHE:HZ    | 2:K:51:MET:CE    | 2.26                     | 0.48              |
| 2:K:58:PHE:HD2   | 2:K:67:TRP:CE2   | 2.31                     | 0.48              |
| 3:L:128:TYR:CE2  | 3:L:165:ILE:HG13 | 2.49                     | 0.48              |
| 3:C:259:ARG:CB   | 3:C:259:ARG:HH11 | 2.27                     | 0.47              |
| 2:E:108:MET:O    | 2:E:159:ARG:HG3  | 2.14                     | 0.47              |
| 2:H:109:GLU:OE1  | 2:H:109:GLU:N    | 2.45                     | 0.47              |
| 3:I:19:GLU:C     | 3:I:20:ASP:O     | 2.48                     | 0.47              |
| 1:A:189:MET:CB   | 1:A:193:LEU:HD22 | 2.44                     | 0.47              |
| 1:D:178:ALA:O    | 1:D:179:MET:HB2  | 2.14                     | 0.47              |
| 1:D:202:GLU:C    | 1:D:204:ALA:H    | 2.16                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:242:SER:O    | 3:I:244:PRO:HD3  | 2.14                     | 0.47              |
| 2:B:40:THR:HB    | 2:B:43:GLU:OE2   | 2.14                     | 0.47              |
| 3:I:122:THR:N    | 3:I:123:PRO:CD   | 2.77                     | 0.47              |
| 1:J:13:LEU:HD12  | 1:J:14:VAL:N     | 2.29                     | 0.47              |
| 1:A:193:LEU:O    | 1:A:196:GLN:NE2  | 2.46                     | 0.47              |
| 3:I:322:VAL:HG12 | 3:I:326:ARG:NH1  | 2.29                     | 0.47              |
| 3:L:18:THR:HG22  | 3:L:21:GLU:CD    | 2.34                     | 0.47              |
| 3:L:261:ALA:CB   | 3:L:286:ILE:HG12 | 2.44                     | 0.47              |
| 3:L:266:ASP:O    | 3:L:269:SER:HB3  | 2.14                     | 0.47              |
| 3:C:309:GLU:HA   | 3:C:338:ASP:OD1  | 2.13                     | 0.47              |
| 2:E:109:GLU:N    | 2:E:109:GLU:CD   | 2.67                     | 0.47              |
| 3:I:100:ARG:HA   | 3:I:128:TYR:HB2  | 1.96                     | 0.47              |
| 1:J:10:GLN:HE21  | 1:J:60:LYS:HD2   | 1.80                     | 0.47              |
| 1:A:163:TRP:CZ2  | 1:A:167:LYS:HE3  | 2.49                     | 0.47              |
| 1:A:95:ARG:HB2   | 1:A:95:ARG:NH1   | 2.30                     | 0.47              |
| 3:F:19:GLU:C     | 3:F:20:ASP:O     | 2.52                     | 0.47              |
| 3:F:303:PRO:O    | 3:F:334:ARG:NH2  | 2.48                     | 0.47              |
| 1:J:178:ALA:O    | 1:J:179:MET:HB2  | 2.15                     | 0.47              |
| 2:K:40:THR:HB    | 2:K:43:GLU:OE2   | 2.14                     | 0.47              |
| 3:L:259:ARG:CB   | 3:L:259:ARG:HH11 | 2.27                     | 0.47              |
| 1:A:13:LEU:HD12  | 1:A:14:VAL:N     | 2.30                     | 0.47              |
| 1:A:16:VAL:HG13  | 1:A:17:GLY:N     | 2.30                     | 0.47              |
| 3:C:322:VAL:HG12 | 3:C:326:ARG:NH1  | 2.30                     | 0.47              |
| 1:D:189:MET:O    | 1:D:190:ASP:CB   | 2.63                     | 0.47              |
| 1:D:81:ILE:HD13  | 1:D:82:GLN:HG3   | 1.96                     | 0.47              |
| 2:E:136:GLU:CG   | 2:E:138:LEU:HD21 | 2.44                     | 0.47              |
| 3:F:100:ARG:HA   | 3:F:128:TYR:HB2  | 1.96                     | 0.47              |
| 3:F:122:THR:N    | 3:F:123:PRO:CD   | 2.78                     | 0.47              |
| 1:J:189:MET:CB   | 1:J:193:LEU:HD22 | 2.45                     | 0.47              |
| 2:E:49:PHE:HZ    | 2:E:51:MET:CE    | 2.28                     | 0.47              |
| 3:F:259:ARG:CB   | 3:F:259:ARG:HH11 | 2.27                     | 0.47              |
| 3:F:295:LYS:HG3  | 3:F:325:ILE:CG1  | 2.45                     | 0.47              |
| 1:J:193:LEU:O    | 1:J:196:GLN:NE2  | 2.47                     | 0.47              |
| 3:C:28:LEU:O     | 3:C:59:LYS:NZ    | 2.48                     | 0.47              |
| 2:E:58:PHE:HD2   | 2:E:67:TRP:CE2   | 2.32                     | 0.47              |
| 1:J:81:ILE:HD13  | 1:J:82:GLN:N     | 2.30                     | 0.47              |
| 2:K:160:LYS:O    | 2:K:164:GLU:HG3  | 2.15                     | 0.47              |
| 3:C:295:LYS:HG3  | 3:C:325:ILE:CG1  | 2.45                     | 0.47              |
| 2:E:57:ARG:HG3   | 2:E:70:ARG:HD3   | 1.97                     | 0.47              |
| 2:E:95:THR:O     | 2:E:96:LEU:HB2   | 2.14                     | 0.47              |
| 3:L:100:ARG:HA   | 3:L:128:TYR:HB2  | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:188:VAL:O    | 1:A:189:MET:HG2  | 2.14                     | 0.47              |
| 3:C:122:THR:N    | 3:C:123:PRO:CD   | 2.78                     | 0.47              |
| 3:C:144:ARG:HG2  | 3:C:178:GLU:CG   | 2.45                     | 0.47              |
| 2:E:86:ILE:HB    | 2:E:162:ILE:CD1  | 2.32                     | 0.47              |
| 3:I:144:ARG:HG2  | 3:I:178:GLU:CG   | 2.45                     | 0.47              |
| 1:J:177:VAL:HG23 | 2:K:38:ILE:CD1   | 2.45                     | 0.47              |
| 1:J:195:ALA:O    | 1:J:197:TYR:N    | 2.48                     | 0.47              |
| 3:L:176:MET:CE   | 3:L:207:LEU:HD13 | 2.45                     | 0.47              |
| 1:G:81:ILE:HD13  | 1:G:82:GLN:N     | 2.30                     | 0.46              |
| 2:H:158:CYS:O    | 2:H:162:ILE:HG13 | 2.15                     | 0.46              |
| 2:H:49:PHE:HZ    | 2:H:51:MET:CE    | 2.28                     | 0.46              |
| 1:A:10:GLN:HE21  | 1:A:60:LYS:HD2   | 1.81                     | 0.46              |
| 3:C:261:ALA:CB   | 3:C:286:ILE:HG12 | 2.45                     | 0.46              |
| 3:C:266:ASP:O    | 3:C:269:SER:HB3  | 2.15                     | 0.46              |
| 3:F:295:LYS:HG3  | 3:F:325:ILE:HG13 | 1.97                     | 0.46              |
| 3:I:242:SER:C    | 3:I:244:PRO:HD3  | 2.35                     | 0.46              |
| 1:J:202:GLU:C    | 1:J:204:ALA:H    | 2.18                     | 0.46              |
| 3:L:19:GLU:C     | 3:L:20:ASP:O     | 2.52                     | 0.46              |
| 1:D:188:VAL:O    | 1:D:189:MET:HG2  | 2.15                     | 0.46              |
| 1:D:205:GLN:HE22 | 2:E:111:LYS:HE2  | 1.79                     | 0.46              |
| 1:J:177:VAL:HG23 | 2:K:38:ILE:HD13  | 1.98                     | 0.46              |
| 1:A:186:GLU:O    | 1:A:187:VAL:HB   | 2.16                     | 0.46              |
| 3:F:144:ARG:HG2  | 3:F:178:GLU:CG   | 2.45                     | 0.46              |
| 2:H:84:GLY:H     | 2:H:165:ARG:HH21 | 1.63                     | 0.46              |
| 6:G:3275:HOH:O   | 3:I:107:GLY:HA3  | 2.14                     | 0.46              |
| 3:I:195:VAL:HG22 | 3:I:224:GLN:HB3  | 1.97                     | 0.46              |
| 3:I:236:LEU:HD21 | 3:I:251:LEU:HD11 | 1.97                     | 0.46              |
| 3:L:195:VAL:HG22 | 3:L:224:GLN:HB3  | 1.97                     | 0.46              |
| 2:E:118:ARG:HA   | 2:E:148:ALA:HB2  | 1.97                     | 0.46              |
| 3:F:322:VAL:HG12 | 3:F:326:ARG:NH1  | 2.30                     | 0.46              |
| 2:H:59:ALA:O     | 2:H:60:SER:CB    | 2.62                     | 0.46              |
| 3:I:314:ARG:NH1  | 3:I:344:GLU:OE1  | 2.49                     | 0.46              |
| 1:J:188:VAL:O    | 1:J:189:MET:HG2  | 2.14                     | 0.46              |
| 2:K:59:ALA:O     | 2:K:60:SER:CB    | 2.63                     | 0.46              |
| 3:C:183:PHE:CE1  | 3:C:207:LEU:HD11 | 2.50                     | 0.46              |
| 3:F:314:ARG:NH1  | 3:F:344:GLU:OE1  | 2.49                     | 0.46              |
| 3:L:122:THR:N    | 3:L:123:PRO:CD   | 2.79                     | 0.46              |
| 2:B:63:ASP:C     | 2:B:65:PRO:HD3   | 2.36                     | 0.46              |
| 1:G:186:GLU:O    | 1:G:187:VAL:HB   | 2.16                     | 0.46              |
| 1:G:31:LEU:HB3   | 1:G:50:LEU:HD21  | 1.98                     | 0.46              |
| 2:H:123:ASN:HD22 | 2:H:124:THR:N    | 2.13                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:144:ASN:HD22 | 2:H:147:ASN:HD21 | 1.64                     | 0.46              |
| 3:L:322:VAL:HG12 | 3:L:326:ARG:NH1  | 2.31                     | 0.46              |
| 3:C:4:PHE:HA     | 6:C:398:HOH:O    | 2.15                     | 0.46              |
| 1:D:124:VAL:HG22 | 1:D:149:ILE:O    | 2.16                     | 0.46              |
| 2:E:109:GLU:OE1  | 2:E:109:GLU:N    | 2.46                     | 0.46              |
| 2:E:63:ASP:C     | 2:E:65:PRO:HD3   | 2.36                     | 0.46              |
| 1:G:135:SER:O    | 1:G:137:VAL:HG23 | 2.16                     | 0.46              |
| 2:H:49:PHE:O     | 2:H:76:LYS:HA    | 2.16                     | 0.46              |
| 2:H:88:LEU:HD23  | 2:H:89:LEU:N     | 2.31                     | 0.46              |
| 3:C:186:HIS:HD2  | 6:C:456:HOH:O    | 1.99                     | 0.45              |
| 2:B:49:PHE:HZ    | 2:B:51:MET:CE    | 2.29                     | 0.45              |
| 3:F:199:ILE:HG22 | 3:F:204:ILE:HD12 | 1.98                     | 0.45              |
| 2:H:63:ASP:C     | 2:H:65:PRO:HD3   | 2.37                     | 0.45              |
| 1:J:112:CYS:HB3  | 1:J:115:ILE:HD13 | 1.99                     | 0.45              |
| 2:B:157:GLU:HA   | 2:B:160:LYS:HE2  | 1.97                     | 0.45              |
| 2:B:59:ALA:O     | 2:B:60:SER:CB    | 2.63                     | 0.45              |
| 3:C:18:THR:HG22  | 3:C:21:GLU:CD    | 2.37                     | 0.45              |
| 1:D:81:ILE:HD13  | 1:D:82:GLN:N     | 2.32                     | 0.45              |
| 3:F:18:THR:HG22  | 3:F:21:GLU:CD    | 2.37                     | 0.45              |
| 1:G:112:CYS:HB3  | 1:G:115:ILE:HD13 | 1.98                     | 0.45              |
| 1:J:169:ILE:HD12 | 2:K:33:LEU:CD1   | 2.45                     | 0.45              |
| 1:J:183:ALA:HA   | 1:J:184:PRO:HD3  | 1.83                     | 0.45              |
| 1:A:112:CYS:HB3  | 1:A:115:ILE:HD13 | 1.97                     | 0.45              |
| 1:A:128:ASP:HB2  | 6:C:430:HOH:O    | 2.17                     | 0.45              |
| 3:C:256:LEU:O    | 3:C:257:SER:CB   | 2.65                     | 0.45              |
| 1:D:16:VAL:HG13  | 1:D:17:GLY:N     | 2.32                     | 0.45              |
| 1:G:178:ALA:O    | 1:G:179:MET:HB2  | 2.16                     | 0.45              |
| 1:D:112:CYS:HB3  | 1:D:115:ILE:HD13 | 1.98                     | 0.45              |
| 1:D:186:GLU:O    | 1:D:187:VAL:HB   | 2.17                     | 0.45              |
| 1:D:205:GLN:NE2  | 2:E:111:LYS:HE2  | 2.31                     | 0.45              |
| 1:G:115:ILE:O    | 1:G:117:ILE:HG13 | 2.16                     | 0.45              |
| 2:K:63:ASP:C     | 2:K:65:PRO:HD3   | 2.37                     | 0.45              |
| 1:G:105:HIS:CD2  | 1:G:144:LEU:HD21 | 2.52                     | 0.45              |
| 3:I:18:THR:HG22  | 3:I:21:GLU:CD    | 2.37                     | 0.45              |
| 3:I:28:LEU:O     | 3:I:59:LYS:NZ    | 2.50                     | 0.45              |
| 1:J:135:SER:O    | 1:J:137:VAL:HG23 | 2.16                     | 0.45              |
| 1:J:209:LEU:HB3  | 2:K:141:ARG:NH2  | 2.31                     | 0.45              |
| 1:A:135:SER:O    | 1:A:137:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:31:LEU:HB3   | 1:A:50:LEU:HD21  | 1.98                     | 0.45              |
| 1:D:12:LYS:HE3   | 1:D:64:TRP:CE2   | 2.51                     | 0.45              |
| 6:J:4278:HOH:O   | 3:L:109:THR:CG2  | 2.65                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:109:GLU:CD   | 2:H:109:GLU:N    | 2.66                     | 0.45              |
| 1:J:93:THR:O     | 1:J:130:LYS:HD2  | 2.17                     | 0.45              |
| 3:I:187:ARG:NH2  | 3:L:270:LYS:O    | 2.39                     | 0.45              |
| 1:A:93:THR:HG21  | 1:A:126:ILE:HG21 | 1.99                     | 0.45              |
| 1:J:103:ASN:OD1  | 1:J:106:ARG:NH2  | 2.50                     | 0.45              |
| 3:L:256:LEU:O    | 3:L:257:SER:CB   | 2.65                     | 0.45              |
| 1:A:195:ALA:O    | 1:A:197:TYR:N    | 2.50                     | 0.45              |
| 2:K:118:ARG:HA   | 2:K:148:ALA:HB2  | 1.97                     | 0.45              |
| 3:L:303:PRO:O    | 3:L:334:ARG:NH2  | 2.50                     | 0.45              |
| 1:A:103:ASN:OD1  | 1:A:106:ARG:NH2  | 2.48                     | 0.44              |
| 1:A:81:ILE:HD13  | 1:A:82:GLN:N     | 2.32                     | 0.44              |
| 3:C:303:PRO:O    | 3:C:334:ARG:NH2  | 2.50                     | 0.44              |
| 6:D:2277:HOH:O   | 3:F:107:GLY:HA3  | 2.17                     | 0.44              |
| 2:K:38:ILE:O     | 2:K:38:ILE:HG13  | 2.16                     | 0.44              |
| 3:L:18:THR:O     | 3:L:20:ASP:O     | 2.35                     | 0.44              |
| 1:D:209:LEU:HD13 | 2:E:67:TRP:CG    | 2.51                     | 0.44              |
| 2:E:149:GLN:O    | 2:E:153:THR:HG22 | 2.17                     | 0.44              |
| 1:G:189:MET:CB   | 1:G:193:LEU:HD22 | 2.47                     | 0.44              |
| 3:L:170:ARG:NH1  | 6:L:405:HOH:O    | 2.50                     | 0.44              |
| 3:I:108:PRO:HD3  | 6:I:435:HOH:O    | 2.16                     | 0.44              |
| 1:D:105:HIS:CD2  | 1:D:144:LEU:HD21 | 2.53                     | 0.44              |
| 3:F:72:THR:HG22  | 6:F:406:HOH:O    | 2.16                     | 0.44              |
| 1:A:178:ALA:O    | 1:A:179:MET:HB2  | 2.17                     | 0.44              |
| 2:E:40:THR:HB    | 2:E:43:GLU:OE2   | 2.17                     | 0.44              |
| 3:I:21:GLU:O     | 3:I:24:VAL:HB    | 2.18                     | 0.44              |
| 3:L:314:ARG:NH1  | 3:L:344:GLU:OE1  | 2.50                     | 0.44              |
| 3:L:295:LYS:HG3  | 3:L:325:ILE:CG1  | 2.47                     | 0.44              |
| 3:L:295:LYS:HG3  | 3:L:325:ILE:HG13 | 2.00                     | 0.44              |
| 1:A:202:GLU:C    | 1:A:204:ALA:N    | 2.70                     | 0.44              |
| 2:B:118:ARG:HA   | 2:B:148:ALA:HB2  | 1.98                     | 0.44              |
| 3:C:21:GLU:O     | 3:C:24:VAL:HB    | 2.17                     | 0.44              |
| 1:D:115:ILE:O    | 1:D:117:ILE:HG13 | 2.18                     | 0.44              |
| 3:I:173:ASN:HD21 | 3:I:200:ARG:N    | 2.10                     | 0.44              |
| 1:J:186:GLU:O    | 1:J:187:VAL:HB   | 2.17                     | 0.44              |
| 1:J:81:ILE:HD13  | 1:J:82:GLN:HG3   | 1.99                     | 0.44              |
| 3:L:84:ARG:O     | 3:L:88:GLN:HB2   | 2.17                     | 0.44              |
| 1:D:133:ALA:N    | 6:D:2269:HOH:O   | 2.37                     | 0.44              |
| 1:D:135:SER:O    | 1:D:137:VAL:HG23 | 2.17                     | 0.44              |
| 1:D:202:GLU:C    | 1:D:204:ALA:N    | 2.71                     | 0.44              |
| 3:F:128:TYR:CE2  | 3:F:165:ILE:HG13 | 2.52                     | 0.44              |
| 1:G:103:ASN:OD1  | 1:G:106:ARG:NH2  | 2.50                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:13:LEU:HD12  | 1:G:14:VAL:N     | 2.33                     | 0.44              |
| 2:H:149:GLN:O    | 2:H:153:THR:HG22 | 2.17                     | 0.44              |
| 3:I:96:LEU:O     | 3:I:121:HIS:HE1  | 2.01                     | 0.44              |
| 3:F:250:GLY:HA2  | 3:F:280:ARG:HB2  | 2.00                     | 0.44              |
| 1:G:125:ASP:OD2  | 1:G:126:ILE:HD12 | 2.17                     | 0.44              |
| 1:J:124:VAL:HG22 | 1:J:149:ILE:O    | 2.18                     | 0.44              |
| 1:A:105:HIS:CD2  | 1:A:144:LEU:HD21 | 2.53                     | 0.44              |
| 2:B:149:GLN:O    | 2:B:153:THR:HG22 | 2.18                     | 0.44              |
| 2:E:93:ASP:O     | 2:E:95:THR:N     | 2.43                     | 0.44              |
| 2:H:70:ARG:HD2   | 2:H:70:ARG:HA    | 1.83                     | 0.44              |
| 1:J:125:ASP:OD2  | 1:J:126:ILE:HD12 | 2.18                     | 0.44              |
| 2:B:49:PHE:O     | 2:B:76:LYS:HA    | 2.17                     | 0.43              |
| 1:D:159:LYS:HB2  | 1:D:160:PRO:HD3  | 2.00                     | 0.43              |
| 3:I:294:LEU:O    | 3:I:298:ILE:HG13 | 2.18                     | 0.43              |
| 1:J:31:LEU:HB3   | 1:J:50:LEU:HD21  | 1.99                     | 0.43              |
| 2:K:49:PHE:O     | 2:K:76:LYS:HA    | 2.18                     | 0.43              |
| 2:K:59:ALA:CB    | 2:K:65:PRO:HA    | 2.47                     | 0.43              |
| 1:A:213:ASP:OD2  | 2:B:141:ARG:NH1  | 2.44                     | 0.43              |
| 1:G:16:VAL:HG13  | 1:G:17:GLY:N     | 2.33                     | 0.43              |
| 3:I:186:HIS:HD2  | 6:I:411:HOH:O    | 2.02                     | 0.43              |
| 1:A:206:THR:O    | 2:B:114:ALA:HB2  | 2.17                     | 0.43              |
| 3:C:199:ILE:HG22 | 3:C:204:ILE:HD12 | 1.98                     | 0.43              |
| 1:D:195:ALA:O    | 1:D:197:TYR:N    | 2.51                     | 0.43              |
| 1:G:202:GLU:C    | 1:G:204:ALA:N    | 2.71                     | 0.43              |
| 1:J:178:ALA:O    | 1:J:179:MET:CB   | 2.66                     | 0.43              |
| 1:J:30:HIS:HD2   | 6:J:4260:HOH:O   | 2.00                     | 0.43              |
| 2:K:123:ASN:HD22 | 2:K:124:THR:N    | 2.14                     | 0.43              |
| 3:C:252:ASN:ND2  | 3:C:280:ARG:HB3  | 2.33                     | 0.43              |
| 3:F:309:GLU:HA   | 3:F:338:ASP:OD1  | 2.18                     | 0.43              |
| 2:H:102:HIS:CE1  | 2:H:122:TRP:HE1  | 2.36                     | 0.43              |
| 2:H:51:MET:HE3   | 2:H:142:PHE:CD1  | 2.54                     | 0.43              |
| 1:D:178:ALA:O    | 1:D:179:MET:CB   | 2.66                     | 0.43              |
| 2:E:57:ARG:HD3   | 2:E:136:GLU:OE2  | 2.18                     | 0.43              |
| 2:E:49:PHE:O     | 2:E:76:LYS:HA    | 2.18                     | 0.43              |
| 3:F:28:LEU:O     | 3:F:59:LYS:NZ    | 2.52                     | 0.43              |
| 1:G:12:LYS:HE3   | 1:G:64:TRP:CE2   | 2.54                     | 0.43              |
| 2:H:118:ARG:HA   | 2:H:148:ALA:HB2  | 2.00                     | 0.43              |
| 3:I:206:HIS:HD2  | 6:I:439:HOH:O    | 2.01                     | 0.43              |
| 1:A:16:VAL:CG1   | 1:A:17:GLY:N     | 2.81                     | 0.43              |
| 3:C:165:ILE:CD1  | 6:C:445:HOH:O    | 2.64                     | 0.43              |
| 2:E:38:ILE:O     | 2:E:38:ILE:HG13  | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:59:ALA:O     | 2:E:60:SER:CB    | 2.62                     | 0.43              |
| 3:F:21:GLU:O     | 3:F:24:VAL:HB    | 2.19                     | 0.43              |
| 1:G:195:ALA:O    | 1:G:197:TYR:N    | 2.51                     | 0.43              |
| 2:H:84:GLY:H     | 2:H:165:ARG:NH2  | 2.17                     | 0.43              |
| 3:I:18:THR:O     | 3:I:20:ASP:O     | 2.36                     | 0.43              |
| 2:K:102:HIS:HB3  | 2:K:127:ASP:HA   | 1.99                     | 0.43              |
| 3:L:176:MET:HE3  | 3:L:207:LEU:HD13 | 1.99                     | 0.43              |
| 1:A:67:ALA:HA    | 6:A:1252:HOH:O   | 2.18                     | 0.43              |
| 2:B:102:HIS:HB3  | 2:B:127:ASP:HA   | 2.01                     | 0.43              |
| 2:E:51:MET:HE2   | 2:E:142:PHE:CE1  | 2.54                     | 0.43              |
| 2:E:58:PHE:O     | 2:E:59:ALA:C     | 2.57                     | 0.43              |
| 3:I:176:MET:CE   | 3:I:207:LEU:HD13 | 2.49                     | 0.43              |
| 2:K:80:HIS:O     | 2:K:83:LYS:O     | 2.37                     | 0.43              |
| 3:L:344:GLU:CG   | 3:L:345:GLU:N    | 2.81                     | 0.43              |
| 3:C:295:LYS:HG3  | 3:C:325:ILE:HG13 | 2.00                     | 0.43              |
| 3:C:329:PHE:CG   | 3:C:335:GLY:HA3  | 2.53                     | 0.43              |
| 3:I:309:GLU:HA   | 3:I:338:ASP:OD1  | 2.18                     | 0.43              |
| 3:L:31:ASP:O     | 3:L:34:VAL:HG23  | 2.18                     | 0.43              |
| 1:G:93:THR:HG21  | 1:G:126:ILE:HG21 | 2.00                     | 0.43              |
| 2:H:95:THR:HG23  | 2:H:97:LYS:H     | 1.84                     | 0.43              |
| 3:I:66:GLU:HG2   | 3:I:100:ARG:HD2  | 2.01                     | 0.43              |
| 3:L:16:ILE:HG22  | 3:L:16:ILE:O     | 2.18                     | 0.43              |
| 3:L:173:ASN:HD21 | 3:L:200:ARG:N    | 2.13                     | 0.43              |
| 3:L:329:PHE:CG   | 3:L:335:GLY:HA3  | 2.54                     | 0.43              |
| 3:C:274:ILE:HG22 | 3:C:276:LEU:H    | 1.84                     | 0.43              |
| 6:G:3274:HOH:O   | 3:I:170:ARG:HG3  | 2.19                     | 0.43              |
| 3:L:144:ARG:HG2  | 3:L:178:GLU:CG   | 2.48                     | 0.43              |
| 2:B:51:MET:HE3   | 2:B:142:PHE:CD1  | 2.54                     | 0.42              |
| 2:B:163:GLU:O    | 2:B:166:GLU:OE2  | 2.37                     | 0.42              |
| 3:C:18:THR:HG22  | 3:C:21:GLU:HG3   | 2.00                     | 0.42              |
| 3:F:207:LEU:HG   | 3:F:212:LEU:HD22 | 2.01                     | 0.42              |
| 1:G:126:ILE:CD1  | 5:G:3250:GNP:N2  | 2.82                     | 0.42              |
| 3:I:183:PHE:CE1  | 3:I:207:LEU:HD11 | 2.53                     | 0.42              |
| 3:L:259:ARG:HB3  | 3:L:259:ARG:CZ   | 2.49                     | 0.42              |
| 2:B:67:TRP:CH2   | 2:B:139:ALA:HB2  | 2.54                     | 0.42              |
| 2:B:70:ARG:HD2   | 2:B:70:ARG:HA    | 1.86                     | 0.42              |
| 3:C:339:GLU:HA   | 3:C:339:GLU:OE1  | 2.19                     | 0.42              |
| 3:F:84:ARG:O     | 3:F:88:GLN:HB2   | 2.19                     | 0.42              |
| 3:I:207:LEU:HG   | 3:I:212:LEU:HD22 | 2.01                     | 0.42              |
| 3:I:339:GLU:OE1  | 3:I:339:GLU:HA   | 2.19                     | 0.42              |
| 1:J:13:LEU:HD13  | 1:J:86:ALA:HA    | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:D:2277:HOH:O   | 3:F:109:THR:HG22 | 2.16                     | 0.42              |
| 3:F:266:ASP:O    | 3:F:269:SER:HB3  | 2.20                     | 0.42              |
| 2:H:144:ASN:HD22 | 2:H:147:ASN:ND2  | 2.17                     | 0.42              |
| 2:K:149:GLN:O    | 2:K:153:THR:HG22 | 2.19                     | 0.42              |
| 3:L:259:ARG:NH1  | 3:L:259:ARG:CB   | 2.78                     | 0.42              |
| 1:G:202:GLU:HA   | 1:G:205:GLN:HG2  | 2.01                     | 0.42              |
| 2:H:93:ASP:O     | 2:H:95:THR:N     | 2.45                     | 0.42              |
| 3:I:18:THR:HG23  | 3:I:20:ASP:C     | 2.40                     | 0.42              |
| 2:K:58:PHE:O     | 2:K:59:ALA:C     | 2.58                     | 0.42              |
| 3:C:291:VAL:HG21 | 3:C:315:PHE:CD2  | 2.54                     | 0.42              |
| 3:C:298:ILE:HD13 | 3:C:305:LEU:CD2  | 2.49                     | 0.42              |
| 2:E:102:HIS:HB3  | 2:E:127:ASP:HA   | 2.02                     | 0.42              |
| 2:E:80:HIS:O     | 2:E:83:LYS:O     | 2.37                     | 0.42              |
| 3:F:339:GLU:OE1  | 3:F:339:GLU:HA   | 2.20                     | 0.42              |
| 1:J:189:MET:O    | 1:J:190:ASP:CB   | 2.63                     | 0.42              |
| 1:J:202:GLU:C    | 1:J:204:ALA:N    | 2.73                     | 0.42              |
| 2:K:160:LYS:HG2  | 2:K:164:GLU:OE2  | 2.20                     | 0.42              |
| 3:F:183:PHE:CE1  | 3:F:207:LEU:HD11 | 2.53                     | 0.42              |
| 3:I:18:THR:HG23  | 3:I:20:ASP:O     | 2.20                     | 0.42              |
| 3:L:252:ASN:ND2  | 3:L:280:ARG:HB3  | 2.35                     | 0.42              |
| 2:B:102:HIS:CE1  | 2:B:122:TRP:HE1  | 2.37                     | 0.42              |
| 1:A:177:VAL:HG23 | 2:B:38:ILE:CD1   | 2.49                     | 0.42              |
| 2:E:88:LEU:HD23  | 2:E:89:LEU:N     | 2.35                     | 0.42              |
| 3:F:344:GLU:CG   | 3:F:345:GLU:N    | 2.83                     | 0.42              |
| 3:I:18:THR:HG22  | 3:I:21:GLU:HG3   | 2.01                     | 0.42              |
| 3:I:344:GLU:CG   | 3:I:345:GLU:N    | 2.82                     | 0.42              |
| 3:L:72:THR:HG23  | 6:L:409:HOH:O    | 2.18                     | 0.42              |
| 1:A:178:ALA:O    | 1:A:179:MET:CB   | 2.67                     | 0.42              |
| 1:D:171:ASP:OD1  | 1:D:173:ASN:N    | 2.49                     | 0.42              |
| 3:I:66:GLU:OE1   | 3:I:100:ARG:HB2  | 2.20                     | 0.42              |
| 2:K:102:HIS:CE1  | 2:K:122:TRP:HE1  | 2.37                     | 0.42              |
| 2:B:59:ALA:CB    | 2:B:65:PRO:HA    | 2.48                     | 0.42              |
| 2:E:164:GLU:O    | 2:E:165:ARG:C    | 2.58                     | 0.42              |
| 3:F:231:LEU:HA   | 3:F:231:LEU:HD12 | 1.91                     | 0.42              |
| 2:H:57:ARG:HD3   | 2:H:136:GLU:OE2  | 2.20                     | 0.42              |
| 2:H:40:THR:HB    | 2:H:43:GLU:OE2   | 2.19                     | 0.42              |
| 2:K:51:MET:HE3   | 2:K:142:PHE:CD1  | 2.55                     | 0.42              |
| 1:A:124:VAL:HG22 | 1:A:149:ILE:O    | 2.19                     | 0.41              |
| 2:B:84:GLY:H     | 2:B:165:ARG:NH2  | 2.17                     | 0.41              |
| 2:B:33:LEU:HA    | 2:B:34:PRO:HD3   | 1.90                     | 0.41              |
| 2:B:88:LEU:HD23  | 2:B:89:LEU:N     | 2.34                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:33:LEU:HA    | 2:H:34:PRO:HD3   | 1.89                     | 0.41              |
| 1:J:205:GLN:OE1  | 2:K:111:LYS:HE2  | 2.20                     | 0.41              |
| 2:K:70:ARG:HG2   | 2:K:70:ARG:HH11  | 1.86                     | 0.41              |
| 3:F:294:LEU:O    | 3:F:298:ILE:HG13 | 2.20                     | 0.41              |
| 3:I:256:LEU:O    | 3:I:257:SER:CB   | 2.69                     | 0.41              |
| 2:K:93:ASP:O     | 2:K:95:THR:N     | 2.47                     | 0.41              |
| 1:A:183:ALA:HA   | 1:A:184:PRO:HD3  | 1.83                     | 0.41              |
| 1:D:143:ASN:HA   | 2:E:22:ASN:HD22  | 1.81                     | 0.41              |
| 1:D:189:MET:CG   | 1:D:193:LEU:HD22 | 2.51                     | 0.41              |
| 3:F:242:SER:C    | 3:F:244:PRO:HD3  | 2.41                     | 0.41              |
| 1:J:137:VAL:O    | 1:J:140:ARG:HB2  | 2.20                     | 0.41              |
| 3:I:238:ILE:HG21 | 3:L:238:ILE:HG21 | 2.02                     | 0.41              |
| 1:A:81:ILE:HD13  | 1:A:82:GLN:HG3   | 2.01                     | 0.41              |
| 3:C:96:LEU:O     | 3:C:121:HIS:HE1  | 2.03                     | 0.41              |
| 3:C:138:ALA:O    | 3:C:142:ILE:HG12 | 2.21                     | 0.41              |
| 3:C:146:LEU:HD12 | 3:C:146:LEU:HA   | 1.91                     | 0.41              |
| 3:C:84:ARG:O     | 3:C:88:GLN:HB2   | 2.20                     | 0.41              |
| 2:E:134:LYS:HA   | 2:E:135:PRO:HD3  | 1.96                     | 0.41              |
| 2:H:167:LYS:HD2  | 2:H:167:LYS:H    | 1.85                     | 0.41              |
| 2:H:46:GLU:O     | 2:H:47:GLU:CB    | 2.69                     | 0.41              |
| 1:J:93:THR:HG21  | 1:J:126:ILE:HG21 | 2.02                     | 0.41              |
| 3:L:18:THR:HG23  | 3:L:20:ASP:C     | 2.41                     | 0.41              |
| 3:L:18:THR:HG23  | 3:L:20:ASP:O     | 2.20                     | 0.41              |
| 2:B:123:ASN:HD22 | 2:B:124:THR:N    | 2.12                     | 0.41              |
| 2:E:59:ALA:CB    | 2:E:65:PRO:HA    | 2.48                     | 0.41              |
| 2:E:86:ILE:HD12  | 2:E:162:ILE:HD11 | 2.02                     | 0.41              |
| 1:J:43:LEU:HD22  | 3:L:76:LYS:HA    | 2.02                     | 0.41              |
| 3:C:231:LEU:HD12 | 3:C:231:LEU:HA   | 1.93                     | 0.41              |
| 3:C:72:THR:HG22  | 6:C:427:HOH:O    | 2.20                     | 0.41              |
| 1:D:16:VAL:CG1   | 1:D:17:GLY:N     | 2.83                     | 0.41              |
| 2:E:144:ASN:HD22 | 2:E:147:ASN:HD21 | 1.69                     | 0.41              |
| 1:D:177:VAL:HG23 | 2:E:38:ILE:CD1   | 2.50                     | 0.41              |
| 2:E:46:GLU:HB3   | 2:E:47:GLU:H     | 1.69                     | 0.41              |
| 3:F:96:LEU:O     | 3:F:121:HIS:HE1  | 2.04                     | 0.41              |
| 3:L:99:VAL:HG12  | 3:L:124:LEU:CD1  | 2.50                     | 0.41              |
| 3:L:329:PHE:CD2  | 3:L:335:GLY:HA3  | 2.56                     | 0.41              |
| 1:A:189:MET:O    | 1:A:190:ASP:CB   | 2.62                     | 0.41              |
| 2:B:144:ASN:HD22 | 2:B:147:ASN:HD21 | 1.69                     | 0.41              |
| 3:F:91:LEU:HA    | 3:F:91:LEU:HD23  | 1.92                     | 0.41              |
| 2:H:109:GLU:O    | 2:H:110:LEU:HD23 | 2.20                     | 0.41              |
| 3:L:199:ILE:HG22 | 3:L:204:ILE:HD12 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:95:THR:HG23  | 2:B:97:LYS:H     | 1.86                     | 0.41              |
| 2:E:113:ASN:O    | 2:E:114:ALA:C    | 2.58                     | 0.41              |
| 1:G:137:VAL:O    | 1:G:140:ARG:HB2  | 2.20                     | 0.41              |
| 2:H:113:ASN:O    | 2:H:114:ALA:C    | 2.58                     | 0.41              |
| 1:J:202:GLU:HA   | 1:J:205:GLN:HG2  | 2.02                     | 0.41              |
| 3:L:242:SER:C    | 3:L:244:PRO:HD3  | 2.40                     | 0.41              |
| 1:A:137:VAL:O    | 1:A:140:ARG:HB2  | 2.21                     | 0.41              |
| 2:B:57:ARG:HD3   | 2:B:136:GLU:OE2  | 2.21                     | 0.41              |
| 3:C:170:ARG:HG2  | 6:C:412:HOH:O    | 2.21                     | 0.41              |
| 3:C:242:SER:C    | 3:C:244:PRO:HD3  | 2.41                     | 0.41              |
| 3:C:329:PHE:CD2  | 3:C:335:GLY:HA3  | 2.56                     | 0.41              |
| 2:H:102:HIS:HB3  | 2:H:127:ASP:HA   | 2.02                     | 0.41              |
| 2:H:67:TRP:CH2   | 2:H:139:ALA:HB2  | 2.56                     | 0.41              |
| 2:K:144:ASN:HD22 | 2:K:147:ASN:HD21 | 1.68                     | 0.41              |
| 3:C:317:GLU:CB   | 6:C:441:HOH:O    | 2.67                     | 0.41              |
| 1:D:28:LYS:O     | 1:D:31:LEU:HD12  | 2.21                     | 0.41              |
| 1:D:72:PHE:HE2   | 1:D:104:TRP:CD2  | 2.39                     | 0.41              |
| 1:J:195:ALA:C    | 1:J:197:TYR:H    | 2.23                     | 0.41              |
| 3:L:274:ILE:HG22 | 3:L:276:LEU:H    | 1.86                     | 0.41              |
| 2:B:113:ASN:O    | 2:B:114:ALA:C    | 2.59                     | 0.41              |
| 2:B:144:ASN:HD22 | 2:B:147:ASN:ND2  | 2.19                     | 0.41              |
| 1:D:178:ALA:HB3  | 2:E:38:ILE:HD11  | 2.03                     | 0.41              |
| 3:I:128:TYR:CE2  | 3:I:165:ILE:HG13 | 2.56                     | 0.41              |
| 1:J:182:LEU:HD12 | 1:J:182:LEU:N    | 2.36                     | 0.41              |
| 1:A:28:LYS:O     | 1:A:31:LEU:HD12  | 2.21                     | 0.40              |
| 3:C:114:LEU:HD12 | 3:C:114:LEU:HA   | 1.94                     | 0.40              |
| 1:D:13:LEU:HD13  | 1:D:86:ALA:HA    | 2.04                     | 0.40              |
| 2:E:67:TRP:CH2   | 2:E:139:ALA:HB2  | 2.56                     | 0.40              |
| 3:I:329:PHE:CG   | 3:I:335:GLY:HA3  | 2.56                     | 0.40              |
| 1:J:146:TYR:CG   | 1:J:147:TYR:N    | 2.89                     | 0.40              |
| 2:K:109:GLU:CD   | 2:K:109:GLU:N    | 2.67                     | 0.40              |
| 3:L:183:PHE:CE1  | 3:L:207:LEU:HD11 | 2.56                     | 0.40              |
| 2:B:46:GLU:HB3   | 2:B:47:GLU:H     | 1.69                     | 0.40              |
| 3:F:146:LEU:HA   | 3:F:146:LEU:HD12 | 1.91                     | 0.40              |
| 1:G:195:ALA:C    | 1:G:197:TYR:H    | 2.25                     | 0.40              |
| 3:I:84:ARG:O     | 3:I:88:GLN:HB2   | 2.21                     | 0.40              |
| 2:K:62:ASN:HB3   | 2:K:64:LEU:CD2   | 2.51                     | 0.40              |
| 1:A:202:GLU:HA   | 1:A:205:GLN:HG2  | 2.03                     | 0.40              |
| 1:D:31:LEU:HB3   | 1:D:50:LEU:HD21  | 2.04                     | 0.40              |
| 3:I:114:LEU:HA   | 3:I:114:LEU:HD12 | 1.95                     | 0.40              |
| 3:I:138:ALA:O    | 3:I:142:ILE:HG12 | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:184:GLN:NE2  | 3:L:270:LYS:NZ   | 2.66                     | 0.40              |
| 1:A:55:ASN:OD1   | 1:A:174:LEU:HD12 | 2.22                     | 0.40              |
| 3:C:344:GLU:CG   | 3:C:345:GLU:N    | 2.83                     | 0.40              |
| 2:E:123:ASN:HD22 | 2:E:124:THR:N    | 2.11                     | 0.40              |
| 2:E:63:ASP:O     | 2:E:65:PRO:HD3   | 2.22                     | 0.40              |
| 3:F:18:THR:HG22  | 3:F:21:GLU:HG3   | 2.02                     | 0.40              |
| 3:I:231:LEU:HA   | 3:I:231:LEU:HD12 | 1.90                     | 0.40              |
| 3:L:207:LEU:HG   | 3:L:212:LEU:HD22 | 2.04                     | 0.40              |
| 3:C:18:THR:HG23  | 3:C:20:ASP:C     | 2.42                     | 0.40              |
| 3:C:207:LEU:HG   | 3:C:212:LEU:HD22 | 2.03                     | 0.40              |
| 3:C:259:ARG:CZ   | 3:C:259:ARG:HB3  | 2.51                     | 0.40              |
| 2:E:70:ARG:HG2   | 2:E:70:ARG:HH11  | 1.87                     | 0.40              |
| 3:F:334:ARG:CZ   | 3:F:334:ARG:HB3  | 2.52                     | 0.40              |
| 1:G:13:LEU:HD13  | 1:G:86:ALA:HA    | 2.04                     | 0.40              |
| 1:G:178:ALA:O    | 1:G:179:MET:CB   | 2.69                     | 0.40              |
| 1:G:203:VAL:O    | 1:G:203:VAL:HG12 | 2.22                     | 0.40              |
| 3:I:259:ARG:NH1  | 3:I:259:ARG:CB   | 2.80                     | 0.40              |
| 3:C:331:THR:CG2  | 1:J:142:LYS:HA   | 2.50                     | 0.40              |
| 1:J:202:GLU:O    | 1:J:206:THR:HG23 | 2.22                     | 0.40              |
| 2:K:70:ARG:HA    | 2:K:70:ARG:HD2   | 1.82                     | 0.40              |
| 3:L:21:GLU:O     | 3:L:24:VAL:HB    | 2.22                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |   |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1   | A     | 204/216 (94%) | 174 (85%) | 17 (8%) | 13 (6%)  | 1           | 2 |
| 1   | D     | 204/216 (94%) | 176 (86%) | 15 (7%) | 13 (6%)  | 1           | 2 |
| 1   | G     | 204/216 (94%) | 174 (85%) | 17 (8%) | 13 (6%)  | 1           | 2 |
| 1   | J     | 204/216 (94%) | 175 (86%) | 16 (8%) | 13 (6%)  | 1           | 2 |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 2   | B     | 144/201 (72%)   | 121 (84%)  | 15 (10%)  | 8 (6%)   | 2           | 3  |
| 2   | E     | 144/201 (72%)   | 119 (83%)  | 17 (12%)  | 8 (6%)   | 2           | 3  |
| 2   | H     | 144/201 (72%)   | 121 (84%)  | 15 (10%)  | 8 (6%)   | 2           | 3  |
| 2   | K     | 144/201 (72%)   | 121 (84%)  | 15 (10%)  | 8 (6%)   | 2           | 3  |
| 3   | C     | 342/386 (89%)   | 301 (88%)  | 38 (11%)  | 3 (1%)   | 19          | 44 |
| 3   | F     | 342/386 (89%)   | 302 (88%)  | 37 (11%)  | 3 (1%)   | 19          | 44 |
| 3   | I     | 342/386 (89%)   | 305 (89%)  | 34 (10%)  | 3 (1%)   | 19          | 44 |
| 3   | L     | 342/386 (89%)   | 305 (89%)  | 34 (10%)  | 3 (1%)   | 19          | 44 |
| All | All   | 2760/3212 (86%) | 2394 (87%) | 270 (10%) | 96 (4%)  | 4           | 9  |

All (96) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 106 | ARG  |
| 1   | A     | 179 | MET  |
| 1   | A     | 189 | MET  |
| 1   | A     | 190 | ASP  |
| 1   | A     | 191 | PRO  |
| 2   | B     | 45  | GLU  |
| 2   | B     | 46  | GLU  |
| 2   | B     | 59  | ALA  |
| 2   | B     | 60  | SER  |
| 2   | B     | 165 | ARG  |
| 1   | D     | 179 | MET  |
| 1   | D     | 189 | MET  |
| 1   | D     | 190 | ASP  |
| 1   | D     | 191 | PRO  |
| 2   | E     | 45  | GLU  |
| 2   | E     | 46  | GLU  |
| 2   | E     | 59  | ALA  |
| 2   | E     | 60  | SER  |
| 2   | E     | 165 | ARG  |
| 1   | G     | 106 | ARG  |
| 1   | G     | 179 | MET  |
| 1   | G     | 189 | MET  |
| 1   | G     | 190 | ASP  |
| 1   | G     | 191 | PRO  |
| 2   | H     | 45  | GLU  |
| 2   | H     | 46  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 59  | ALA  |
| 2   | H     | 60  | SER  |
| 2   | H     | 165 | ARG  |
| 1   | J     | 106 | ARG  |
| 1   | J     | 179 | MET  |
| 1   | J     | 189 | MET  |
| 1   | J     | 190 | ASP  |
| 1   | J     | 191 | PRO  |
| 2   | K     | 45  | GLU  |
| 2   | K     | 46  | GLU  |
| 2   | K     | 59  | ALA  |
| 2   | K     | 60  | SER  |
| 2   | K     | 165 | ARG  |
| 1   | A     | 178 | ALA  |
| 1   | A     | 196 | GLN  |
| 2   | B     | 116 | SER  |
| 1   | D     | 106 | ARG  |
| 1   | D     | 178 | ALA  |
| 1   | D     | 196 | GLN  |
| 2   | E     | 116 | SER  |
| 3   | F     | 172 | GLU  |
| 1   | G     | 178 | ALA  |
| 1   | G     | 196 | GLN  |
| 2   | H     | 116 | SER  |
| 1   | J     | 178 | ALA  |
| 1   | J     | 196 | GLN  |
| 1   | A     | 194 | ALA  |
| 3   | C     | 172 | GLU  |
| 1   | D     | 194 | ALA  |
| 2   | E     | 47  | GLU  |
| 1   | G     | 194 | ALA  |
| 2   | H     | 47  | GLU  |
| 3   | I     | 172 | GLU  |
| 1   | J     | 194 | ALA  |
| 2   | K     | 47  | GLU  |
| 2   | K     | 116 | SER  |
| 3   | L     | 172 | GLU  |
| 3   | L     | 336 | GLU  |
| 1   | A     | 186 | GLU  |
| 1   | A     | 187 | VAL  |
| 1   | A     | 195 | ALA  |
| 2   | B     | 47  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 336 | GLU  |
| 1   | D     | 186 | GLU  |
| 1   | D     | 187 | VAL  |
| 1   | D     | 195 | ALA  |
| 3   | F     | 336 | GLU  |
| 1   | G     | 186 | GLU  |
| 1   | G     | 187 | VAL  |
| 1   | G     | 195 | ALA  |
| 3   | I     | 336 | GLU  |
| 1   | J     | 186 | GLU  |
| 1   | J     | 195 | ALA  |
| 1   | A     | 188 | VAL  |
| 1   | D     | 188 | VAL  |
| 1   | D     | 210 | PRO  |
| 1   | G     | 188 | VAL  |
| 1   | G     | 210 | PRO  |
| 1   | J     | 187 | VAL  |
| 1   | J     | 188 | VAL  |
| 1   | J     | 210 | PRO  |
| 1   | A     | 210 | PRO  |
| 2   | H     | 65  | PRO  |
| 2   | B     | 65  | PRO  |
| 2   | K     | 65  | PRO  |
| 2   | E     | 65  | PRO  |
| 3   | C     | 16  | ILE  |
| 3   | F     | 16  | ILE  |
| 3   | I     | 16  | ILE  |
| 3   | L     | 16  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A     | 178/185 (96%) | 165 (93%) | 13 (7%)  | 15          | 36 |
| 1   | D     | 178/185 (96%) | 165 (93%) | 13 (7%)  | 15          | 36 |
| 1   | G     | 178/185 (96%) | 165 (93%) | 13 (7%)  | 15          | 36 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | J     | 178/185 (96%)   | 166 (93%)  | 12 (7%)  | 18          | 40 |
| 2   | B     | 131/176 (74%)   | 119 (91%)  | 12 (9%)  | 10          | 23 |
| 2   | E     | 131/176 (74%)   | 119 (91%)  | 12 (9%)  | 10          | 23 |
| 2   | H     | 131/176 (74%)   | 119 (91%)  | 12 (9%)  | 10          | 23 |
| 2   | K     | 131/176 (74%)   | 119 (91%)  | 12 (9%)  | 10          | 23 |
| 3   | C     | 295/334 (88%)   | 277 (94%)  | 18 (6%)  | 20          | 45 |
| 3   | F     | 295/334 (88%)   | 277 (94%)  | 18 (6%)  | 20          | 45 |
| 3   | I     | 295/334 (88%)   | 277 (94%)  | 18 (6%)  | 20          | 45 |
| 3   | L     | 295/334 (88%)   | 277 (94%)  | 18 (6%)  | 20          | 45 |
| All | All   | 2416/2780 (87%) | 2245 (93%) | 171 (7%) | 16          | 38 |

All (171) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 13  | LEU  |
| 1   | A     | 16  | VAL  |
| 1   | A     | 28  | LYS  |
| 1   | A     | 31  | LEU  |
| 1   | A     | 81  | ILE  |
| 1   | A     | 97  | THR  |
| 1   | A     | 111 | VAL  |
| 1   | A     | 118 | VAL  |
| 1   | A     | 140 | ARG  |
| 1   | A     | 141 | LYS  |
| 1   | A     | 157 | PHE  |
| 1   | A     | 158 | GLU  |
| 1   | A     | 186 | GLU  |
| 2   | B     | 26  | GLN  |
| 2   | B     | 46  | GLU  |
| 2   | B     | 57  | ARG  |
| 2   | B     | 63  | ASP  |
| 2   | B     | 64  | LEU  |
| 2   | B     | 75  | VAL  |
| 2   | B     | 109 | GLU  |
| 2   | B     | 118 | ARG  |
| 2   | B     | 123 | ASN  |
| 2   | B     | 146 | GLU  |
| 2   | B     | 156 | GLU  |
| 2   | B     | 166 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 19  | GLU  |
| 3   | C     | 29  | LEU  |
| 3   | C     | 43  | THR  |
| 3   | C     | 66  | GLU  |
| 3   | C     | 78  | GLU  |
| 3   | C     | 81  | GLU  |
| 3   | C     | 109 | THR  |
| 3   | C     | 112 | GLU  |
| 3   | C     | 114 | LEU  |
| 3   | C     | 146 | LEU  |
| 3   | C     | 192 | VAL  |
| 3   | C     | 196 | GLN  |
| 3   | C     | 208 | LEU  |
| 3   | C     | 212 | LEU  |
| 3   | C     | 247 | ARG  |
| 3   | C     | 278 | THR  |
| 3   | C     | 293 | THR  |
| 3   | C     | 296 | THR  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 16  | VAL  |
| 1   | D     | 28  | LYS  |
| 1   | D     | 31  | LEU  |
| 1   | D     | 81  | ILE  |
| 1   | D     | 97  | THR  |
| 1   | D     | 111 | VAL  |
| 1   | D     | 118 | VAL  |
| 1   | D     | 140 | ARG  |
| 1   | D     | 141 | LYS  |
| 1   | D     | 157 | PHE  |
| 1   | D     | 158 | GLU  |
| 1   | D     | 186 | GLU  |
| 2   | E     | 26  | GLN  |
| 2   | E     | 46  | GLU  |
| 2   | E     | 57  | ARG  |
| 2   | E     | 63  | ASP  |
| 2   | E     | 64  | LEU  |
| 2   | E     | 75  | VAL  |
| 2   | E     | 109 | GLU  |
| 2   | E     | 118 | ARG  |
| 2   | E     | 123 | ASN  |
| 2   | E     | 146 | GLU  |
| 2   | E     | 156 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 166 | GLU  |
| 3   | F     | 19  | GLU  |
| 3   | F     | 29  | LEU  |
| 3   | F     | 43  | THR  |
| 3   | F     | 66  | GLU  |
| 3   | F     | 78  | GLU  |
| 3   | F     | 81  | GLU  |
| 3   | F     | 109 | THR  |
| 3   | F     | 112 | GLU  |
| 3   | F     | 114 | LEU  |
| 3   | F     | 146 | LEU  |
| 3   | F     | 192 | VAL  |
| 3   | F     | 196 | GLN  |
| 3   | F     | 208 | LEU  |
| 3   | F     | 212 | LEU  |
| 3   | F     | 247 | ARG  |
| 3   | F     | 278 | THR  |
| 3   | F     | 293 | THR  |
| 3   | F     | 296 | THR  |
| 1   | G     | 13  | LEU  |
| 1   | G     | 16  | VAL  |
| 1   | G     | 28  | LYS  |
| 1   | G     | 31  | LEU  |
| 1   | G     | 81  | ILE  |
| 1   | G     | 97  | THR  |
| 1   | G     | 111 | VAL  |
| 1   | G     | 118 | VAL  |
| 1   | G     | 140 | ARG  |
| 1   | G     | 141 | LYS  |
| 1   | G     | 157 | PHE  |
| 1   | G     | 158 | GLU  |
| 1   | G     | 186 | GLU  |
| 2   | H     | 26  | GLN  |
| 2   | H     | 46  | GLU  |
| 2   | H     | 57  | ARG  |
| 2   | H     | 63  | ASP  |
| 2   | H     | 64  | LEU  |
| 2   | H     | 75  | VAL  |
| 2   | H     | 109 | GLU  |
| 2   | H     | 118 | ARG  |
| 2   | H     | 123 | ASN  |
| 2   | H     | 146 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | H     | 156 | GLU  |
| 2   | H     | 166 | GLU  |
| 3   | I     | 19  | GLU  |
| 3   | I     | 29  | LEU  |
| 3   | I     | 43  | THR  |
| 3   | I     | 66  | GLU  |
| 3   | I     | 78  | GLU  |
| 3   | I     | 81  | GLU  |
| 3   | I     | 109 | THR  |
| 3   | I     | 112 | GLU  |
| 3   | I     | 114 | LEU  |
| 3   | I     | 146 | LEU  |
| 3   | I     | 192 | VAL  |
| 3   | I     | 196 | GLN  |
| 3   | I     | 208 | LEU  |
| 3   | I     | 212 | LEU  |
| 3   | I     | 247 | ARG  |
| 3   | I     | 278 | THR  |
| 3   | I     | 293 | THR  |
| 3   | I     | 296 | THR  |
| 1   | J     | 13  | LEU  |
| 1   | J     | 16  | VAL  |
| 1   | J     | 28  | LYS  |
| 1   | J     | 31  | LEU  |
| 1   | J     | 81  | ILE  |
| 1   | J     | 97  | THR  |
| 1   | J     | 118 | VAL  |
| 1   | J     | 140 | ARG  |
| 1   | J     | 141 | LYS  |
| 1   | J     | 157 | PHE  |
| 1   | J     | 158 | GLU  |
| 1   | J     | 186 | GLU  |
| 2   | K     | 26  | GLN  |
| 2   | K     | 46  | GLU  |
| 2   | K     | 57  | ARG  |
| 2   | K     | 63  | ASP  |
| 2   | K     | 64  | LEU  |
| 2   | K     | 75  | VAL  |
| 2   | K     | 109 | GLU  |
| 2   | K     | 118 | ARG  |
| 2   | K     | 123 | ASN  |
| 2   | K     | 146 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 156 | GLU  |
| 2   | K     | 166 | GLU  |
| 3   | L     | 19  | GLU  |
| 3   | L     | 29  | LEU  |
| 3   | L     | 43  | THR  |
| 3   | L     | 66  | GLU  |
| 3   | L     | 78  | GLU  |
| 3   | L     | 81  | GLU  |
| 3   | L     | 109 | THR  |
| 3   | L     | 112 | GLU  |
| 3   | L     | 114 | LEU  |
| 3   | L     | 146 | LEU  |
| 3   | L     | 192 | VAL  |
| 3   | L     | 196 | GLN  |
| 3   | L     | 208 | LEU  |
| 3   | L     | 212 | LEU  |
| 3   | L     | 247 | ARG  |
| 3   | L     | 278 | THR  |
| 3   | L     | 293 | THR  |
| 3   | L     | 296 | THR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 10  | GLN  |
| 1   | A     | 30  | HIS  |
| 1   | A     | 100 | ASN  |
| 1   | A     | 143 | ASN  |
| 1   | A     | 156 | ASN  |
| 2   | B     | 22  | ASN  |
| 2   | B     | 102 | HIS  |
| 2   | B     | 113 | ASN  |
| 2   | B     | 123 | ASN  |
| 2   | B     | 147 | ASN  |
| 3   | C     | 111 | GLN  |
| 3   | C     | 121 | HIS  |
| 3   | C     | 130 | HIS  |
| 3   | C     | 131 | ASN  |
| 3   | C     | 173 | ASN  |
| 3   | C     | 186 | HIS  |
| 3   | C     | 206 | HIS  |
| 3   | C     | 252 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 10  | GLN  |
| 1   | D     | 30  | HIS  |
| 1   | D     | 143 | ASN  |
| 1   | D     | 156 | ASN  |
| 2   | E     | 22  | ASN  |
| 2   | E     | 102 | HIS  |
| 2   | E     | 113 | ASN  |
| 2   | E     | 123 | ASN  |
| 2   | E     | 147 | ASN  |
| 3   | F     | 111 | GLN  |
| 3   | F     | 121 | HIS  |
| 3   | F     | 130 | HIS  |
| 3   | F     | 131 | ASN  |
| 3   | F     | 173 | ASN  |
| 3   | F     | 186 | HIS  |
| 3   | F     | 206 | HIS  |
| 3   | F     | 245 | ASN  |
| 3   | F     | 252 | ASN  |
| 1   | G     | 10  | GLN  |
| 1   | G     | 30  | HIS  |
| 1   | G     | 100 | ASN  |
| 1   | G     | 143 | ASN  |
| 1   | G     | 156 | ASN  |
| 2   | H     | 22  | ASN  |
| 2   | H     | 102 | HIS  |
| 2   | H     | 113 | ASN  |
| 2   | H     | 123 | ASN  |
| 2   | H     | 147 | ASN  |
| 3   | I     | 111 | GLN  |
| 3   | I     | 121 | HIS  |
| 3   | I     | 130 | HIS  |
| 3   | I     | 131 | ASN  |
| 3   | I     | 147 | GLN  |
| 3   | I     | 173 | ASN  |
| 3   | I     | 184 | GLN  |
| 3   | I     | 186 | HIS  |
| 3   | I     | 252 | ASN  |
| 1   | J     | 10  | GLN  |
| 1   | J     | 30  | HIS  |
| 1   | J     | 100 | ASN  |
| 1   | J     | 143 | ASN  |
| 1   | J     | 156 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K     | 22  | ASN  |
| 2   | K     | 102 | HIS  |
| 2   | K     | 113 | ASN  |
| 2   | K     | 123 | ASN  |
| 2   | K     | 147 | ASN  |
| 3   | L     | 111 | GLN  |
| 3   | L     | 121 | HIS  |
| 3   | L     | 130 | HIS  |
| 3   | L     | 131 | ASN  |
| 3   | L     | 173 | ASN  |
| 3   | L     | 186 | HIS  |
| 3   | L     | 206 | HIS  |
| 3   | L     | 252 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | GNP  | A     | 1250 | 4    | 27,34,34     | 2.22 | 8 (29%)     | 30,54,54    | 2.02 | 6 (20%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | GNP  | D     | 2250 | 4    | 27,34,34     | 2.22 | 8 (29%)  | 30,54,54    | 2.03 | 7 (23%)  |
| 5   | GNP  | G     | 3250 | 4    | 27,34,34     | 2.18 | 6 (22%)  | 30,54,54    | 1.99 | 6 (20%)  |
| 5   | GNP  | J     | 4250 | 4    | 27,34,34     | 2.26 | 8 (29%)  | 30,54,54    | 1.97 | 8 (26%)  |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 5   | GNP  | A     | 1250 | 4    | -       | 1/16/38/38 | 0/3/3/3 |
| 5   | GNP  | D     | 2250 | 4    | -       | 1/16/38/38 | 0/3/3/3 |
| 5   | GNP  | G     | 3250 | 4    | -       | 1/16/38/38 | 0/3/3/3 |
| 5   | GNP  | J     | 4250 | 4    | -       | 1/16/38/38 | 0/3/3/3 |

All (30) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 5   | A     | 1250 | GNP  | C4-N9  | -7.02 | 1.38        | 1.47     |
| 5   | J     | 4250 | GNP  | C4-N9  | -6.80 | 1.38        | 1.47     |
| 5   | D     | 2250 | GNP  | C4-N9  | -6.64 | 1.38        | 1.47     |
| 5   | G     | 3250 | GNP  | C4-N9  | -6.46 | 1.39        | 1.47     |
| 5   | A     | 1250 | GNP  | C5-C6  | -4.11 | 1.45        | 1.52     |
| 5   | D     | 2250 | GNP  | PG-O2G | -4.00 | 1.45        | 1.56     |
| 5   | D     | 2250 | GNP  | PB-O2B | -3.89 | 1.46        | 1.56     |
| 5   | A     | 1250 | GNP  | PG-O2G | -3.84 | 1.46        | 1.56     |
| 5   | G     | 3250 | GNP  | PG-O2G | -3.82 | 1.46        | 1.56     |
| 5   | G     | 3250 | GNP  | C5-C6  | -3.69 | 1.46        | 1.52     |
| 5   | G     | 3250 | GNP  | PB-O2B | -3.67 | 1.46        | 1.56     |
| 5   | J     | 4250 | GNP  | PB-O2B | -3.63 | 1.46        | 1.56     |
| 5   | J     | 4250 | GNP  | C5-C6  | -3.51 | 1.46        | 1.52     |
| 5   | J     | 4250 | GNP  | PG-O2G | -3.34 | 1.47        | 1.56     |
| 5   | D     | 2250 | GNP  | C5-C6  | -3.31 | 1.47        | 1.52     |
| 5   | A     | 1250 | GNP  | PB-O2B | -3.04 | 1.48        | 1.56     |
| 5   | A     | 1250 | GNP  | C8-N9  | -2.55 | 1.39        | 1.46     |
| 5   | D     | 2250 | GNP  | C8-N9  | -2.29 | 1.40        | 1.46     |
| 5   | J     | 4250 | GNP  | C8-N9  | -2.20 | 1.40        | 1.46     |
| 5   | J     | 4250 | GNP  | C5-C4  | -2.14 | 1.39        | 1.52     |
| 5   | D     | 2250 | GNP  | C5-C4  | -2.12 | 1.39        | 1.52     |
| 5   | A     | 1250 | GNP  | C5-C4  | -2.08 | 1.39        | 1.52     |
| 5   | G     | 3250 | GNP  | C8-N9  | -2.03 | 1.40        | 1.46     |
| 5   | D     | 2250 | GNP  | PB-O3A | 2.47  | 1.62        | 1.59     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 5   | A     | 1250 | GNP  | PB-O3A | 2.78 | 1.62        | 1.59     |
| 5   | A     | 1250 | GNP  | C6-N1  | 3.46 | 1.39        | 1.33     |
| 5   | J     | 4250 | GNP  | PB-O3A | 3.51 | 1.63        | 1.59     |
| 5   | D     | 2250 | GNP  | C6-N1  | 3.87 | 1.39        | 1.33     |
| 5   | J     | 4250 | GNP  | C6-N1  | 4.15 | 1.40        | 1.33     |
| 5   | G     | 3250 | GNP  | C6-N1  | 4.23 | 1.40        | 1.33     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 5   | G     | 3250 | GNP  | C5-C6-N1   | -4.86 | 112.48      | 118.27   |
| 5   | A     | 1250 | GNP  | C5-C6-N1   | -4.84 | 112.50      | 118.27   |
| 5   | D     | 2250 | GNP  | C5-C6-N1   | -4.78 | 112.58      | 118.27   |
| 5   | J     | 4250 | GNP  | C5-C6-N1   | -4.66 | 112.72      | 118.27   |
| 5   | G     | 3250 | GNP  | O3G-PG-O1G | -3.53 | 104.46      | 113.43   |
| 5   | A     | 1250 | GNP  | O3G-PG-O1G | -3.51 | 104.50      | 113.43   |
| 5   | D     | 2250 | GNP  | O6-C6-N1   | -3.45 | 118.13      | 122.71   |
| 5   | D     | 2250 | GNP  | O3G-PG-O1G | -3.43 | 104.72      | 113.43   |
| 5   | J     | 4250 | GNP  | O6-C6-N1   | -3.19 | 118.47      | 122.71   |
| 5   | A     | 1250 | GNP  | O6-C6-N1   | -3.18 | 118.49      | 122.71   |
| 5   | J     | 4250 | GNP  | O3G-PG-O1G | -3.14 | 105.45      | 113.43   |
| 5   | G     | 3250 | GNP  | O6-C6-N1   | -2.86 | 118.91      | 122.71   |
| 5   | D     | 2250 | GNP  | O2G-PG-O1G | -2.13 | 108.00      | 113.43   |
| 5   | J     | 4250 | GNP  | O2G-PG-O1G | -2.04 | 108.25      | 113.43   |
| 5   | J     | 4250 | GNP  | O1B-PB-N3B | 2.06  | 114.88      | 111.79   |
| 5   | J     | 4250 | GNP  | O1G-PG-N3B | 2.18  | 115.05      | 111.79   |
| 5   | G     | 3250 | GNP  | O1G-PG-N3B | 2.28  | 115.20      | 111.79   |
| 5   | D     | 2250 | GNP  | O1G-PG-N3B | 2.43  | 115.42      | 111.79   |
| 5   | A     | 1250 | GNP  | O1G-PG-N3B | 2.52  | 115.56      | 111.79   |
| 5   | G     | 3250 | GNP  | O6-C6-C5   | 4.26  | 128.60      | 119.82   |
| 5   | J     | 4250 | GNP  | O6-C6-C5   | 4.36  | 128.81      | 119.82   |
| 5   | A     | 1250 | GNP  | O6-C6-C5   | 4.46  | 129.01      | 119.82   |
| 5   | D     | 2250 | GNP  | O6-C6-C5   | 4.59  | 129.29      | 119.82   |
| 5   | J     | 4250 | GNP  | C4-C5-N7   | 5.63  | 109.92      | 102.46   |
| 5   | D     | 2250 | GNP  | C4-C5-N7   | 5.66  | 109.96      | 102.46   |
| 5   | A     | 1250 | GNP  | C4-C5-N7   | 5.68  | 109.99      | 102.46   |
| 5   | G     | 3250 | GNP  | C4-C5-N7   | 5.83  | 110.18      | 102.46   |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 5   | G     | 3250 | GNP  | O1B-PB-N3B-PG |
| 5   | D     | 2250 | GNP  | O1B-PB-N3B-PG |
| 5   | A     | 1250 | GNP  | O1B-PB-N3B-PG |
| 5   | J     | 4250 | GNP  | O1B-PB-N3B-PG |

There are no ring outliers.

4 monomers are involved in 14 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5   | A     | 1250 | GNP  | 2       | 0            |
| 5   | D     | 2250 | GNP  | 3       | 0            |
| 5   | G     | 3250 | GNP  | 3       | 0            |
| 5   | J     | 4250 | GNP  | 6       | 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     | 206/216 (95%)   | 0.36   | 23 (11%) 5 4  | 27, 46, 132, 170      | 0     |
| 1   | D     | 206/216 (95%)   | 0.54   | 22 (10%) 6 4  | 21, 46, 146, 188      | 0     |
| 1   | G     | 206/216 (95%)   | 0.44   | 23 (11%) 5 4  | 28, 49, 127, 168      | 0     |
| 1   | J     | 206/216 (95%)   | 0.31   | 19 (9%) 9 7   | 24, 47, 117, 170      | 0     |
| 2   | B     | 146/201 (72%)   | 0.73   | 24 (16%) 1 1  | 36, 72, 130, 159      | 0     |
| 2   | E     | 146/201 (72%)   | 1.38   | 42 (28%) 0 0  | 41, 88, 138, 159      | 0     |
| 2   | H     | 146/201 (72%)   | 0.96   | 24 (16%) 1 1  | 41, 71, 138, 176      | 0     |
| 2   | K     | 146/201 (72%)   | 0.63   | 21 (14%) 2 1  | 28, 73, 126, 149      | 0     |
| 3   | C     | 344/386 (89%)   | -0.07  | 4 (1%) 79 80  | 21, 42, 76, 135       | 0     |
| 3   | F     | 344/386 (89%)   | -0.04  | 14 (4%) 37 35 | 24, 45, 83, 135       | 0     |
| 3   | I     | 344/386 (89%)   | -0.05  | 5 (1%) 73 75  | 23, 45, 81, 114       | 0     |
| 3   | L     | 344/386 (89%)   | 0.02   | 10 (2%) 51 51 | 22, 45, 90, 143       | 0     |
| All | All   | 2784/3212 (86%) | 0.30   | 231 (8%) 11 9 | 21, 49, 120, 188      | 0     |

All (231) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 189 | MET  | 14.5 |
| 1   | D     | 191 | PRO  | 12.0 |
| 1   | D     | 192 | ALA  | 11.8 |
| 1   | G     | 192 | ALA  | 10.9 |
| 1   | D     | 188 | VAL  | 10.5 |
| 2   | H     | 63  | ASP  | 10.3 |
| 1   | G     | 191 | PRO  | 10.2 |
| 1   | D     | 187 | VAL  | 10.1 |
| 1   | A     | 190 | ASP  | 9.2  |
| 1   | D     | 190 | ASP  | 8.2  |
| 1   | D     | 195 | ALA  | 8.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 187 | VAL  | 7.5  |
| 2   | H     | 22  | ASN  | 7.5  |
| 1   | J     | 189 | MET  | 7.4  |
| 2   | B     | 63  | ASP  | 7.4  |
| 1   | A     | 192 | ALA  | 7.4  |
| 1   | D     | 194 | ALA  | 7.3  |
| 2   | E     | 107 | MET  | 6.8  |
| 1   | A     | 212 | GLU  | 6.7  |
| 1   | A     | 188 | VAL  | 6.6  |
| 1   | A     | 191 | PRO  | 6.6  |
| 2   | H     | 23  | HIS  | 6.5  |
| 2   | E     | 116 | SER  | 6.3  |
| 1   | J     | 190 | ASP  | 6.3  |
| 1   | G     | 197 | TYR  | 6.2  |
| 1   | A     | 197 | TYR  | 6.1  |
| 3   | F     | 20  | ASP  | 6.0  |
| 1   | G     | 199 | HIS  | 5.9  |
| 1   | D     | 193 | LEU  | 5.9  |
| 2   | E     | 63  | ASP  | 5.8  |
| 2   | E     | 61  | GLU  | 5.8  |
| 1   | A     | 194 | ALA  | 5.7  |
| 1   | D     | 197 | TYR  | 5.7  |
| 1   | D     | 141 | LYS  | 5.6  |
| 1   | G     | 186 | GLU  | 5.6  |
| 2   | B     | 23  | HIS  | 5.5  |
| 2   | E     | 117 | ASP  | 5.3  |
| 1   | A     | 186 | GLU  | 5.2  |
| 1   | A     | 193 | LEU  | 5.2  |
| 2   | B     | 65  | PRO  | 5.2  |
| 2   | H     | 116 | SER  | 5.1  |
| 1   | G     | 196 | GLN  | 5.1  |
| 2   | H     | 65  | PRO  | 5.1  |
| 1   | D     | 199 | HIS  | 5.0  |
| 1   | G     | 140 | ARG  | 5.0  |
| 2   | B     | 61  | GLU  | 5.0  |
| 1   | G     | 212 | GLU  | 5.0  |
| 2   | E     | 145 | ALA  | 4.9  |
| 1   | G     | 193 | LEU  | 4.9  |
| 1   | G     | 141 | LYS  | 4.8  |
| 2   | E     | 49  | PHE  | 4.7  |
| 2   | E     | 23  | HIS  | 4.7  |
| 1   | A     | 199 | HIS  | 4.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 195 | ALA  | 4.6  |
| 2   | H     | 37  | GLU  | 4.5  |
| 2   | K     | 61  | GLU  | 4.5  |
| 2   | E     | 160 | LYS  | 4.5  |
| 2   | E     | 22  | ASN  | 4.4  |
| 2   | H     | 64  | LEU  | 4.3  |
| 2   | H     | 61  | GLU  | 4.2  |
| 1   | D     | 186 | GLU  | 4.2  |
| 2   | E     | 82  | GLU  | 4.2  |
| 1   | A     | 141 | LYS  | 4.2  |
| 1   | J     | 191 | PRO  | 4.1  |
| 1   | D     | 198 | GLU  | 4.1  |
| 1   | A     | 195 | ALA  | 4.1  |
| 1   | J     | 192 | ALA  | 4.0  |
| 1   | D     | 212 | GLU  | 4.0  |
| 2   | E     | 115 | GLY  | 4.0  |
| 2   | H     | 82  | GLU  | 3.9  |
| 3   | I     | 334 | ARG  | 3.9  |
| 2   | B     | 64  | LEU  | 3.8  |
| 2   | E     | 167 | LYS  | 3.8  |
| 2   | K     | 115 | GLY  | 3.8  |
| 3   | I     | 345 | GLU  | 3.8  |
| 1   | J     | 193 | LEU  | 3.8  |
| 1   | A     | 189 | MET  | 3.8  |
| 2   | H     | 167 | LYS  | 3.8  |
| 1   | A     | 211 | ASP  | 3.8  |
| 2   | B     | 24  | ASP  | 3.8  |
| 2   | H     | 114 | ALA  | 3.8  |
| 1   | G     | 187 | VAL  | 3.8  |
| 2   | B     | 117 | ASP  | 3.7  |
| 2   | B     | 82  | GLU  | 3.7  |
| 1   | G     | 194 | ALA  | 3.7  |
| 1   | D     | 196 | GLN  | 3.7  |
| 2   | K     | 23  | HIS  | 3.7  |
| 3   | I     | 333 | GLY  | 3.6  |
| 2   | B     | 167 | LYS  | 3.6  |
| 2   | K     | 63  | ASP  | 3.6  |
| 2   | B     | 115 | GLY  | 3.6  |
| 1   | J     | 212 | GLU  | 3.5  |
| 2   | H     | 115 | GLY  | 3.5  |
| 1   | J     | 196 | GLN  | 3.5  |
| 2   | B     | 22  | ASN  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 28  | GLU  | 3.4  |
| 2   | K     | 38  | ILE  | 3.4  |
| 2   | E     | 143 | LEU  | 3.4  |
| 2   | E     | 144 | ASN  | 3.3  |
| 1   | D     | 202 | GLU  | 3.3  |
| 1   | D     | 213 | ASP  | 3.3  |
| 2   | K     | 132 | CYS  | 3.3  |
| 1   | J     | 197 | TYR  | 3.3  |
| 2   | E     | 67  | TRP  | 3.2  |
| 2   | H     | 117 | ASP  | 3.2  |
| 3   | C     | 341 | ASP  | 3.2  |
| 2   | H     | 24  | ASP  | 3.2  |
| 1   | G     | 189 | MET  | 3.2  |
| 2   | E     | 46  | GLU  | 3.2  |
| 1   | G     | 190 | ASP  | 3.2  |
| 3   | F     | 31  | ASP  | 3.2  |
| 1   | G     | 211 | ASP  | 3.1  |
| 3   | F     | 32  | ASP  | 3.1  |
| 2   | E     | 62  | ASN  | 3.1  |
| 2   | B     | 45  | GLU  | 3.1  |
| 3   | F     | 345 | GLU  | 3.1  |
| 2   | B     | 28  | GLU  | 3.1  |
| 3   | L     | 345 | GLU  | 3.1  |
| 1   | A     | 213 | ASP  | 3.1  |
| 1   | A     | 202 | GLU  | 3.1  |
| 2   | B     | 166 | GLU  | 3.0  |
| 2   | E     | 65  | PRO  | 3.0  |
| 2   | E     | 140 | ILE  | 3.0  |
| 2   | E     | 45  | GLU  | 3.0  |
| 2   | B     | 26  | GLN  | 3.0  |
| 2   | B     | 140 | ILE  | 3.0  |
| 1   | G     | 213 | ASP  | 2.9  |
| 2   | E     | 149 | GLN  | 2.9  |
| 2   | B     | 37  | GLU  | 2.9  |
| 2   | E     | 66  | GLU  | 2.9  |
| 2   | K     | 64  | LEU  | 2.9  |
| 1   | A     | 140 | ARG  | 2.9  |
| 2   | E     | 165 | ARG  | 2.9  |
| 3   | C     | 310 | LEU  | 2.9  |
| 3   | L     | 20  | ASP  | 2.9  |
| 3   | L     | 52  | LEU  | 2.8  |
| 2   | E     | 163 | GLU  | 2.8  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 198 | GLU  | 2.8  |
| 1   | J     | 195 | ALA  | 2.8  |
| 3   | C     | 230 | HIS  | 2.8  |
| 3   | F     | 19  | GLU  | 2.8  |
| 2   | K     | 145 | ALA  | 2.8  |
| 2   | H     | 140 | ILE  | 2.7  |
| 2   | E     | 132 | CYS  | 2.7  |
| 2   | K     | 114 | ALA  | 2.7  |
| 1   | D     | 211 | ASP  | 2.7  |
| 1   | G     | 144 | LEU  | 2.7  |
| 2   | H     | 164 | GLU  | 2.7  |
| 2   | K     | 62  | ASN  | 2.7  |
| 1   | J     | 188 | VAL  | 2.7  |
| 1   | J     | 200 | ASP  | 2.7  |
| 2   | K     | 117 | ASP  | 2.7  |
| 1   | A     | 209 | LEU  | 2.7  |
| 2   | B     | 163 | GLU  | 2.7  |
| 2   | B     | 59  | ALA  | 2.6  |
| 2   | E     | 121 | VAL  | 2.6  |
| 2   | K     | 82  | GLU  | 2.6  |
| 2   | H     | 160 | LYS  | 2.6  |
| 3   | F     | 157 | ASN  | 2.6  |
| 1   | G     | 198 | GLU  | 2.6  |
| 2   | E     | 108 | MET  | 2.6  |
| 2   | H     | 66  | GLU  | 2.6  |
| 2   | E     | 119 | ALA  | 2.6  |
| 3   | F     | 155 | ALA  | 2.6  |
| 1   | J     | 187 | VAL  | 2.6  |
| 2   | E     | 24  | ASP  | 2.5  |
| 3   | L     | 30  | GLU  | 2.5  |
| 2   | K     | 110 | LEU  | 2.5  |
| 2   | H     | 26  | GLN  | 2.5  |
| 3   | F     | 2   | ALA  | 2.5  |
| 3   | L     | 230 | HIS  | 2.5  |
| 2   | E     | 64  | LEU  | 2.5  |
| 2   | B     | 62  | ASN  | 2.5  |
| 2   | K     | 65  | PRO  | 2.5  |
| 2   | B     | 116 | SER  | 2.5  |
| 2   | E     | 84  | GLY  | 2.5  |
| 1   | A     | 137 | VAL  | 2.5  |
| 1   | J     | 211 | ASP  | 2.4  |
| 1   | J     | 199 | HIS  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 188 | VAL  | 2.4  |
| 2   | K     | 144 | ASN  | 2.4  |
| 2   | K     | 84  | GLY  | 2.4  |
| 1   | J     | 186 | GLU  | 2.4  |
| 2   | E     | 38  | ILE  | 2.4  |
| 2   | K     | 166 | GLU  | 2.4  |
| 1   | J     | 134 | LYS  | 2.3  |
| 3   | L     | 320 | ASP  | 2.3  |
| 3   | F     | 30  | GLU  | 2.3  |
| 3   | L     | 327 | GLU  | 2.3  |
| 1   | G     | 185 | PRO  | 2.3  |
| 1   | J     | 67  | ALA  | 2.3  |
| 2   | E     | 28  | GLU  | 2.3  |
| 2   | E     | 146 | GLU  | 2.3  |
| 2   | H     | 163 | GLU  | 2.3  |
| 3   | L     | 32  | ASP  | 2.3  |
| 2   | H     | 145 | ALA  | 2.3  |
| 3   | F     | 333 | GLY  | 2.3  |
| 2   | H     | 45  | GLU  | 2.3  |
| 3   | F     | 67  | PHE  | 2.2  |
| 2   | E     | 60  | SER  | 2.2  |
| 2   | H     | 53  | ALA  | 2.2  |
| 3   | F     | 39  | LEU  | 2.2  |
| 2   | E     | 112 | PRO  | 2.2  |
| 3   | L     | 310 | LEU  | 2.2  |
| 1   | A     | 196 | GLN  | 2.2  |
| 3   | F     | 52  | LEU  | 2.1  |
| 2   | E     | 51  | MET  | 2.1  |
| 2   | B     | 60  | SER  | 2.1  |
| 2   | E     | 26  | GLN  | 2.1  |
| 1   | G     | 67  | ALA  | 2.1  |
| 2   | B     | 139 | ALA  | 2.1  |
| 2   | K     | 107 | MET  | 2.1  |
| 1   | J     | 213 | ASP  | 2.1  |
| 3   | C     | 19  | GLU  | 2.1  |
| 1   | D     | 206 | THR  | 2.1  |
| 2   | E     | 133 | PRO  | 2.1  |
| 2   | B     | 146 | GLU  | 2.1  |
| 2   | K     | 156 | GLU  | 2.1  |
| 3   | I     | 281 | LEU  | 2.1  |
| 3   | F     | 146 | LEU  | 2.0  |
| 1   | D     | 137 | VAL  | 2.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 203 | VAL  | 2.0  |
| 2   | K     | 146 | GLU  | 2.0  |
| 3   | I     | 341 | ASP  | 2.0  |
| 3   | L     | 313 | ASN  | 2.0  |
| 1   | G     | 66  | THR  | 2.0  |
| 1   | J     | 206 | THR  | 2.0  |
| 2   | E     | 88  | LEU  | 2.0  |
| 2   | E     | 80  | HIS  | 2.0  |
| 2   | K     | 163 | GLU  | 2.0  |
| 1   | A     | 210 | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | MG   | D     | 2251 | 1/1   | 0.95 | 0.09 | 44,44,44,44                 | 0     |
| 4   | MG   | G     | 3251 | 1/1   | 0.96 | 0.13 | 36,36,36,36                 | 0     |
| 5   | GNP  | A     | 1250 | 32/32 | 0.96 | 0.13 | 37,37,37,37                 | 0     |
| 5   | GNP  | G     | 3250 | 32/32 | 0.96 | 0.15 | 37,37,37,37                 | 0     |
| 5   | GNP  | J     | 4250 | 32/32 | 0.97 | 0.13 | 36,36,36,36                 | 0     |
| 4   | MG   | J     | 4251 | 1/1   | 0.98 | 0.08 | 44,44,44,44                 | 0     |
| 5   | GNP  | D     | 2250 | 32/32 | 0.98 | 0.13 | 37,37,37,37                 | 0     |
| 4   | MG   | A     | 1251 | 1/1   | 0.99 | 0.07 | 29,29,29,29                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.