



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:32 am BST

PDB ID : 3QYM  
Title : Structure of p63 DNA Binding Domain in Complex with a 10 Base Pair A/T  
Rich Response Element Half Site  
Authors : Herzberg, O.; Chen, C.  
Deposited on : 2011-03-03  
Resolution : 3.20 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  |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

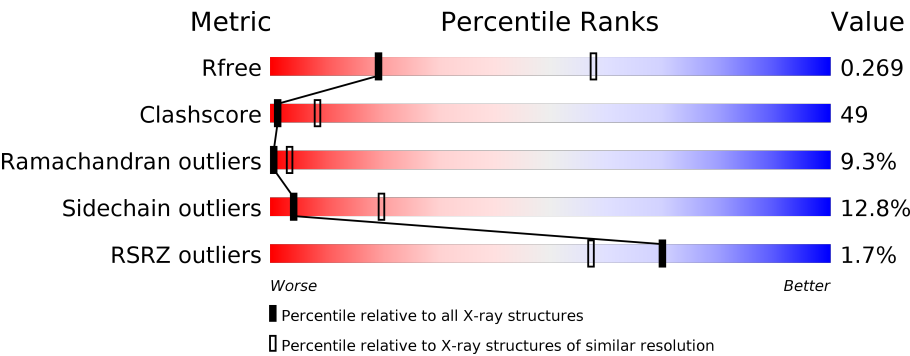
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1133 (3.20-3.20)                                      |
| Clashscore            | 141614                      | 1253 (3.20-3.20)                                      |
| Ramachandran outliers | 138981                      | 1234 (3.20-3.20)                                      |
| Sidechain outliers    | 138945                      | 1233 (3.20-3.20)                                      |
| RSRZ outliers         | 127900                      | 1095 (3.20-3.20)                                      |

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

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 203    | <div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>35%45%13%• 5%</div></div> |
| 1   | B     | 203    | <div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>34%45%14%• 6%</div></div> |
| 1   | C     | 203    | <div><div></div><div><div></div><div></div><div></div><div></div></div><div>33%49%14%• •</div></div>    |
| 1   | D     | 203    | <div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>33%49%14%• •</div></div>   |
| 1   | E     | 203    | <div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>34%46%16%• •</div></div>   |
| 1   | F     | 203    | <div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>34%47%14%• •</div></div>   |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | G     | 203    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%33%46%13%6%</div></div> |
| 1   | H     | 203    | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>%31%47%14%7%</div></div>  |
| 2   | I     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>100%</div></div>          |
| 2   | J     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>100%</div></div>          |
| 2   | K     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |
| 2   | L     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |
| 2   | M     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |
| 2   | N     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |
| 2   | O     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |
| 2   | P     | 10     | <div><div><div></div><div></div><div></div><div></div><div></div></div><div>10%90%</div></div>        |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13681 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 Tumor protein 63.

| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| 1   | A     | 192      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1497  | 937 | 266 | 282 | 12 |         |         |       |
| 1   | B     | 191      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1496  | 936 | 266 | 282 | 12 |         |         |       |
| 1   | C     | 195      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1518  | 948 | 270 | 288 | 12 |         |         |       |
| 1   | D     | 196      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1523  | 951 | 271 | 289 | 12 |         |         |       |
| 1   | E     | 197      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1534  | 957 | 275 | 290 | 12 |         |         |       |
| 1   | F     | 195      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1518  | 948 | 270 | 288 | 12 |         |         |       |
| 1   | G     | 190      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1487  | 930 | 265 | 280 | 12 |         |         |       |
| 1   | H     | 189      | Total | C   | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1484  | 930 | 264 | 278 | 12 |         |         |       |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| A     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| A     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| A     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| A     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| A     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| B     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| C     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| C     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| C     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| C     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| C     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| D     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| E     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| F     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| G     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 121     | GLY      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 122     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 123     | HIS      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 124     | MET      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 125     | ALA      | -      | EXPRESSION TAG | UNP Q9H3D4 |
| H     | 126     | SER      | -      | EXPRESSION TAG | UNP Q9H3D4 |

- Molecule 2 is a DNA chain called 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'.

| Mol | Chain | Residues | Atoms        |         |         |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|--------|---------|---------|-------|
| 2   | I     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | J     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |         |         |         |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|--------|---------|---------|-------|
| 2   | K     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | L     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | M     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | N     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | O     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |
| 2   | P     | 10       | Total<br>202 | C<br>99 | N<br>36 | O<br>58 | P<br>9 | 0       | 0       | 0     |

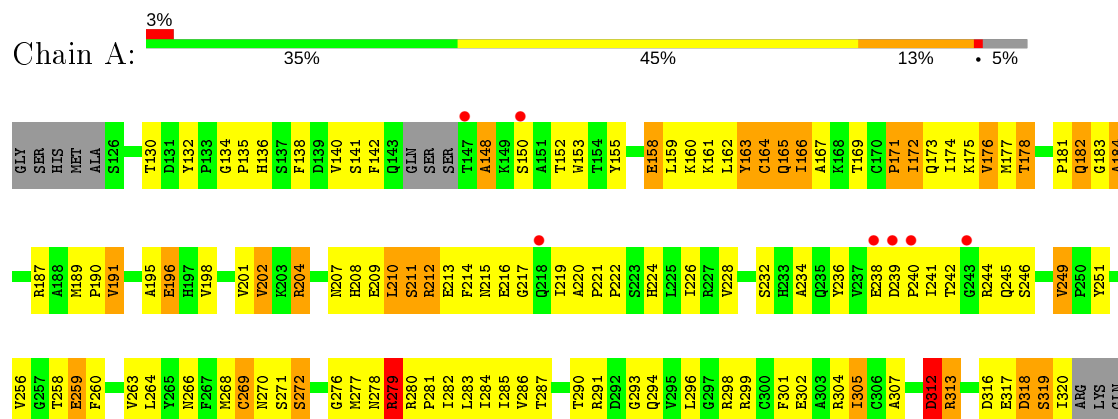
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3   | G     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | D     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | E     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | H     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | B     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | C     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | A     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |
| 3   | F     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

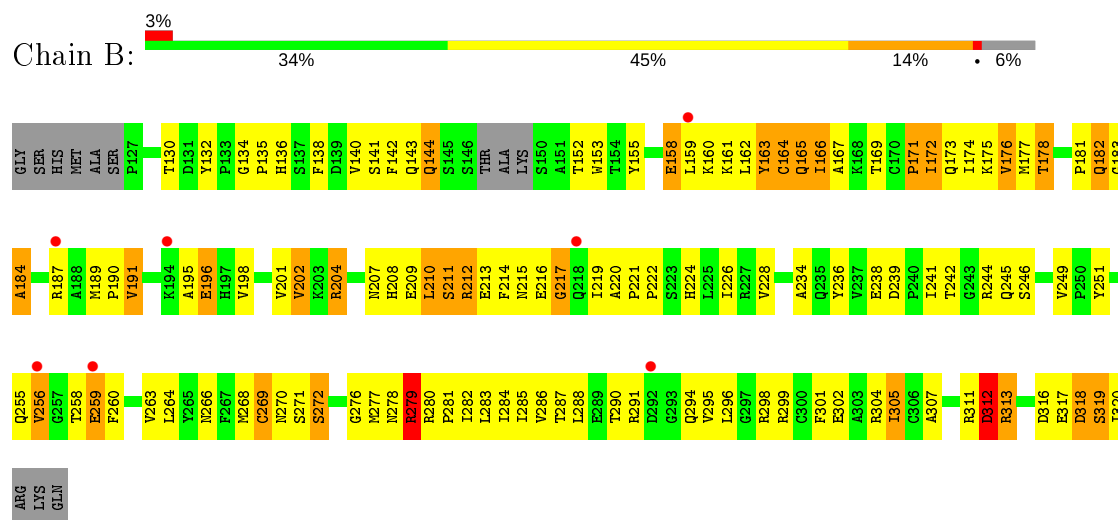
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

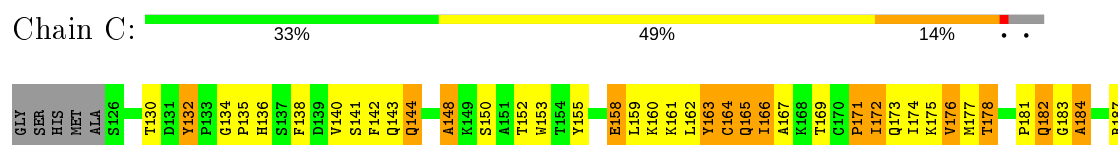
#### • Molecule 1: Tumor protein 63

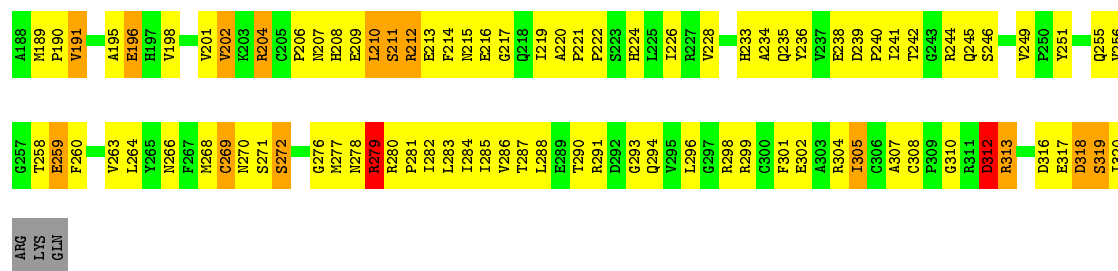


#### • Molecule 1: Tumor protein 63

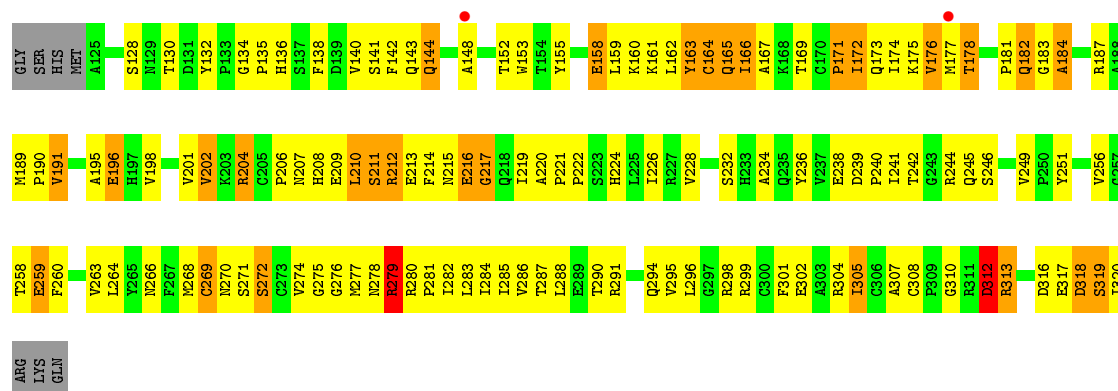


#### • Molecule 1: Tumor protein 63

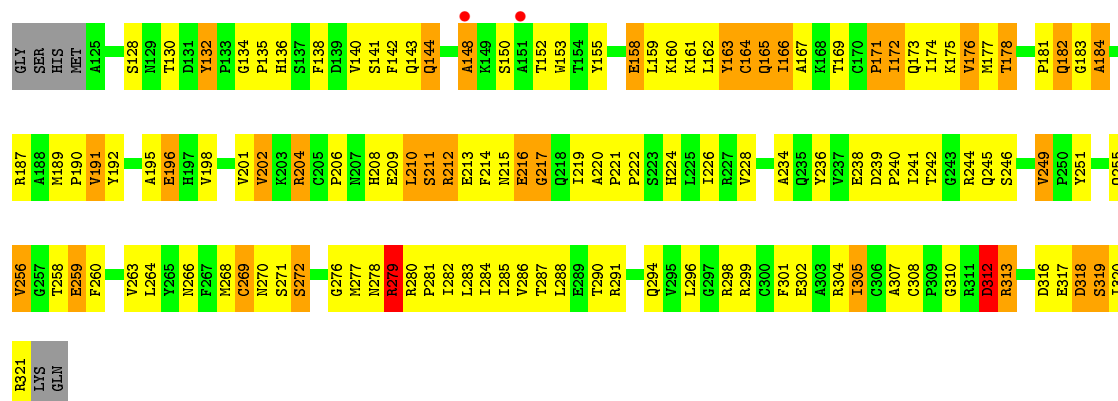




• Molecule 1: Tumor protein 63



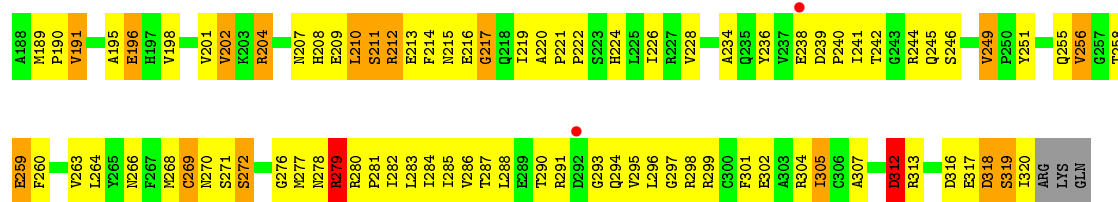
• Molecule 1: Tumor protein 63



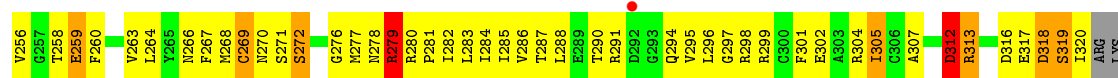
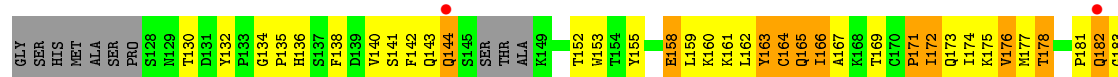
• Molecule 1: Tumor protein 63





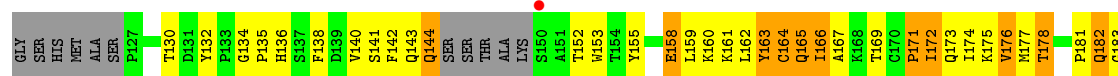


• Molecule 1: Tumor protein 63



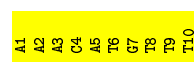
GLN

• Molecule 1: Tumor protein 63



ARG  
LYS  
GLN

• Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'



|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain K:  10% 90%

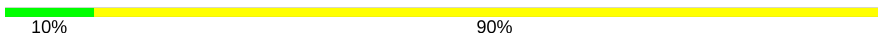
|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain L:  10% 90%

|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain M:  10% 90%

|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain N:  10% 90%

|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain O:  10% 90%

|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

- Molecule 2: 5'-D(\*AP\*AP\*AP\*CP\*AP\*TP\*GP\*TP\*TP\*T)-3'

Chain P:  10% 90%

|    |    |    |    |    |    |    |    |    |     |
|----|----|----|----|----|----|----|----|----|-----|
| A1 | A2 | A3 | C4 | A5 | T6 | C7 | T8 | T9 | T10 |
|----|----|----|----|----|----|----|----|----|-----|

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 123.87Å 180.20Å 104.38Å<br>90.00° 92.62° 90.00°             | Depositor        |
| Resolution (Å)  | 19.72 – 3.20<br>19.72 – 3.15                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 97.5 (19.72-3.20)<br>97.4 (19.72-3.15)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.14  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.41 (at 3.15Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.6.4_486)                           | Depositor        |
| R, $R_{free}$   | 0.245 , 0.271<br>0.240 , 0.269                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1917 reflections (5.00%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 82.2  | Xtriage          |
| Anisotropy  | 0.282   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 66.7   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction   | 0.085 for -h,-k,l   | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 13681   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 137.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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 [i](#)

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

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

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     | 0.38         | 0/1532  | 0.66        | 0/2082         |
| 1   | B     | 0.37         | 0/1531  | 0.65        | 1/2079 (0.0%)  |
| 1   | C     | 0.43         | 0/1554  | 0.66        | 0/2113         |
| 1   | D     | 0.40         | 0/1559  | 0.66        | 1/2120 (0.0%)  |
| 1   | E     | 0.43         | 0/1570  | 0.67        | 1/2134 (0.0%)  |
| 1   | F     | 0.40         | 0/1554  | 0.66        | 1/2113 (0.0%)  |
| 1   | G     | 0.39         | 0/1521  | 0.65        | 0/2065         |
| 1   | H     | 0.40         | 0/1519  | 0.66        | 1/2063 (0.0%)  |
| 2   | I     | 0.67         | 0/226   | 0.79        | 0/347          |
| 2   | J     | 0.74         | 0/226   | 0.78        | 0/347          |
| 2   | K     | 0.75         | 0/226   | 0.82        | 0/347          |
| 2   | L     | 0.64         | 0/226   | 0.83        | 0/347          |
| 2   | M     | 0.57         | 0/226   | 0.78        | 0/347          |
| 2   | N     | 0.57         | 0/226   | 0.80        | 0/347          |
| 2   | O     | 0.55         | 0/226   | 0.78        | 0/347          |
| 2   | P     | 0.55         | 0/226   | 0.79        | 0/347          |
| All | All   | 0.44         | 0/14148 | 0.68        | 5/19545 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 217 | GLY  | N-CA-C | -5.11 | 100.32      | 113.10   |
| 1   | H     | 217 | GLY  | N-CA-C | -5.10 | 100.36      | 113.10   |
| 1   | B     | 217 | GLY  | N-CA-C | -5.07 | 100.43      | 113.10   |
| 1   | E     | 217 | GLY  | N-CA-C | -5.07 | 100.44      | 113.10   |
| 1   | D     | 217 | GLY  | N-CA-C | -5.05 | 100.46      | 113.10   |

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     | 1497  | 0        | 1472     | 147     | 0            |
| 1   | B     | 1496  | 0        | 1473     | 143     | 0            |
| 1   | C     | 1518  | 0        | 1491     | 163     | 3            |
| 1   | D     | 1523  | 0        | 1496     | 169     | 0            |
| 1   | E     | 1534  | 0        | 1509     | 174     | 2            |
| 1   | F     | 1518  | 0        | 1491     | 154     | 0            |
| 1   | G     | 1487  | 0        | 1461     | 140     | 0            |
| 1   | H     | 1484  | 0        | 1463     | 150     | 1            |
| 2   | I     | 202   | 0        | 116      | 8       | 0            |
| 2   | J     | 202   | 0        | 116      | 20      | 0            |
| 2   | K     | 202   | 0        | 116      | 7       | 0            |
| 2   | L     | 202   | 0        | 116      | 17      | 0            |
| 2   | M     | 202   | 0        | 116      | 22      | 0            |
| 2   | N     | 202   | 0        | 116      | 8       | 0            |
| 2   | O     | 202   | 0        | 116      | 23      | 0            |
| 2   | P     | 202   | 0        | 116      | 8       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | C     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | F     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 13681 | 0        | 12784    | 1290    | 4            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (1290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:A:204:ARG:HD2 | 1:A:268:MET:HB2 | 1.34                     | 1.08              |
| 1:H:204:ARG:HD2 | 1:H:268:MET:HB2 | 1.35                     | 1.07              |
| 1:C:204:ARG:HD2 | 1:C:268:MET:HB2 | 1.35                     | 1.06              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:204:ARG:HD2  | 1:E:268:MET:HB2  | 1.35                     | 1.06              |
| 1:D:204:ARG:HD2  | 1:D:268:MET:HB2  | 1.35                     | 1.05              |
| 1:F:204:ARG:HD2  | 1:F:268:MET:HB2  | 1.34                     | 1.04              |
| 1:B:204:ARG:HD2  | 1:B:268:MET:HB2  | 1.35                     | 1.04              |
| 1:G:204:ARG:HD2  | 1:G:268:MET:HB2  | 1.35                     | 1.03              |
| 1:C:207:ASN:ND2  | 1:D:274:VAL:O    | 1.94                     | 1.00              |
| 1:C:169:THR:HG21 | 1:E:196:GLU:N    | 1.76                     | 1.00              |
| 2:L:8:DT:H2"     | 2:L:9:DT:H5"     | 1.43                     | 1.00              |
| 1:G:238:GLU:HG2  | 1:G:245:GLN:HG2  | 1.45                     | 0.99              |
| 1:D:166:ILE:HG13 | 1:D:167:ALA:H    | 1.28                     | 0.99              |
| 1:H:238:GLU:HG2  | 1:H:245:GLN:HG2  | 1.45                     | 0.98              |
| 1:B:166:ILE:HG13 | 1:B:167:ALA:H    | 1.28                     | 0.98              |
| 1:F:238:GLU:HG2  | 1:F:245:GLN:HG2  | 1.45                     | 0.98              |
| 1:B:238:GLU:HG2  | 1:B:245:GLN:HG2  | 1.45                     | 0.97              |
| 1:G:166:ILE:HG13 | 1:G:167:ALA:H    | 1.27                     | 0.97              |
| 1:G:136:HIS:HA   | 1:G:178:THR:HG23 | 1.46                     | 0.97              |
| 1:A:166:ILE:HG13 | 1:A:167:ALA:H    | 1.28                     | 0.97              |
| 1:D:238:GLU:HG2  | 1:D:245:GLN:HG2  | 1.45                     | 0.97              |
| 1:A:136:HIS:HA   | 1:A:178:THR:HG23 | 1.47                     | 0.97              |
| 1:A:238:GLU:HG2  | 1:A:245:GLN:HG2  | 1.46                     | 0.96              |
| 1:C:136:HIS:HA   | 1:C:178:THR:HG23 | 1.46                     | 0.96              |
| 2:O:8:DT:H2"     | 2:O:9:DT:H5"     | 1.45                     | 0.96              |
| 2:M:8:DT:H2"     | 2:M:9:DT:H5"     | 1.46                     | 0.96              |
| 2:J:8:DT:H2"     | 2:J:9:DT:H5"     | 1.47                     | 0.96              |
| 1:C:166:ILE:HG13 | 1:C:167:ALA:H    | 1.28                     | 0.95              |
| 1:D:136:HIS:HA   | 1:D:178:THR:HG23 | 1.48                     | 0.95              |
| 1:H:166:ILE:HG13 | 1:H:167:ALA:H    | 1.29                     | 0.95              |
| 1:F:166:ILE:HG13 | 1:F:167:ALA:H    | 1.28                     | 0.95              |
| 1:B:136:HIS:HA   | 1:B:178:THR:HG23 | 1.47                     | 0.94              |
| 1:F:136:HIS:HA   | 1:F:178:THR:HG23 | 1.47                     | 0.94              |
| 1:E:136:HIS:HA   | 1:E:178:THR:HG23 | 1.48                     | 0.94              |
| 1:H:136:HIS:HA   | 1:H:178:THR:HG23 | 1.47                     | 0.93              |
| 2:M:9:DT:H2"     | 2:M:10:DT:H5'    | 1.48                     | 0.93              |
| 2:O:9:DT:H2"     | 2:O:10:DT:H5'    | 1.49                     | 0.93              |
| 1:E:238:GLU:HG2  | 1:E:245:GLN:HG2  | 1.46                     | 0.93              |
| 2:L:9:DT:H2"     | 2:L:10:DT:H5'    | 1.48                     | 0.93              |
| 1:E:166:ILE:HG13 | 1:E:167:ALA:H    | 1.33                     | 0.93              |
| 1:C:238:GLU:HG2  | 1:C:245:GLN:HG2  | 1.46                     | 0.92              |
| 1:D:196:GLU:N    | 1:F:169:THR:HG21 | 1.85                     | 0.92              |
| 1:E:216:GLU:HG3  | 1:H:264:LEU:HD11 | 1.51                     | 0.91              |
| 1:C:255:GLN:HE21 | 1:E:128:SER:N    | 1.69                     | 0.90              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:9:DT:H2'     | 2:J:10:DT:H5'    | 1.50                     | 0.90              |
| 1:A:264:LEU:HD11 | 1:D:216:GLU:HG3  | 1.56                     | 0.88              |
| 1:D:166:ILE:HG13 | 1:D:167:ALA:N    | 1.89                     | 0.88              |
| 1:G:166:ILE:HG13 | 1:G:167:ALA:N    | 1.89                     | 0.87              |
| 1:E:166:ILE:HG13 | 1:E:167:ALA:N    | 1.90                     | 0.87              |
| 2:O:3:DA:H1'     | 2:O:4:DC:H5'     | 1.57                     | 0.87              |
| 2:L:3:DA:H1'     | 2:L:4:DC:H5'     | 1.55                     | 0.86              |
| 1:A:166:ILE:HG13 | 1:A:167:ALA:N    | 1.90                     | 0.86              |
| 2:J:3:DA:H1'     | 2:J:4:DC:H5'     | 1.57                     | 0.86              |
| 1:C:166:ILE:HG13 | 1:C:167:ALA:N    | 1.90                     | 0.86              |
| 2:M:3:DA:H1'     | 2:M:4:DC:H5'     | 1.56                     | 0.86              |
| 1:F:166:ILE:HG13 | 1:F:167:ALA:N    | 1.89                     | 0.86              |
| 1:B:166:ILE:HG13 | 1:B:167:ALA:N    | 1.91                     | 0.85              |
| 1:H:272:SER:HA   | 1:H:279:ARG:H    | 1.42                     | 0.85              |
| 1:H:166:ILE:HG13 | 1:H:167:ALA:N    | 1.90                     | 0.84              |
| 1:D:212:ARG:HA   | 1:D:212:ARG:HE   | 1.43                     | 0.84              |
| 1:C:212:ARG:HE   | 1:C:212:ARG:HA   | 1.43                     | 0.83              |
| 1:G:290:THR:HB   | 1:G:296:LEU:HD21 | 1.59                     | 0.83              |
| 1:A:290:THR:HB   | 1:A:296:LEU:HD21 | 1.60                     | 0.83              |
| 1:G:272:SER:HA   | 1:G:279:ARG:H    | 1.43                     | 0.83              |
| 1:H:212:ARG:HE   | 1:H:212:ARG:HA   | 1.42                     | 0.83              |
| 1:F:272:SER:HA   | 1:F:279:ARG:H    | 1.43                     | 0.83              |
| 1:G:212:ARG:HA   | 1:G:212:ARG:HE   | 1.43                     | 0.83              |
| 1:A:212:ARG:HA   | 1:A:212:ARG:HE   | 1.42                     | 0.83              |
| 1:D:290:THR:HB   | 1:D:296:LEU:HD21 | 1.61                     | 0.83              |
| 1:F:290:THR:HB   | 1:F:296:LEU:HD21 | 1.61                     | 0.82              |
| 1:E:290:THR:HB   | 1:E:296:LEU:HD21 | 1.59                     | 0.82              |
| 1:B:212:ARG:HA   | 1:B:212:ARG:HE   | 1.42                     | 0.82              |
| 1:D:196:GLU:CA   | 1:F:169:THR:HG21 | 2.10                     | 0.82              |
| 1:C:272:SER:HA   | 1:C:279:ARG:H    | 1.42                     | 0.82              |
| 1:E:272:SER:HA   | 1:E:279:ARG:H    | 1.44                     | 0.82              |
| 1:D:272:SER:HA   | 1:D:279:ARG:H    | 1.43                     | 0.82              |
| 1:B:290:THR:HB   | 1:B:296:LEU:HD21 | 1.59                     | 0.81              |
| 1:F:212:ARG:HA   | 1:F:212:ARG:HE   | 1.43                     | 0.81              |
| 1:B:272:SER:HA   | 1:B:279:ARG:H    | 1.45                     | 0.81              |
| 1:H:290:THR:HB   | 1:H:296:LEU:HD21 | 1.60                     | 0.81              |
| 1:C:290:THR:HB   | 1:C:296:LEU:HD21 | 1.62                     | 0.81              |
| 1:B:241:ILE:HG23 | 1:B:242:THR:HG23 | 1.63                     | 0.81              |
| 1:D:241:ILE:HG23 | 1:D:242:THR:HG23 | 1.62                     | 0.81              |
| 1:F:241:ILE:HG23 | 1:F:242:THR:HG23 | 1.63                     | 0.81              |
| 1:A:272:SER:HA   | 1:A:279:ARG:H    | 1.44                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:241:ILE:HG23 | 1:H:242:THR:HG23 | 1.63                     | 0.80              |
| 1:E:212:ARG:HE   | 1:E:212:ARG:HA   | 1.44                     | 0.80              |
| 1:E:269:CYS:C    | 1:E:305:ILE:HD11 | 2.02                     | 0.80              |
| 1:C:269:CYS:C    | 1:C:305:ILE:HD11 | 2.02                     | 0.80              |
| 1:G:241:ILE:HG23 | 1:G:242:THR:HG23 | 1.63                     | 0.80              |
| 1:E:241:ILE:HG23 | 1:E:242:THR:HG23 | 1.62                     | 0.80              |
| 1:A:241:ILE:HG23 | 1:A:242:THR:HG23 | 1.63                     | 0.79              |
| 1:C:241:ILE:HG23 | 1:C:242:THR:HG23 | 1.62                     | 0.79              |
| 1:F:269:CYS:C    | 1:F:305:ILE:HD11 | 2.03                     | 0.79              |
| 1:C:206:PRO:HB2  | 1:D:207:ASN:ND2  | 1.96                     | 0.79              |
| 1:A:172:ILE:HG22 | 1:A:263:VAL:O    | 1.83                     | 0.79              |
| 1:F:172:ILE:HG22 | 1:F:263:VAL:O    | 1.83                     | 0.79              |
| 1:A:269:CYS:C    | 1:A:305:ILE:HD11 | 2.04                     | 0.78              |
| 1:E:172:ILE:HG22 | 1:E:263:VAL:O    | 1.83                     | 0.78              |
| 1:D:172:ILE:HG22 | 1:D:263:VAL:O    | 1.84                     | 0.78              |
| 1:H:172:ILE:HG22 | 1:H:263:VAL:O    | 1.84                     | 0.78              |
| 1:H:269:CYS:C    | 1:H:305:ILE:HD11 | 2.04                     | 0.78              |
| 1:G:269:CYS:C    | 1:G:305:ILE:HD11 | 2.03                     | 0.78              |
| 1:B:269:CYS:C    | 1:B:305:ILE:HD11 | 2.03                     | 0.77              |
| 1:B:172:ILE:HG22 | 1:B:263:VAL:O    | 1.84                     | 0.77              |
| 1:D:269:CYS:C    | 1:D:305:ILE:HD11 | 2.05                     | 0.77              |
| 1:G:172:ILE:HG22 | 1:G:263:VAL:O    | 1.84                     | 0.77              |
| 1:F:226:ILE:HD11 | 1:F:284:ILE:HD12 | 1.67                     | 0.76              |
| 1:A:264:LEU:HD11 | 1:D:216:GLU:CB   | 2.15                     | 0.76              |
| 1:C:172:ILE:HG22 | 1:C:263:VAL:O    | 1.84                     | 0.76              |
| 1:D:226:ILE:HD11 | 1:D:284:ILE:HD12 | 1.67                     | 0.76              |
| 1:E:226:ILE:HD11 | 1:E:284:ILE:HD12 | 1.68                     | 0.76              |
| 1:D:196:GLU:HB3  | 1:F:169:THR:HG22 | 1.66                     | 0.75              |
| 1:A:264:LEU:HD11 | 1:D:216:GLU:CG   | 2.16                     | 0.75              |
| 1:A:207:ASN:OD1  | 1:B:207:ASN:ND2  | 2.18                     | 0.75              |
| 1:G:204:ARG:HD2  | 1:G:268:MET:CB   | 2.16                     | 0.75              |
| 2:L:8:DT:H2''    | 2:L:9:DT:C5'     | 2.14                     | 0.75              |
| 1:H:226:ILE:HD11 | 1:H:284:ILE:HD12 | 1.68                     | 0.75              |
| 2:L:1:DA:HO5'    | 2:L:1:DA:H8      | 1.35                     | 0.75              |
| 1:C:255:GLN:NE2  | 1:E:128:SER:N    | 2.35                     | 0.74              |
| 1:F:204:ARG:HD2  | 1:F:268:MET:CB   | 2.16                     | 0.74              |
| 1:G:226:ILE:HD11 | 1:G:284:ILE:HD12 | 1.68                     | 0.74              |
| 2:O:8:DT:H2''    | 2:O:9:DT:C5'     | 2.16                     | 0.74              |
| 1:A:204:ARG:HD2  | 1:A:268:MET:CB   | 2.14                     | 0.74              |
| 1:B:226:ILE:HD11 | 1:B:284:ILE:HD12 | 1.67                     | 0.74              |
| 1:D:204:ARG:HD2  | 1:D:268:MET:CB   | 2.15                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:320:ILE:HG13 | 1:E:321:ARG:N    | 2.01                     | 0.74              |
| 2:M:8:DT:H2''    | 2:M:9:DT:C5'     | 2.16                     | 0.74              |
| 2:J:8:DT:H2''    | 2:J:9:DT:C5'     | 2.16                     | 0.74              |
| 1:H:239:ASP:OD1  | 1:H:241:ILE:HG22 | 1.88                     | 0.74              |
| 1:E:216:GLU:CG   | 1:H:264:LEU:HD11 | 2.18                     | 0.73              |
| 1:A:226:ILE:HD11 | 1:A:284:ILE:HD12 | 1.69                     | 0.73              |
| 1:B:204:ARG:HD2  | 1:B:268:MET:CB   | 2.16                     | 0.73              |
| 1:C:204:ARG:HD2  | 1:C:268:MET:CB   | 2.16                     | 0.73              |
| 1:E:204:ARG:HD2  | 1:E:268:MET:CB   | 2.16                     | 0.73              |
| 1:E:317:GLU:O    | 1:E:320:ILE:HG12 | 1.87                     | 0.73              |
| 1:D:239:ASP:OD1  | 1:D:241:ILE:HG22 | 1.89                     | 0.72              |
| 1:F:183:GLY:HA2  | 1:F:291:ARG:HH21 | 1.54                     | 0.72              |
| 2:M:10:DT:H2'    | 2:O:1:DA:O4'     | 1.89                     | 0.72              |
| 1:A:239:ASP:OD1  | 1:A:241:ILE:HG22 | 1.88                     | 0.72              |
| 1:B:183:GLY:HA2  | 1:B:291:ARG:HH21 | 1.54                     | 0.72              |
| 1:F:239:ASP:OD1  | 1:F:241:ILE:HG22 | 1.89                     | 0.72              |
| 1:D:183:GLY:HA2  | 1:D:291:ARG:HH21 | 1.55                     | 0.72              |
| 1:B:239:ASP:OD1  | 1:B:241:ILE:HG22 | 1.89                     | 0.72              |
| 1:C:183:GLY:HA2  | 1:C:291:ARG:HH21 | 1.53                     | 0.72              |
| 1:A:183:GLY:HA2  | 1:A:291:ARG:HH21 | 1.54                     | 0.72              |
| 1:H:183:GLY:HA2  | 1:H:291:ARG:HH21 | 1.55                     | 0.72              |
| 1:C:255:GLN:HB3  | 1:E:128:SER:HB2  | 1.70                     | 0.72              |
| 1:G:239:ASP:OD1  | 1:G:241:ILE:HG22 | 1.89                     | 0.72              |
| 1:G:183:GLY:HA2  | 1:G:291:ARG:HH21 | 1.55                     | 0.72              |
| 1:C:169:THR:HG21 | 1:E:196:GLU:H    | 1.52                     | 0.71              |
| 1:C:169:THR:CG2  | 1:E:196:GLU:HB3  | 2.21                     | 0.71              |
| 1:E:183:GLY:HA2  | 1:E:291:ARG:HH21 | 1.55                     | 0.71              |
| 2:O:8:DT:C2'     | 2:O:9:DT:H5''    | 2.21                     | 0.71              |
| 2:L:9:DT:C2'     | 2:L:10:DT:H5'    | 2.21                     | 0.71              |
| 1:C:226:ILE:HD11 | 1:C:284:ILE:HD12 | 1.71                     | 0.71              |
| 1:E:239:ASP:OD1  | 1:E:241:ILE:HG22 | 1.91                     | 0.71              |
| 1:D:169:THR:HA   | 1:D:266:ASN:ND2  | 2.06                     | 0.70              |
| 2:M:1:DA:HO5'    | 2:M:1:DA:H8      | 1.39                     | 0.70              |
| 1:H:317:GLU:O    | 1:H:320:ILE:HG12 | 1.91                     | 0.70              |
| 1:C:239:ASP:OD1  | 1:C:241:ILE:HG22 | 1.90                     | 0.70              |
| 1:C:258:THR:HG22 | 1:C:259:GLU:H    | 1.57                     | 0.70              |
| 1:C:317:GLU:O    | 1:C:320:ILE:HG12 | 1.91                     | 0.70              |
| 1:H:204:ARG:HD2  | 1:H:268:MET:CB   | 2.16                     | 0.70              |
| 1:C:169:THR:HG21 | 1:E:196:GLU:CA   | 2.22                     | 0.70              |
| 1:E:234:ALA:HB2  | 1:E:249:VAL:HG12 | 1.74                     | 0.70              |
| 2:L:8:DT:C2'     | 2:L:9:DT:H5''    | 2.20                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:5:DA:H2''    | 2:N:6:DT:H5'     | 1.73                     | 0.70              |
| 1:A:290:THR:HG22 | 1:A:294:GLN:O    | 1.92                     | 0.70              |
| 2:K:5:DA:H2''    | 2:K:6:DT:H5'     | 1.74                     | 0.70              |
| 2:J:8:DT:C2'     | 2:J:9:DT:H5''    | 2.22                     | 0.69              |
| 2:P:5:DA:H2''    | 2:P:6:DT:H5'     | 1.74                     | 0.69              |
| 1:G:169:THR:HA   | 1:G:266:ASN:ND2  | 2.07                     | 0.69              |
| 1:G:207:ASN:ND2  | 1:H:207:ASN:OD1  | 2.25                     | 0.69              |
| 1:G:290:THR:HG22 | 1:G:294:GLN:O    | 1.92                     | 0.69              |
| 1:H:169:THR:HA   | 1:H:266:ASN:ND2  | 2.07                     | 0.69              |
| 2:I:5:DA:H2''    | 2:I:6:DT:H5'     | 1.74                     | 0.69              |
| 1:C:169:THR:HA   | 1:C:266:ASN:ND2  | 2.07                     | 0.69              |
| 1:F:290:THR:HG22 | 1:F:294:GLN:O    | 1.92                     | 0.69              |
| 1:F:158:GLU:CD   | 1:F:159:LEU:H    | 1.96                     | 0.69              |
| 1:H:290:THR:HG22 | 1:H:294:GLN:O    | 1.92                     | 0.69              |
| 2:M:9:DT:C2'     | 2:M:10:DT:H5'    | 2.21                     | 0.69              |
| 2:O:9:DT:C2'     | 2:O:10:DT:H5'    | 2.22                     | 0.69              |
| 1:E:169:THR:HA   | 1:E:266:ASN:ND2  | 2.07                     | 0.69              |
| 1:A:169:THR:HA   | 1:A:266:ASN:ND2  | 2.08                     | 0.69              |
| 1:B:234:ALA:HB2  | 1:B:249:VAL:HG12 | 1.75                     | 0.69              |
| 1:D:290:THR:HG22 | 1:D:294:GLN:O    | 1.93                     | 0.68              |
| 1:G:234:ALA:HB2  | 1:G:249:VAL:HG12 | 1.75                     | 0.68              |
| 1:G:258:THR:HG22 | 1:G:259:GLU:H    | 1.58                     | 0.68              |
| 1:B:290:THR:HG22 | 1:B:294:GLN:O    | 1.93                     | 0.68              |
| 1:F:317:GLU:O    | 1:F:320:ILE:HG12 | 1.93                     | 0.68              |
| 1:A:158:GLU:CD   | 1:A:159:LEU:H    | 1.96                     | 0.68              |
| 1:D:317:GLU:O    | 1:D:320:ILE:HG12 | 1.94                     | 0.68              |
| 1:C:290:THR:HG22 | 1:C:294:GLN:O    | 1.92                     | 0.68              |
| 1:F:258:THR:HG22 | 1:F:259:GLU:H    | 1.57                     | 0.68              |
| 1:G:158:GLU:CD   | 1:G:159:LEU:H    | 1.97                     | 0.68              |
| 1:A:190:PRO:HG2  | 1:A:202:VAL:CG2  | 2.24                     | 0.68              |
| 1:D:234:ALA:HB2  | 1:D:249:VAL:HG12 | 1.75                     | 0.68              |
| 1:F:169:THR:HA   | 1:F:266:ASN:ND2  | 2.08                     | 0.68              |
| 1:F:234:ALA:HB2  | 1:F:249:VAL:HG12 | 1.75                     | 0.68              |
| 2:M:5:DA:H2''    | 2:M:6:DT:H5'     | 1.74                     | 0.68              |
| 1:B:169:THR:HA   | 1:B:266:ASN:ND2  | 2.08                     | 0.68              |
| 2:O:5:DA:H2''    | 2:O:6:DT:H5'     | 1.75                     | 0.68              |
| 1:A:153:TRP:HB3  | 1:A:164:CYS:HB2  | 1.76                     | 0.68              |
| 1:E:190:PRO:HG2  | 1:E:202:VAL:CG2  | 2.24                     | 0.68              |
| 1:A:317:GLU:O    | 1:A:320:ILE:HG12 | 1.94                     | 0.68              |
| 1:E:258:THR:HG22 | 1:E:259:GLU:H    | 1.59                     | 0.68              |
| 1:E:290:THR:HG22 | 1:E:294:GLN:O    | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:234:ALA:HB2  | 1:C:249:VAL:HG12 | 1.76                     | 0.68              |
| 2:L:5:DA:H2"     | 2:L:6:DT:H5'     | 1.75                     | 0.68              |
| 1:D:196:GLU:HA   | 1:F:169:THR:HG21 | 1.75                     | 0.67              |
| 2:M:8:DT:C2'     | 2:M:9:DT:H5"     | 2.22                     | 0.67              |
| 1:A:258:THR:HG22 | 1:A:259:GLU:H    | 1.59                     | 0.67              |
| 1:H:158:GLU:CD   | 1:H:159:LEU:H    | 1.97                     | 0.67              |
| 2:J:5:DA:H2"     | 2:J:6:DT:H5'     | 1.75                     | 0.67              |
| 1:B:258:THR:HG22 | 1:B:259:GLU:H    | 1.59                     | 0.67              |
| 1:D:190:PRO:HG2  | 1:D:202:VAL:CG2  | 2.24                     | 0.67              |
| 2:J:9:DT:C2'     | 2:J:10:DT:H5'    | 2.22                     | 0.67              |
| 1:H:258:THR:HG22 | 1:H:259:GLU:H    | 1.58                     | 0.67              |
| 1:C:158:GLU:CD   | 1:C:159:LEU:H    | 1.98                     | 0.66              |
| 1:D:158:GLU:CD   | 1:D:159:LEU:H    | 1.98                     | 0.66              |
| 1:F:190:PRO:HG2  | 1:F:202:VAL:CG2  | 2.25                     | 0.66              |
| 1:H:234:ALA:HB2  | 1:H:249:VAL:HG12 | 1.75                     | 0.66              |
| 1:E:158:GLU:CD   | 1:E:159:LEU:H    | 1.97                     | 0.66              |
| 1:A:234:ALA:HB2  | 1:A:249:VAL:HG12 | 1.76                     | 0.66              |
| 1:C:190:PRO:HG2  | 1:C:202:VAL:CG2  | 2.26                     | 0.66              |
| 1:A:204:ARG:NH1  | 1:A:208:HIS:HB3  | 2.11                     | 0.66              |
| 1:G:317:GLU:O    | 1:G:320:ILE:HG12 | 1.95                     | 0.66              |
| 1:H:190:PRO:HG2  | 1:H:202:VAL:CG2  | 2.26                     | 0.66              |
| 1:B:190:PRO:HG2  | 1:B:202:VAL:CG2  | 2.26                     | 0.66              |
| 1:B:158:GLU:CD   | 1:B:159:LEU:H    | 1.99                     | 0.66              |
| 1:H:204:ARG:NH1  | 1:H:208:HIS:HB3  | 2.11                     | 0.66              |
| 1:B:317:GLU:O    | 1:B:320:ILE:HG12 | 1.96                     | 0.66              |
| 1:D:204:ARG:NH1  | 1:D:208:HIS:HB3  | 2.11                     | 0.66              |
| 1:G:140:VAL:HG11 | 1:G:286:VAL:HG21 | 1.78                     | 0.66              |
| 1:C:204:ARG:NH1  | 1:C:208:HIS:HB3  | 2.11                     | 0.65              |
| 1:D:171:PRO:O    | 1:D:172:ILE:HB   | 1.96                     | 0.65              |
| 1:E:216:GLU:CB   | 1:H:264:LEU:HD11 | 2.27                     | 0.65              |
| 1:A:171:PRO:O    | 1:A:172:ILE:HB   | 1.97                     | 0.65              |
| 1:F:171:PRO:O    | 1:F:172:ILE:HB   | 1.94                     | 0.65              |
| 1:G:204:ARG:NH1  | 1:G:208:HIS:HB3  | 2.11                     | 0.65              |
| 1:B:153:TRP:HB3  | 1:B:164:CYS:HB2  | 1.79                     | 0.65              |
| 1:B:204:ARG:NH1  | 1:B:208:HIS:HB3  | 2.12                     | 0.65              |
| 1:D:258:THR:HG22 | 1:D:259:GLU:H    | 1.60                     | 0.65              |
| 1:H:140:VAL:HG11 | 1:H:286:VAL:HG21 | 1.78                     | 0.65              |
| 1:E:171:PRO:O    | 1:E:172:ILE:HB   | 1.97                     | 0.65              |
| 1:G:153:TRP:HB3  | 1:G:164:CYS:HB2  | 1.77                     | 0.65              |
| 1:H:153:TRP:HB3  | 1:H:164:CYS:HB2  | 1.77                     | 0.65              |
| 1:C:153:TRP:HB3  | 1:C:164:CYS:HB2  | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:140:VAL:HG11 | 1:C:286:VAL:HG21 | 1.78                     | 0.64              |
| 1:F:204:ARG:NH1  | 1:F:208:HIS:HB3  | 2.12                     | 0.64              |
| 1:D:169:THR:HA   | 1:D:266:ASN:HD21 | 1.61                     | 0.64              |
| 1:E:153:TRP:HB3  | 1:E:164:CYS:HB2  | 1.80                     | 0.64              |
| 1:G:169:THR:HA   | 1:G:266:ASN:HD21 | 1.62                     | 0.64              |
| 1:H:171:PRO:O    | 1:H:172:ILE:HB   | 1.96                     | 0.64              |
| 1:F:140:VAL:HG11 | 1:F:286:VAL:HG21 | 1.78                     | 0.64              |
| 1:G:190:PRO:HG2  | 1:G:202:VAL:CG2  | 2.27                     | 0.64              |
| 1:B:171:PRO:O    | 1:B:172:ILE:HB   | 1.97                     | 0.64              |
| 1:G:171:PRO:O    | 1:G:172:ILE:HB   | 1.97                     | 0.64              |
| 1:D:140:VAL:HG11 | 1:D:286:VAL:HG21 | 1.79                     | 0.64              |
| 1:E:169:THR:HA   | 1:E:266:ASN:HD21 | 1.63                     | 0.64              |
| 1:D:153:TRP:HB3  | 1:D:164:CYS:HB2  | 1.80                     | 0.63              |
| 1:F:153:TRP:HB3  | 1:F:164:CYS:HB2  | 1.79                     | 0.63              |
| 1:B:140:VAL:HG11 | 1:B:286:VAL:HG21 | 1.78                     | 0.63              |
| 1:C:171:PRO:O    | 1:C:172:ILE:HB   | 1.97                     | 0.63              |
| 1:D:152:THR:HG23 | 1:D:153:TRP:HD1  | 1.64                     | 0.63              |
| 1:D:166:ILE:CG1  | 1:D:167:ALA:N    | 2.60                     | 0.63              |
| 1:F:169:THR:HA   | 1:F:266:ASN:HD21 | 1.64                     | 0.63              |
| 1:E:140:VAL:HG11 | 1:E:286:VAL:HG21 | 1.80                     | 0.63              |
| 1:E:152:THR:HG23 | 1:E:153:TRP:HD1  | 1.63                     | 0.63              |
| 1:E:204:ARG:NH1  | 1:E:208:HIS:HB3  | 2.12                     | 0.63              |
| 1:A:264:LEU:CD1  | 1:D:216:GLU:HB2  | 2.29                     | 0.63              |
| 1:A:140:VAL:HG11 | 1:A:286:VAL:HG21 | 1.79                     | 0.63              |
| 1:B:169:THR:HA   | 1:B:266:ASN:HD21 | 1.64                     | 0.63              |
| 1:B:209:GLU:O    | 1:B:209:GLU:HG3  | 1.99                     | 0.63              |
| 1:D:190:PRO:HG2  | 1:D:202:VAL:HG21 | 1.80                     | 0.63              |
| 1:F:290:THR:HG21 | 1:F:294:GLN:HG2  | 1.81                     | 0.63              |
| 1:A:204:ARG:HD3  | 1:A:224:HIS:O    | 1.99                     | 0.62              |
| 1:C:169:THR:HA   | 1:C:266:ASN:HD21 | 1.62                     | 0.62              |
| 1:G:204:ARG:HD3  | 1:G:224:HIS:O    | 2.00                     | 0.62              |
| 1:F:204:ARG:HD3  | 1:F:224:HIS:O    | 1.99                     | 0.62              |
| 1:H:169:THR:HA   | 1:H:266:ASN:HD21 | 1.63                     | 0.62              |
| 1:A:190:PRO:HG2  | 1:A:202:VAL:HG21 | 1.81                     | 0.62              |
| 1:D:204:ARG:HD3  | 1:D:224:HIS:O    | 1.99                     | 0.62              |
| 1:E:152:THR:HG23 | 1:E:153:TRP:CD1  | 2.35                     | 0.62              |
| 1:B:290:THR:HG21 | 1:B:294:GLN:HG2  | 1.82                     | 0.62              |
| 1:A:290:THR:HG21 | 1:A:294:GLN:HG2  | 1.82                     | 0.62              |
| 1:B:204:ARG:HD3  | 1:B:224:HIS:O    | 2.00                     | 0.62              |
| 1:E:209:GLU:O    | 1:E:209:GLU:HG3  | 1.99                     | 0.62              |
| 1:G:290:THR:HG21 | 1:G:294:GLN:HG2  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:172:ILE:HG23 | 1:C:172:ILE:O    | 1.99                     | 0.62              |
| 1:D:209:GLU:O    | 1:D:209:GLU:HG3  | 1.99                     | 0.62              |
| 1:A:166:ILE:CG1  | 1:A:167:ALA:H    | 2.01                     | 0.62              |
| 1:H:290:THR:HG21 | 1:H:294:GLN:HG2  | 1.82                     | 0.62              |
| 1:D:152:THR:HG23 | 1:D:153:TRP:CD1  | 2.35                     | 0.61              |
| 1:C:204:ARG:HD3  | 1:C:224:HIS:O    | 1.99                     | 0.61              |
| 1:F:190:PRO:HG2  | 1:F:202:VAL:HG21 | 1.82                     | 0.61              |
| 1:G:132:TYR:CE2  | 1:G:134:GLY:HA2  | 2.35                     | 0.61              |
| 1:C:152:THR:HG23 | 1:C:153:TRP:HD1  | 1.66                     | 0.61              |
| 1:C:204:ARG:HH21 | 1:C:215:ASN:HD21 | 1.48                     | 0.61              |
| 1:E:290:THR:HG21 | 1:E:294:GLN:HG2  | 1.82                     | 0.61              |
| 2:O:1:DA:H8      | 2:O:1:DA:HO5'    | 1.48                     | 0.61              |
| 1:A:172:ILE:O    | 1:A:172:ILE:HG23 | 2.00                     | 0.61              |
| 1:B:172:ILE:HG23 | 1:B:172:ILE:O    | 2.00                     | 0.61              |
| 1:C:255:GLN:HB3  | 1:E:128:SER:CB   | 2.31                     | 0.61              |
| 1:G:172:ILE:O    | 1:G:172:ILE:HG23 | 1.99                     | 0.61              |
| 1:B:132:TYR:CE2  | 1:B:134:GLY:HA2  | 2.36                     | 0.61              |
| 1:F:132:TYR:CE2  | 1:F:134:GLY:HA2  | 2.35                     | 0.61              |
| 1:H:204:ARG:HD3  | 1:H:224:HIS:O    | 2.00                     | 0.61              |
| 1:D:172:ILE:HG23 | 1:D:172:ILE:O    | 2.01                     | 0.61              |
| 1:G:209:GLU:HG3  | 1:G:209:GLU:O    | 2.00                     | 0.61              |
| 1:H:209:GLU:O    | 1:H:209:GLU:HG3  | 2.00                     | 0.61              |
| 1:B:152:THR:HG23 | 1:B:153:TRP:HD1  | 1.65                     | 0.61              |
| 1:C:290:THR:HG21 | 1:C:294:GLN:HG2  | 1.82                     | 0.61              |
| 1:E:320:ILE:HD11 | 1:E:321:ARG:NH1  | 2.16                     | 0.61              |
| 1:G:204:ARG:HH21 | 1:G:215:ASN:HD21 | 1.49                     | 0.61              |
| 1:H:132:TYR:CE2  | 1:H:134:GLY:HA2  | 2.35                     | 0.61              |
| 1:A:132:TYR:CE2  | 1:A:134:GLY:HA2  | 2.36                     | 0.60              |
| 1:A:169:THR:HA   | 1:A:266:ASN:HD21 | 1.64                     | 0.60              |
| 1:E:204:ARG:HD3  | 1:E:224:HIS:O    | 2.00                     | 0.60              |
| 1:B:152:THR:HG23 | 1:B:153:TRP:CD1  | 2.36                     | 0.60              |
| 1:D:132:TYR:CE2  | 1:D:134:GLY:HA2  | 2.36                     | 0.60              |
| 1:H:190:PRO:HG2  | 1:H:202:VAL:HG21 | 1.83                     | 0.60              |
| 1:E:132:TYR:CE2  | 1:E:134:GLY:HA2  | 2.36                     | 0.60              |
| 1:F:152:THR:HG23 | 1:F:153:TRP:HD1  | 1.66                     | 0.60              |
| 1:A:204:ARG:HH21 | 1:A:215:ASN:HD21 | 1.49                     | 0.60              |
| 1:C:152:THR:HG23 | 1:C:153:TRP:CD1  | 2.37                     | 0.60              |
| 1:D:290:THR:HG21 | 1:D:294:GLN:HG2  | 1.82                     | 0.60              |
| 1:C:132:TYR:CE2  | 1:C:134:GLY:HA2  | 2.36                     | 0.60              |
| 1:D:196:GLU:CA   | 1:F:169:THR:CG2  | 2.79                     | 0.60              |
| 1:B:190:PRO:HG2  | 1:B:202:VAL:HG21 | 1.83                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:190:PRO:HG2  | 1:C:202:VAL:HG21 | 1.82                     | 0.60              |
| 1:C:209:GLU:HG3  | 1:C:209:GLU:O    | 2.00                     | 0.60              |
| 1:E:166:ILE:HG23 | 1:E:167:ALA:N    | 2.15                     | 0.60              |
| 1:F:172:ILE:O    | 1:F:172:ILE:HG23 | 2.01                     | 0.60              |
| 1:F:258:THR:HG22 | 1:F:259:GLU:N    | 2.17                     | 0.60              |
| 1:H:173:GLN:HB3  | 1:H:260:PHE:CG   | 2.37                     | 0.60              |
| 1:B:173:GLN:HB3  | 1:B:260:PHE:CG   | 2.37                     | 0.60              |
| 1:F:209:GLU:O    | 1:F:209:GLU:HG3  | 2.01                     | 0.60              |
| 1:A:152:THR:HG23 | 1:A:153:TRP:HD1  | 1.67                     | 0.60              |
| 1:C:278:ASN:N    | 1:C:278:ASN:HD22 | 2.00                     | 0.60              |
| 1:E:190:PRO:HG2  | 1:E:202:VAL:HG21 | 1.82                     | 0.60              |
| 1:F:173:GLN:HB3  | 1:F:260:PHE:CG   | 2.37                     | 0.60              |
| 1:H:166:ILE:CG1  | 1:H:167:ALA:N    | 2.61                     | 0.60              |
| 1:H:172:ILE:HG23 | 1:H:172:ILE:O    | 2.01                     | 0.59              |
| 1:E:172:ILE:HG23 | 1:E:172:ILE:O    | 2.01                     | 0.59              |
| 1:F:204:ARG:HH21 | 1:F:215:ASN:HD21 | 1.49                     | 0.59              |
| 1:H:152:THR:HG23 | 1:H:153:TRP:CD1  | 2.37                     | 0.59              |
| 1:C:312:ASP:O    | 1:C:316:ASP:HB2  | 2.02                     | 0.59              |
| 1:F:152:THR:HG23 | 1:F:153:TRP:CD1  | 2.38                     | 0.59              |
| 1:A:173:GLN:HB3  | 1:A:260:PHE:CG   | 2.37                     | 0.59              |
| 1:D:173:GLN:HB3  | 1:D:260:PHE:CG   | 2.37                     | 0.59              |
| 1:E:204:ARG:HH21 | 1:E:215:ASN:HD21 | 1.48                     | 0.59              |
| 1:G:173:GLN:HB3  | 1:G:260:PHE:CG   | 2.37                     | 0.59              |
| 1:H:204:ARG:HH21 | 1:H:215:ASN:HD21 | 1.49                     | 0.59              |
| 1:C:173:GLN:HB3  | 1:C:260:PHE:CG   | 2.37                     | 0.59              |
| 1:C:258:THR:HG22 | 1:C:259:GLU:N    | 2.16                     | 0.59              |
| 1:H:152:THR:HG23 | 1:H:153:TRP:HD1  | 1.67                     | 0.59              |
| 1:A:209:GLU:O    | 1:A:209:GLU:HG3  | 2.00                     | 0.59              |
| 1:C:169:THR:HG22 | 1:E:196:GLU:CD   | 2.23                     | 0.59              |
| 1:E:173:GLN:HB3  | 1:E:260:PHE:CG   | 2.37                     | 0.59              |
| 1:F:312:ASP:O    | 1:F:316:ASP:HB2  | 2.02                     | 0.59              |
| 2:J:1:DA:HO5'    | 2:J:1:DA:H8      | 1.51                     | 0.59              |
| 1:G:152:THR:HG23 | 1:G:153:TRP:HD1  | 1.66                     | 0.59              |
| 1:A:258:THR:HG22 | 1:A:259:GLU:N    | 2.18                     | 0.59              |
| 1:E:189:MET:HE3  | 1:E:246:SER:HB2  | 1.85                     | 0.59              |
| 1:A:152:THR:HG23 | 1:A:153:TRP:CD1  | 2.37                     | 0.58              |
| 1:B:312:ASP:O    | 1:B:316:ASP:HB2  | 2.02                     | 0.58              |
| 1:F:166:ILE:HG23 | 1:F:167:ALA:N    | 2.18                     | 0.58              |
| 1:G:166:ILE:HG23 | 1:G:167:ALA:N    | 2.18                     | 0.58              |
| 1:B:204:ARG:HH21 | 1:B:215:ASN:HD21 | 1.50                     | 0.58              |
| 1:C:169:THR:HG22 | 1:E:196:GLU:HB3  | 1.84                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:152:THR:HA   | 1:C:165:GLN:OE1  | 2.03                     | 0.58              |
| 1:C:278:ASN:H    | 1:C:278:ASN:HD22 | 1.51                     | 0.58              |
| 1:D:196:GLU:HB3  | 1:F:169:THR:CG2  | 2.34                     | 0.58              |
| 1:G:152:THR:HG23 | 1:G:153:TRP:CD1  | 2.37                     | 0.58              |
| 1:H:130:THR:O    | 1:H:298:ARG:NH1  | 2.36                     | 0.58              |
| 1:C:130:THR:O    | 1:C:298:ARG:NH1  | 2.36                     | 0.58              |
| 1:C:166:ILE:HG23 | 1:C:167:ALA:N    | 2.18                     | 0.58              |
| 1:H:258:THR:HG22 | 1:H:259:GLU:N    | 2.18                     | 0.58              |
| 1:E:130:THR:O    | 1:E:298:ARG:NH1  | 2.37                     | 0.58              |
| 1:E:163:TYR:O    | 1:E:164:CYS:HB3  | 2.03                     | 0.58              |
| 1:H:312:ASP:O    | 1:H:316:ASP:HB2  | 2.04                     | 0.58              |
| 1:E:312:ASP:O    | 1:E:316:ASP:HB2  | 2.03                     | 0.57              |
| 1:D:204:ARG:HH21 | 1:D:215:ASN:HD21 | 1.50                     | 0.57              |
| 1:E:269:CYS:O    | 1:E:305:ILE:HD11 | 2.05                     | 0.57              |
| 1:F:163:TYR:CD1  | 1:F:163:TYR:N    | 2.72                     | 0.57              |
| 1:G:312:ASP:O    | 1:G:316:ASP:HB2  | 2.04                     | 0.57              |
| 1:C:169:THR:HG22 | 1:E:196:GLU:OE1  | 2.04                     | 0.57              |
| 1:B:130:THR:O    | 1:B:298:ARG:NH1  | 2.38                     | 0.57              |
| 1:D:166:ILE:HG23 | 1:D:167:ALA:N    | 2.20                     | 0.57              |
| 1:G:258:THR:HG22 | 1:G:259:GLU:N    | 2.18                     | 0.57              |
| 1:B:166:ILE:CG1  | 1:B:167:ALA:N    | 2.61                     | 0.57              |
| 1:B:166:ILE:HG23 | 1:B:167:ALA:N    | 2.20                     | 0.57              |
| 1:G:190:PRO:HG2  | 1:G:202:VAL:HG21 | 1.84                     | 0.57              |
| 1:G:209:GLU:O    | 1:G:210:LEU:HG   | 2.04                     | 0.57              |
| 1:G:269:CYS:O    | 1:G:305:ILE:HD11 | 2.04                     | 0.57              |
| 1:E:278:ASN:HD22 | 1:E:278:ASN:H    | 1.51                     | 0.57              |
| 1:G:163:TYR:CD1  | 1:G:163:TYR:N    | 2.73                     | 0.57              |
| 1:H:163:TYR:O    | 1:H:164:CYS:HB3  | 2.04                     | 0.57              |
| 1:C:269:CYS:O    | 1:C:305:ILE:HD11 | 2.05                     | 0.57              |
| 1:E:258:THR:HG22 | 1:E:259:GLU:N    | 2.19                     | 0.57              |
| 1:G:152:THR:HA   | 1:G:165:GLN:OE1  | 2.05                     | 0.57              |
| 1:H:166:ILE:HG23 | 1:H:167:ALA:N    | 2.19                     | 0.57              |
| 2:L:3:DA:H1'     | 2:L:4:DC:C5'     | 2.33                     | 0.57              |
| 1:A:163:TYR:N    | 1:A:163:TYR:CD1  | 2.73                     | 0.57              |
| 1:H:278:ASN:HD22 | 1:H:278:ASN:N    | 2.03                     | 0.57              |
| 1:A:312:ASP:O    | 1:A:316:ASP:HB2  | 2.04                     | 0.57              |
| 1:D:204:ARG:NH2  | 1:D:208:HIS:O    | 2.38                     | 0.57              |
| 1:D:312:ASP:O    | 1:D:316:ASP:HB2  | 2.04                     | 0.57              |
| 1:H:204:ARG:NH2  | 1:H:208:HIS:O    | 2.38                     | 0.57              |
| 1:A:130:THR:O    | 1:A:298:ARG:NH1  | 2.38                     | 0.57              |
| 1:D:258:THR:HG22 | 1:D:259:GLU:N    | 2.20                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:278:ASN:N    | 1:E:278:ASN:HD22 | 2.01                     | 0.57              |
| 1:B:258:THR:HG22 | 1:B:259:GLU:N    | 2.18                     | 0.56              |
| 1:C:163:TYR:CD1  | 1:C:163:TYR:N    | 2.72                     | 0.56              |
| 1:G:130:THR:O    | 1:G:298:ARG:NH1  | 2.38                     | 0.56              |
| 1:C:255:GLN:NE2  | 1:E:128:SER:H    | 2.02                     | 0.56              |
| 1:E:163:TYR:CD1  | 1:E:163:TYR:N    | 2.72                     | 0.56              |
| 1:A:153:TRP:CB   | 1:A:164:CYS:HB2  | 2.35                     | 0.56              |
| 1:C:209:GLU:O    | 1:C:210:LEU:HG   | 2.05                     | 0.56              |
| 1:D:189:MET:HE3  | 1:D:246:SER:HB2  | 1.87                     | 0.56              |
| 1:E:166:ILE:HG23 | 1:E:167:ALA:H    | 1.70                     | 0.56              |
| 1:F:278:ASN:H    | 1:F:278:ASN:HD22 | 1.54                     | 0.56              |
| 1:A:270:ASN:O    | 1:A:272:SER:N    | 2.37                     | 0.56              |
| 1:B:278:ASN:H    | 1:B:278:ASN:HD22 | 1.53                     | 0.56              |
| 1:E:209:GLU:O    | 1:E:210:LEU:HG   | 2.05                     | 0.56              |
| 1:B:204:ARG:NH2  | 1:B:208:HIS:O    | 2.38                     | 0.56              |
| 1:D:163:TYR:N    | 1:D:163:TYR:CD1  | 2.73                     | 0.56              |
| 1:F:152:THR:HA   | 1:F:165:GLN:OE1  | 2.06                     | 0.56              |
| 1:B:152:THR:HA   | 1:B:165:GLN:OE1  | 2.06                     | 0.56              |
| 1:B:270:ASN:O    | 1:B:272:SER:N    | 2.37                     | 0.56              |
| 1:B:278:ASN:HD22 | 1:B:278:ASN:N    | 2.03                     | 0.56              |
| 1:D:270:ASN:O    | 1:D:272:SER:N    | 2.38                     | 0.56              |
| 1:H:163:TYR:CD1  | 1:H:163:TYR:N    | 2.72                     | 0.56              |
| 2:O:3:DA:H1'     | 2:O:4:DC:C5'     | 2.34                     | 0.56              |
| 1:A:166:ILE:HG23 | 1:A:167:ALA:N    | 2.20                     | 0.56              |
| 1:C:182:GLN:OE1  | 1:C:182:GLN:HA   | 2.06                     | 0.56              |
| 1:G:270:ASN:O    | 1:G:272:SER:N    | 2.38                     | 0.56              |
| 1:G:278:ASN:HD22 | 1:G:278:ASN:N    | 2.04                     | 0.56              |
| 1:F:204:ARG:NH2  | 1:F:215:ASN:HD21 | 2.04                     | 0.56              |
| 1:A:264:LEU:HD11 | 1:D:216:GLU:HB2  | 1.85                     | 0.56              |
| 1:B:204:ARG:NH2  | 1:B:215:ASN:HD21 | 2.04                     | 0.56              |
| 1:B:269:CYS:O    | 1:B:305:ILE:HD11 | 2.05                     | 0.56              |
| 1:G:204:ARG:NH2  | 1:G:215:ASN:HD21 | 2.04                     | 0.56              |
| 1:H:278:ASN:H    | 1:H:278:ASN:HD22 | 1.53                     | 0.56              |
| 1:A:204:ARG:NH2  | 1:A:208:HIS:O    | 2.39                     | 0.56              |
| 1:C:204:ARG:NH2  | 1:C:215:ASN:HD21 | 2.03                     | 0.56              |
| 1:E:204:ARG:NH2  | 1:E:215:ASN:HD21 | 2.03                     | 0.56              |
| 1:A:278:ASN:HD22 | 1:A:278:ASN:H    | 1.54                     | 0.55              |
| 1:B:163:TYR:O    | 1:B:164:CYS:HB3  | 2.06                     | 0.55              |
| 1:H:152:THR:HA   | 1:H:165:GLN:OE1  | 2.06                     | 0.55              |
| 1:G:204:ARG:NH2  | 1:G:208:HIS:O    | 2.38                     | 0.55              |
| 1:C:286:VAL:HG23 | 1:C:286:VAL:O    | 2.06                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:204:ARG:NH2  | 1:E:208:HIS:O    | 2.38                     | 0.55              |
| 1:H:210:LEU:O    | 1:H:212:ARG:N    | 2.40                     | 0.55              |
| 1:B:163:TYR:N    | 1:B:163:TYR:CD1  | 2.73                     | 0.55              |
| 1:D:182:GLN:OE1  | 1:D:182:GLN:HA   | 2.07                     | 0.55              |
| 1:F:209:GLU:O    | 1:F:210:LEU:HG   | 2.06                     | 0.55              |
| 1:D:278:ASN:N    | 1:D:278:ASN:HD22 | 2.03                     | 0.55              |
| 1:F:130:THR:O    | 1:F:298:ARG:NH1  | 2.39                     | 0.55              |
| 1:A:210:LEU:O    | 1:A:212:ARG:N    | 2.40                     | 0.55              |
| 1:B:209:GLU:O    | 1:B:210:LEU:HG   | 2.06                     | 0.55              |
| 1:D:163:TYR:O    | 1:D:164:CYS:HB3  | 2.05                     | 0.55              |
| 1:E:152:THR:HA   | 1:E:165:GLN:OE1  | 2.06                     | 0.55              |
| 1:G:163:TYR:O    | 1:G:164:CYS:HB3  | 2.05                     | 0.55              |
| 1:A:163:TYR:O    | 1:A:164:CYS:HB3  | 2.06                     | 0.55              |
| 1:D:204:ARG:NH2  | 1:D:215:ASN:HD21 | 2.05                     | 0.55              |
| 1:F:269:CYS:O    | 1:F:305:ILE:HD11 | 2.06                     | 0.55              |
| 1:G:153:TRP:CB   | 1:G:164:CYS:HB2  | 2.37                     | 0.55              |
| 1:A:209:GLU:O    | 1:A:210:LEU:HG   | 2.07                     | 0.55              |
| 1:A:286:VAL:O    | 1:A:286:VAL:HG23 | 2.07                     | 0.55              |
| 1:F:182:GLN:HA   | 1:F:182:GLN:OE1  | 2.07                     | 0.55              |
| 1:H:153:TRP:CB   | 1:H:164:CYS:HB2  | 2.37                     | 0.55              |
| 1:A:278:ASN:N    | 1:A:278:ASN:HD22 | 2.03                     | 0.55              |
| 1:B:238:GLU:CG   | 1:B:245:GLN:HG2  | 2.31                     | 0.55              |
| 1:C:169:THR:CG2  | 1:E:196:GLU:CB   | 2.85                     | 0.55              |
| 1:D:130:THR:O    | 1:D:298:ARG:NH1  | 2.39                     | 0.55              |
| 1:E:270:ASN:O    | 1:E:272:SER:N    | 2.37                     | 0.55              |
| 1:F:258:THR:HG22 | 1:F:260:PHE:H    | 1.72                     | 0.55              |
| 1:B:214:PHE:C    | 1:B:215:ASN:HD22 | 2.11                     | 0.54              |
| 1:D:214:PHE:C    | 1:D:215:ASN:HD22 | 2.10                     | 0.54              |
| 1:E:182:GLN:HA   | 1:E:182:GLN:OE1  | 2.07                     | 0.54              |
| 1:F:204:ARG:NH2  | 1:F:208:HIS:O    | 2.40                     | 0.54              |
| 1:H:182:GLN:OE1  | 1:H:182:GLN:HA   | 2.07                     | 0.54              |
| 1:C:183:GLY:HA2  | 1:C:291:ARG:NH2  | 2.22                     | 0.54              |
| 1:F:278:ASN:N    | 1:F:278:ASN:HD22 | 2.03                     | 0.54              |
| 1:A:183:GLY:O    | 1:A:184:ALA:C    | 2.46                     | 0.54              |
| 1:B:155:TYR:OH   | 1:B:160:LYS:HD3  | 2.08                     | 0.54              |
| 1:C:204:ARG:NH2  | 1:C:208:HIS:O    | 2.40                     | 0.54              |
| 1:G:278:ASN:H    | 1:G:278:ASN:HD22 | 1.55                     | 0.54              |
| 1:A:258:THR:HG22 | 1:A:260:PHE:H    | 1.73                     | 0.54              |
| 1:D:209:GLU:O    | 1:D:210:LEU:HG   | 2.08                     | 0.54              |
| 1:F:286:VAL:O    | 1:F:286:VAL:HG23 | 2.07                     | 0.54              |
| 1:C:183:GLY:O    | 1:C:184:ALA:C    | 2.45                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:182:GLN:OE1  | 1:G:182:GLN:HA   | 2.08                     | 0.54              |
| 1:H:270:ASN:O    | 1:H:272:SER:N    | 2.40                     | 0.54              |
| 1:H:286:VAL:O    | 1:H:286:VAL:HG23 | 2.08                     | 0.54              |
| 1:C:214:PHE:C    | 1:C:215:ASN:HD22 | 2.11                     | 0.54              |
| 1:G:304:ARG:HG2  | 1:G:304:ARG:O    | 2.07                     | 0.54              |
| 1:H:204:ARG:NH2  | 1:H:215:ASN:HD21 | 2.04                     | 0.54              |
| 1:H:269:CYS:O    | 1:H:305:ILE:HD11 | 2.07                     | 0.54              |
| 1:B:210:LEU:O    | 1:B:212:ARG:N    | 2.41                     | 0.54              |
| 1:B:286:VAL:HG23 | 1:B:286:VAL:O    | 2.07                     | 0.54              |
| 2:J:3:DA:H1'     | 2:J:4:DC:C5'     | 2.34                     | 0.54              |
| 1:B:182:GLN:HA   | 1:B:182:GLN:OE1  | 2.07                     | 0.54              |
| 1:C:153:TRP:CB   | 1:C:164:CYS:HB2  | 2.38                     | 0.54              |
| 1:D:152:THR:HA   | 1:D:165:GLN:OE1  | 2.07                     | 0.54              |
| 1:D:278:ASN:HD22 | 1:D:278:ASN:H    | 1.55                     | 0.54              |
| 1:F:210:LEU:O    | 1:F:212:ARG:N    | 2.41                     | 0.54              |
| 1:G:210:LEU:O    | 1:G:212:ARG:N    | 2.41                     | 0.54              |
| 2:J:2:DA:H2''    | 2:J:3:DA:OP2     | 2.06                     | 0.54              |
| 2:L:2:DA:H2''    | 2:L:3:DA:OP2     | 2.08                     | 0.54              |
| 1:A:204:ARG:NH2  | 1:A:215:ASN:HD21 | 2.04                     | 0.54              |
| 1:D:183:GLY:O    | 1:D:184:ALA:C    | 2.46                     | 0.54              |
| 1:B:183:GLY:O    | 1:B:184:ALA:C    | 2.47                     | 0.53              |
| 1:C:258:THR:HG22 | 1:C:260:PHE:H    | 1.73                     | 0.53              |
| 1:F:183:GLY:O    | 1:F:184:ALA:C    | 2.46                     | 0.53              |
| 1:G:258:THR:HG22 | 1:G:260:PHE:H    | 1.72                     | 0.53              |
| 1:A:278:ASN:O    | 1:A:279:ARG:HG2  | 2.09                     | 0.53              |
| 1:E:286:VAL:O    | 1:E:286:VAL:HG23 | 2.07                     | 0.53              |
| 1:F:155:TYR:OH   | 1:F:160:LYS:HD3  | 2.08                     | 0.53              |
| 1:A:269:CYS:O    | 1:A:305:ILE:HD11 | 2.07                     | 0.53              |
| 1:C:255:GLN:CB   | 1:E:128:SER:HB2  | 2.39                     | 0.53              |
| 1:E:278:ASN:O    | 1:E:279:ARG:HG2  | 2.08                     | 0.53              |
| 1:F:163:TYR:O    | 1:F:164:CYS:HB3  | 2.08                     | 0.53              |
| 1:H:304:ARG:O    | 1:H:304:ARG:HG2  | 2.08                     | 0.53              |
| 1:A:152:THR:HA   | 1:A:165:GLN:OE1  | 2.08                     | 0.53              |
| 1:C:238:GLU:CG   | 1:C:245:GLN:HG2  | 2.31                     | 0.53              |
| 1:E:258:THR:HG22 | 1:E:260:PHE:H    | 1.74                     | 0.53              |
| 1:F:160:LYS:O    | 1:F:301:PHE:HB2  | 2.08                     | 0.53              |
| 1:F:304:ARG:O    | 1:F:304:ARG:HG2  | 2.09                     | 0.53              |
| 1:G:286:VAL:O    | 1:G:286:VAL:HG23 | 2.07                     | 0.53              |
| 1:A:162:LEU:HD23 | 1:A:163:TYR:N    | 2.24                     | 0.53              |
| 1:B:153:TRP:CB   | 1:B:164:CYS:HB2  | 2.39                     | 0.53              |
| 1:C:163:TYR:O    | 1:C:164:CYS:HB3  | 2.06                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:162:LEU:HD23 | 1:D:163:TYR:N    | 2.23                     | 0.53              |
| 1:E:214:PHE:C    | 1:E:215:ASN:HD22 | 2.12                     | 0.53              |
| 1:G:214:PHE:C    | 1:G:215:ASN:HD22 | 2.12                     | 0.53              |
| 2:O:2:DA:H2''    | 2:O:3:DA:OP2     | 2.07                     | 0.53              |
| 1:A:182:GLN:OE1  | 1:A:182:GLN:HA   | 2.07                     | 0.53              |
| 1:B:278:ASN:O    | 1:B:279:ARG:HG2  | 2.09                     | 0.53              |
| 1:C:270:ASN:O    | 1:C:272:SER:N    | 2.41                     | 0.53              |
| 1:E:318:ASP:O    | 1:E:320:ILE:N    | 2.41                     | 0.53              |
| 1:H:209:GLU:O    | 1:H:210:LEU:HG   | 2.07                     | 0.53              |
| 2:M:2:DA:H2''    | 2:M:3:DA:OP2     | 2.06                     | 0.53              |
| 1:E:183:GLY:O    | 1:E:184:ALA:C    | 2.46                     | 0.53              |
| 1:E:190:PRO:HG2  | 1:E:202:VAL:HG23 | 1.91                     | 0.53              |
| 1:A:166:ILE:CG1  | 1:A:167:ALA:N    | 2.60                     | 0.53              |
| 1:B:258:THR:HG22 | 1:B:260:PHE:H    | 1.74                     | 0.53              |
| 1:E:210:LEU:O    | 1:E:212:ARG:N    | 2.42                     | 0.53              |
| 1:H:155:TYR:OH   | 1:H:160:LYS:HD3  | 2.09                     | 0.53              |
| 2:N:9:DT:H1'     | 2:N:10:DT:H5'    | 1.91                     | 0.53              |
| 1:C:207:ASN:HD22 | 1:D:275:GLY:HA3  | 1.74                     | 0.53              |
| 1:D:155:TYR:OH   | 1:D:160:LYS:HD3  | 2.08                     | 0.53              |
| 1:E:162:LEU:HD23 | 1:E:163:TYR:N    | 2.24                     | 0.53              |
| 1:F:278:ASN:O    | 1:F:279:ARG:HG2  | 2.09                     | 0.53              |
| 1:H:258:THR:HG22 | 1:H:260:PHE:H    | 1.73                     | 0.53              |
| 1:F:171:PRO:O    | 1:F:172:ILE:CB   | 2.57                     | 0.53              |
| 1:H:214:PHE:C    | 1:H:215:ASN:HD22 | 2.12                     | 0.53              |
| 1:B:278:ASN:C    | 1:B:279:ARG:HG2  | 2.30                     | 0.52              |
| 1:D:258:THR:HG22 | 1:D:260:PHE:H    | 1.74                     | 0.52              |
| 1:E:155:TYR:OH   | 1:E:160:LYS:HD3  | 2.09                     | 0.52              |
| 1:G:183:GLY:HA2  | 1:G:291:ARG:NH2  | 2.24                     | 0.52              |
| 1:H:162:LEU:HD23 | 1:H:163:TYR:N    | 2.24                     | 0.52              |
| 1:D:160:LYS:O    | 1:D:301:PHE:HB2  | 2.09                     | 0.52              |
| 1:D:278:ASN:O    | 1:D:279:ARG:HG2  | 2.09                     | 0.52              |
| 1:B:183:GLY:HA2  | 1:B:291:ARG:NH2  | 2.23                     | 0.52              |
| 1:C:155:TYR:OH   | 1:C:160:LYS:HD3  | 2.09                     | 0.52              |
| 1:D:153:TRP:CB   | 1:D:164:CYS:HB2  | 2.39                     | 0.52              |
| 1:D:171:PRO:O    | 1:D:172:ILE:CB   | 2.58                     | 0.52              |
| 1:G:155:TYR:OH   | 1:G:160:LYS:HD3  | 2.09                     | 0.52              |
| 1:H:278:ASN:O    | 1:H:279:ARG:HG2  | 2.09                     | 0.52              |
| 1:A:155:TYR:OH   | 1:A:160:LYS:HD3  | 2.09                     | 0.52              |
| 1:A:214:PHE:C    | 1:A:215:ASN:HD22 | 2.12                     | 0.52              |
| 1:D:286:VAL:O    | 1:D:286:VAL:HG23 | 2.08                     | 0.52              |
| 1:G:278:ASN:O    | 1:G:279:ARG:HG2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:183:GLY:O    | 1:H:184:ALA:C    | 2.47                     | 0.52              |
| 2:M:10:DT:H2'    | 2:O:1:DA:H1'     | 1.90                     | 0.52              |
| 1:A:190:PRO:HG2  | 1:A:202:VAL:HG23 | 1.91                     | 0.52              |
| 1:D:210:LEU:O    | 1:D:212:ARG:N    | 2.43                     | 0.52              |
| 1:E:153:TRP:CB   | 1:E:164:CYS:HB2  | 2.39                     | 0.52              |
| 1:C:162:LEU:HD23 | 1:C:163:TYR:N    | 2.24                     | 0.52              |
| 1:E:278:ASN:C    | 1:E:279:ARG:HG2  | 2.30                     | 0.52              |
| 1:B:162:LEU:HD23 | 1:B:163:TYR:N    | 2.25                     | 0.52              |
| 1:C:210:LEU:O    | 1:C:212:ARG:N    | 2.43                     | 0.52              |
| 1:D:269:CYS:O    | 1:D:305:ILE:HD11 | 2.09                     | 0.52              |
| 1:F:270:ASN:O    | 1:F:272:SER:N    | 2.40                     | 0.52              |
| 1:F:278:ASN:C    | 1:F:279:ARG:HG2  | 2.30                     | 0.52              |
| 1:H:173:GLN:N    | 1:H:173:GLN:OE1  | 2.43                     | 0.52              |
| 1:C:173:GLN:OE1  | 1:C:173:GLN:N    | 2.43                     | 0.52              |
| 1:G:160:LYS:O    | 1:G:301:PHE:HB2  | 2.10                     | 0.52              |
| 1:G:162:LEU:HD23 | 1:G:163:TYR:N    | 2.24                     | 0.52              |
| 1:B:304:ARG:HG2  | 1:B:304:ARG:O    | 2.10                     | 0.52              |
| 1:F:214:PHE:C    | 1:F:215:ASN:HD22 | 2.12                     | 0.52              |
| 1:H:160:LYS:O    | 1:H:301:PHE:HB2  | 2.10                     | 0.52              |
| 1:F:153:TRP:CB   | 1:F:164:CYS:HB2  | 2.39                     | 0.51              |
| 1:G:183:GLY:O    | 1:G:184:ALA:C    | 2.47                     | 0.51              |
| 1:A:160:LYS:O    | 1:A:301:PHE:HB2  | 2.10                     | 0.51              |
| 1:A:278:ASN:C    | 1:A:279:ARG:HG2  | 2.30                     | 0.51              |
| 1:G:207:ASN:HD21 | 1:H:207:ASN:H    | 1.58                     | 0.51              |
| 2:M:10:DT:C2'    | 2:O:1:DA:O4'     | 2.57                     | 0.51              |
| 1:A:173:GLN:OE1  | 1:A:173:GLN:N    | 2.44                     | 0.51              |
| 1:B:160:LYS:O    | 1:B:301:PHE:HB2  | 2.11                     | 0.51              |
| 1:C:160:LYS:O    | 1:C:301:PHE:HB2  | 2.10                     | 0.51              |
| 1:E:183:GLY:HA2  | 1:E:291:ARG:NH2  | 2.24                     | 0.51              |
| 1:F:162:LEU:HD23 | 1:F:163:TYR:N    | 2.24                     | 0.51              |
| 1:H:190:PRO:HG2  | 1:H:202:VAL:HG23 | 1.92                     | 0.51              |
| 1:A:189:MET:HE3  | 1:A:246:SER:HB2  | 1.93                     | 0.51              |
| 1:A:304:ARG:O    | 1:A:304:ARG:HG2  | 2.10                     | 0.51              |
| 1:E:189:MET:CE   | 1:E:246:SER:HB2  | 2.40                     | 0.51              |
| 1:H:213:GLU:O    | 1:H:214:PHE:HB2  | 2.11                     | 0.51              |
| 1:C:318:ASP:O    | 1:C:320:ILE:N    | 2.44                     | 0.51              |
| 1:D:173:GLN:N    | 1:D:173:GLN:OE1  | 2.44                     | 0.51              |
| 1:D:278:ASN:C    | 1:D:279:ARG:HG2  | 2.30                     | 0.51              |
| 1:E:171:PRO:O    | 1:E:172:ILE:CB   | 2.59                     | 0.51              |
| 1:G:278:ASN:C    | 1:G:279:ARG:HG2  | 2.31                     | 0.51              |
| 1:C:210:LEU:HD12 | 1:D:206:PRO:HB3  | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:9:DT:H1'     | 2:I:10:DT:H5'    | 1.92                     | 0.51              |
| 1:B:196:GLU:H    | 1:B:196:GLU:CD   | 2.14                     | 0.51              |
| 1:E:173:GLN:OE1  | 1:E:173:GLN:N    | 2.44                     | 0.51              |
| 2:M:3:DA:H1'     | 2:M:4:DC:C5'     | 2.33                     | 0.51              |
| 1:D:213:GLU:O    | 1:D:214:PHE:HB2  | 2.11                     | 0.51              |
| 1:E:160:LYS:O    | 1:E:301:PHE:HB2  | 2.10                     | 0.51              |
| 1:F:173:GLN:N    | 1:F:173:GLN:OE1  | 2.43                     | 0.51              |
| 1:B:173:GLN:OE1  | 1:B:173:GLN:N    | 2.44                     | 0.51              |
| 1:C:278:ASN:O    | 1:C:279:ARG:HG2  | 2.11                     | 0.51              |
| 1:F:213:GLU:O    | 1:F:214:PHE:HB2  | 2.11                     | 0.51              |
| 2:M:5:DA:C2'     | 2:M:6:DT:H5'     | 2.41                     | 0.51              |
| 1:A:189:MET:CE   | 1:A:246:SER:HB2  | 2.42                     | 0.50              |
| 1:D:189:MET:CE   | 1:D:246:SER:HB2  | 2.41                     | 0.50              |
| 1:D:190:PRO:HG2  | 1:D:202:VAL:HG23 | 1.92                     | 0.50              |
| 1:B:171:PRO:O    | 1:B:172:ILE:CB   | 2.59                     | 0.50              |
| 1:C:278:ASN:C    | 1:C:279:ARG:HG2  | 2.32                     | 0.50              |
| 1:E:269:CYS:O    | 1:E:305:ILE:CD1  | 2.59                     | 0.50              |
| 1:E:304:ARG:HG2  | 1:E:304:ARG:O    | 2.10                     | 0.50              |
| 1:G:189:MET:HE3  | 1:G:246:SER:HB2  | 1.93                     | 0.50              |
| 1:H:318:ASP:O    | 1:H:320:ILE:N    | 2.44                     | 0.50              |
| 1:A:211:SER:HB3  | 1:A:213:GLU:HG2  | 1.94                     | 0.50              |
| 1:C:211:SER:HB3  | 1:C:213:GLU:HG2  | 1.94                     | 0.50              |
| 1:C:269:CYS:O    | 1:C:305:ILE:CD1  | 2.59                     | 0.50              |
| 1:B:213:GLU:O    | 1:B:214:PHE:HB2  | 2.12                     | 0.50              |
| 1:E:213:GLU:O    | 1:E:214:PHE:HB2  | 2.12                     | 0.50              |
| 1:G:165:GLN:O    | 1:G:166:ILE:O    | 2.30                     | 0.50              |
| 1:G:269:CYS:O    | 1:G:305:ILE:CD1  | 2.60                     | 0.50              |
| 2:P:9:DT:H1'     | 2:P:10:DT:H5'    | 1.93                     | 0.50              |
| 1:B:190:PRO:HG2  | 1:B:202:VAL:HG23 | 1.93                     | 0.50              |
| 1:E:211:SER:HB3  | 1:E:213:GLU:HG2  | 1.94                     | 0.50              |
| 1:E:228:VAL:HG11 | 1:E:234:ALA:CB   | 2.42                     | 0.50              |
| 1:C:189:MET:HE3  | 1:C:246:SER:HB2  | 1.94                     | 0.50              |
| 1:C:190:PRO:HG2  | 1:C:202:VAL:HG23 | 1.94                     | 0.50              |
| 1:D:166:ILE:CG1  | 1:D:167:ALA:H    | 2.01                     | 0.50              |
| 1:G:171:PRO:O    | 1:G:172:ILE:CB   | 2.59                     | 0.50              |
| 2:O:5:DA:C2'     | 2:O:6:DT:H5'     | 2.42                     | 0.50              |
| 1:A:171:PRO:O    | 1:A:172:ILE:CB   | 2.59                     | 0.50              |
| 1:B:165:GLN:O    | 1:B:166:ILE:O    | 2.30                     | 0.50              |
| 1:E:196:GLU:CD   | 1:E:196:GLU:H    | 2.15                     | 0.50              |
| 1:F:173:GLN:HB3  | 1:F:260:PHE:HB3  | 1.94                     | 0.50              |
| 1:H:143:GLN:HG2  | 1:H:144:GLN:N    | 2.27                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:143:GLN:HG2  | 1:F:144:GLN:N    | 2.26                     | 0.50              |
| 1:F:189:MET:CE   | 1:F:246:SER:HB2  | 2.42                     | 0.50              |
| 1:H:171:PRO:O    | 1:H:172:ILE:CB   | 2.59                     | 0.50              |
| 1:H:278:ASN:C    | 1:H:279:ARG:HG2  | 2.30                     | 0.50              |
| 1:E:238:GLU:CG   | 1:E:245:GLN:HG2  | 2.31                     | 0.49              |
| 1:F:190:PRO:HG2  | 1:F:202:VAL:HG23 | 1.93                     | 0.49              |
| 1:G:161:LYS:HA   | 1:G:302:GLU:O    | 2.12                     | 0.49              |
| 1:H:165:GLN:O    | 1:H:166:ILE:O    | 2.30                     | 0.49              |
| 1:A:318:ASP:O    | 1:A:320:ILE:N    | 2.44                     | 0.49              |
| 1:C:228:VAL:HG11 | 1:C:234:ALA:CB   | 2.43                     | 0.49              |
| 1:E:318:ASP:O    | 1:E:319:SER:C    | 2.49                     | 0.49              |
| 1:F:165:GLN:O    | 1:F:166:ILE:O    | 2.30                     | 0.49              |
| 1:G:173:GLN:N    | 1:G:173:GLN:OE1  | 2.45                     | 0.49              |
| 1:H:228:VAL:HA   | 1:H:264:LEU:O    | 2.12                     | 0.49              |
| 1:B:228:VAL:HA   | 1:B:264:LEU:O    | 2.13                     | 0.49              |
| 1:C:143:GLN:HG2  | 1:C:144:GLN:N    | 2.27                     | 0.49              |
| 1:D:196:GLU:N    | 1:F:169:THR:CG2  | 2.66                     | 0.49              |
| 1:F:269:CYS:O    | 1:F:305:ILE:CD1  | 2.60                     | 0.49              |
| 1:H:162:LEU:C    | 1:H:162:LEU:HD23 | 2.33                     | 0.49              |
| 1:A:196:GLU:H    | 1:A:196:GLU:CD   | 2.16                     | 0.49              |
| 1:A:212:ARG:NE   | 1:A:212:ARG:HA   | 2.21                     | 0.49              |
| 1:D:304:ARG:HG2  | 1:D:304:ARG:O    | 2.12                     | 0.49              |
| 1:E:161:LYS:HA   | 1:E:302:GLU:O    | 2.13                     | 0.49              |
| 1:H:183:GLY:HA2  | 1:H:291:ARG:NH2  | 2.24                     | 0.49              |
| 2:K:9:DT:H1'     | 2:K:10:DT:H5'    | 1.93                     | 0.49              |
| 1:C:165:GLN:O    | 1:C:166:ILE:O    | 2.30                     | 0.49              |
| 1:D:211:SER:HB3  | 1:D:213:GLU:HG2  | 1.95                     | 0.49              |
| 1:D:228:VAL:HG11 | 1:D:234:ALA:CB   | 2.42                     | 0.49              |
| 1:E:165:GLN:O    | 1:E:166:ILE:O    | 2.30                     | 0.49              |
| 1:F:318:ASP:O    | 1:F:320:ILE:N    | 2.46                     | 0.49              |
| 1:A:238:GLU:CG   | 1:A:245:GLN:HG2  | 2.31                     | 0.49              |
| 1:B:269:CYS:O    | 1:B:305:ILE:CD1  | 2.60                     | 0.49              |
| 1:C:255:GLN:CG   | 1:E:128:SER:HB2  | 2.42                     | 0.49              |
| 1:H:196:GLU:H    | 1:H:196:GLU:CD   | 2.16                     | 0.49              |
| 1:H:211:SER:HB3  | 1:H:213:GLU:HG2  | 1.93                     | 0.49              |
| 1:B:135:PRO:HD2  | 1:B:296:LEU:O    | 2.12                     | 0.49              |
| 1:D:318:ASP:O    | 1:D:320:ILE:N    | 2.45                     | 0.49              |
| 1:E:220:ALA:HB2  | 1:E:236:TYR:CE1  | 2.48                     | 0.49              |
| 1:F:183:GLY:HA2  | 1:F:291:ARG:NH2  | 2.24                     | 0.49              |
| 1:G:189:MET:CE   | 1:G:246:SER:HB2  | 2.43                     | 0.49              |
| 2:N:2:DA:H2''    | 2:N:3:DA:OP2     | 2.11                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:162:LEU:HD23 | 1:A:162:LEU:C    | 2.33                     | 0.49              |
| 1:B:173:GLN:HB3  | 1:B:260:PHE:HB3  | 1.95                     | 0.49              |
| 1:C:162:LEU:C    | 1:C:162:LEU:HD23 | 2.33                     | 0.49              |
| 1:C:140:VAL:HG12 | 1:C:174:ILE:CD1  | 2.43                     | 0.49              |
| 1:D:162:LEU:HD23 | 1:D:162:LEU:C    | 2.33                     | 0.49              |
| 1:D:165:GLN:O    | 1:D:166:ILE:O    | 2.30                     | 0.49              |
| 1:D:183:GLY:HA2  | 1:D:291:ARG:NH2  | 2.24                     | 0.49              |
| 1:E:162:LEU:C    | 1:E:162:LEU:HD23 | 2.33                     | 0.49              |
| 1:F:228:VAL:HG11 | 1:F:234:ALA:CB   | 2.43                     | 0.49              |
| 2:J:5:DA:C2'     | 2:J:6:DT:H5'     | 2.43                     | 0.49              |
| 1:A:173:GLN:HB3  | 1:A:260:PHE:HB3  | 1.95                     | 0.49              |
| 1:A:135:PRO:HD2  | 1:A:296:LEU:O    | 2.13                     | 0.49              |
| 1:B:162:LEU:C    | 1:B:162:LEU:HD23 | 2.34                     | 0.49              |
| 1:F:162:LEU:HD23 | 1:F:162:LEU:C    | 2.33                     | 0.49              |
| 1:H:161:LYS:HA   | 1:H:302:GLU:O    | 2.12                     | 0.49              |
| 2:K:2:DA:H2''    | 2:K:3:DA:OP2     | 2.12                     | 0.49              |
| 1:A:140:VAL:HG12 | 1:A:174:ILE:CD1  | 2.43                     | 0.49              |
| 1:A:213:GLU:O    | 1:A:214:PHE:HB2  | 2.13                     | 0.49              |
| 1:C:171:PRO:O    | 1:C:172:ILE:CB   | 2.59                     | 0.49              |
| 1:G:143:GLN:HG2  | 1:G:144:GLN:N    | 2.28                     | 0.49              |
| 1:G:162:LEU:HD23 | 1:G:162:LEU:C    | 2.33                     | 0.49              |
| 1:G:166:ILE:CG1  | 1:G:167:ALA:N    | 2.60                     | 0.49              |
| 1:A:161:LYS:HA   | 1:A:302:GLU:O    | 2.12                     | 0.48              |
| 1:B:189:MET:CE   | 1:B:246:SER:HB2  | 2.42                     | 0.48              |
| 1:C:212:ARG:NE   | 1:C:212:ARG:HA   | 2.21                     | 0.48              |
| 1:A:165:GLN:O    | 1:A:166:ILE:O    | 2.30                     | 0.48              |
| 1:A:318:ASP:O    | 1:A:319:SER:C    | 2.51                     | 0.48              |
| 1:B:143:GLN:HG2  | 1:B:144:GLN:N    | 2.28                     | 0.48              |
| 1:B:211:SER:HB3  | 1:B:213:GLU:HG2  | 1.94                     | 0.48              |
| 1:D:173:GLN:HB3  | 1:D:260:PHE:HB3  | 1.94                     | 0.48              |
| 1:B:159:LEU:C    | 1:B:161:LYS:N    | 2.66                     | 0.48              |
| 1:C:189:MET:CE   | 1:C:246:SER:HB2  | 2.43                     | 0.48              |
| 1:D:228:VAL:HA   | 1:D:264:LEU:O    | 2.13                     | 0.48              |
| 1:F:142:PHE:CZ   | 1:F:162:LEU:HD12 | 2.48                     | 0.48              |
| 1:F:211:SER:HB3  | 1:F:213:GLU:HG2  | 1.94                     | 0.48              |
| 1:F:161:LYS:HA   | 1:F:302:GLU:O    | 2.14                     | 0.48              |
| 1:G:220:ALA:HB2  | 1:G:236:TYR:CE1  | 2.48                     | 0.48              |
| 1:G:318:ASP:O    | 1:G:320:ILE:N    | 2.47                     | 0.48              |
| 1:H:166:ILE:HG23 | 1:H:167:ALA:H    | 1.79                     | 0.48              |
| 1:H:318:ASP:O    | 1:H:319:SER:C    | 2.51                     | 0.48              |
| 1:A:183:GLY:HA2  | 1:A:291:ARG:NH2  | 2.24                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:228:VAL:HA   | 1:C:264:LEU:O    | 2.13                     | 0.48              |
| 1:E:140:VAL:HG12 | 1:E:174:ILE:CD1  | 2.43                     | 0.48              |
| 1:G:135:PRO:HD2  | 1:G:296:LEU:O    | 2.13                     | 0.48              |
| 1:G:278:ASN:O    | 1:G:280:ARG:N    | 2.47                     | 0.48              |
| 1:H:189:MET:CE   | 1:H:246:SER:HB2  | 2.43                     | 0.48              |
| 1:H:173:GLN:HB3  | 1:H:260:PHE:HB3  | 1.94                     | 0.48              |
| 1:A:244:ARG:HH11 | 1:A:244:ARG:HG2  | 1.79                     | 0.48              |
| 1:F:196:GLU:H    | 1:F:196:GLU:CD   | 2.15                     | 0.48              |
| 1:G:195:ALA:O    | 1:G:198:VAL:HG22 | 2.14                     | 0.48              |
| 1:H:189:MET:HE3  | 1:H:246:SER:HB2  | 1.94                     | 0.48              |
| 1:A:228:VAL:HG11 | 1:A:234:ALA:CB   | 2.44                     | 0.48              |
| 1:C:213:GLU:O    | 1:C:214:PHE:HB2  | 2.13                     | 0.48              |
| 1:E:143:GLN:HG2  | 1:E:144:GLN:N    | 2.28                     | 0.48              |
| 1:F:189:MET:HE3  | 1:F:246:SER:HB2  | 1.96                     | 0.48              |
| 1:G:213:GLU:O    | 1:G:214:PHE:HB2  | 2.13                     | 0.48              |
| 1:H:228:VAL:HG11 | 1:H:234:ALA:CB   | 2.43                     | 0.48              |
| 2:P:1:DA:H2''    | 2:P:2:DA:O5'     | 2.13                     | 0.48              |
| 1:A:204:ARG:HH12 | 1:A:208:HIS:HB3  | 1.79                     | 0.48              |
| 1:B:161:LYS:HA   | 1:B:302:GLU:O    | 2.14                     | 0.48              |
| 1:C:318:ASP:O    | 1:C:319:SER:C    | 2.51                     | 0.48              |
| 1:D:135:PRO:HD2  | 1:D:296:LEU:O    | 2.14                     | 0.48              |
| 1:E:142:PHE:CZ   | 1:E:162:LEU:HD12 | 2.49                     | 0.48              |
| 1:F:228:VAL:HA   | 1:F:264:LEU:O    | 2.13                     | 0.48              |
| 1:G:211:SER:HB3  | 1:G:213:GLU:HG2  | 1.95                     | 0.48              |
| 1:G:280:ARG:O    | 1:G:281:PRO:C    | 2.52                     | 0.48              |
| 1:H:135:PRO:HD2  | 1:H:296:LEU:O    | 2.13                     | 0.48              |
| 2:L:4:DC:H2''    | 2:L:5:DA:OP2     | 2.13                     | 0.48              |
| 1:A:228:VAL:HA   | 1:A:264:LEU:O    | 2.14                     | 0.48              |
| 1:D:140:VAL:HG12 | 1:D:174:ILE:CD1  | 2.44                     | 0.48              |
| 1:F:135:PRO:HD2  | 1:F:296:LEU:O    | 2.14                     | 0.48              |
| 1:G:140:VAL:HG12 | 1:G:174:ILE:CD1  | 2.44                     | 0.48              |
| 1:G:173:GLN:HB3  | 1:G:260:PHE:HB3  | 1.94                     | 0.48              |
| 1:G:228:VAL:HA   | 1:G:264:LEU:O    | 2.14                     | 0.48              |
| 1:H:220:ALA:HA   | 1:H:236:TYR:CD1  | 2.49                     | 0.48              |
| 1:A:269:CYS:O    | 1:A:305:ILE:CD1  | 2.61                     | 0.48              |
| 1:B:220:ALA:HB2  | 1:B:236:TYR:CE1  | 2.49                     | 0.48              |
| 1:B:271:SER:O    | 1:B:272:SER:HB3  | 2.14                     | 0.48              |
| 1:E:228:VAL:HA   | 1:E:264:LEU:O    | 2.14                     | 0.48              |
| 1:G:228:VAL:HG11 | 1:G:234:ALA:CB   | 2.44                     | 0.48              |
| 2:L:3:DA:C1'     | 2:L:4:DC:H5'     | 2.38                     | 0.48              |
| 2:L:5:DA:C2'     | 2:L:6:DT:H5'     | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:135:PRO:HD2  | 1:C:296:LEU:O    | 2.14                     | 0.47              |
| 1:D:161:LYS:HA   | 1:D:302:GLU:O    | 2.14                     | 0.47              |
| 1:D:212:ARG:HA   | 1:D:212:ARG:NE   | 2.21                     | 0.47              |
| 1:H:142:PHE:CZ   | 1:H:162:LEU:HD12 | 2.49                     | 0.47              |
| 1:A:195:ALA:O    | 1:A:198:VAL:HG22 | 2.14                     | 0.47              |
| 1:A:220:ALA:HB2  | 1:A:236:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:158:GLU:H    | 1:C:158:GLU:CD   | 2.18                     | 0.47              |
| 1:D:196:GLU:CD   | 1:D:196:GLU:H    | 2.16                     | 0.47              |
| 1:E:173:GLN:HB3  | 1:E:260:PHE:HB3  | 1.95                     | 0.47              |
| 1:C:244:ARG:HG2  | 1:C:244:ARG:HH11 | 1.79                     | 0.47              |
| 1:C:173:GLN:HB3  | 1:C:260:PHE:HB3  | 1.95                     | 0.47              |
| 1:E:244:ARG:HG2  | 1:E:244:ARG:HH11 | 1.79                     | 0.47              |
| 1:F:318:ASP:O    | 1:F:319:SER:C    | 2.53                     | 0.47              |
| 1:G:196:GLU:CD   | 1:G:196:GLU:H    | 2.16                     | 0.47              |
| 2:I:2:DA:H2"     | 2:I:3:DA:OP2     | 2.13                     | 0.47              |
| 1:A:142:PHE:CZ   | 1:A:162:LEU:HD12 | 2.49                     | 0.47              |
| 1:B:228:VAL:HG11 | 1:B:234:ALA:CB   | 2.43                     | 0.47              |
| 1:B:290:THR:HB   | 1:B:296:LEU:CD2  | 2.39                     | 0.47              |
| 1:D:166:ILE:HG23 | 1:D:167:ALA:H    | 1.79                     | 0.47              |
| 1:D:204:ARG:HH12 | 1:D:208:HIS:HB3  | 1.80                     | 0.47              |
| 1:F:220:ALA:HB2  | 1:F:236:TYR:CE1  | 2.49                     | 0.47              |
| 1:H:278:ASN:O    | 1:H:280:ARG:N    | 2.47                     | 0.47              |
| 1:C:166:ILE:HG23 | 1:C:167:ALA:H    | 1.78                     | 0.47              |
| 1:D:195:ALA:O    | 1:D:198:VAL:HG22 | 2.15                     | 0.47              |
| 1:D:220:ALA:HB2  | 1:D:236:TYR:CE1  | 2.50                     | 0.47              |
| 1:F:166:ILE:HG23 | 1:F:167:ALA:H    | 1.79                     | 0.47              |
| 1:G:212:ARG:HA   | 1:G:212:ARG:NE   | 2.21                     | 0.47              |
| 1:H:140:VAL:HG12 | 1:H:174:ILE:CD1  | 2.45                     | 0.47              |
| 1:H:220:ALA:HB2  | 1:H:236:TYR:CE1  | 2.48                     | 0.47              |
| 1:B:212:ARG:HA   | 1:B:212:ARG:NE   | 2.21                     | 0.47              |
| 1:C:220:ALA:HB2  | 1:C:236:TYR:CE1  | 2.49                     | 0.47              |
| 1:C:161:LYS:HA   | 1:C:302:GLU:O    | 2.14                     | 0.47              |
| 1:F:158:GLU:H    | 1:F:158:GLU:CD   | 2.18                     | 0.47              |
| 1:H:159:LEU:C    | 1:H:161:LYS:N    | 2.66                     | 0.47              |
| 1:H:204:ARG:HH12 | 1:H:208:HIS:HB3  | 1.79                     | 0.47              |
| 1:B:142:PHE:CZ   | 1:B:162:LEU:HD12 | 2.50                     | 0.47              |
| 1:C:204:ARG:HH12 | 1:C:208:HIS:HB3  | 1.79                     | 0.47              |
| 1:D:269:CYS:O    | 1:D:305:ILE:CD1  | 2.63                     | 0.47              |
| 1:D:196:GLU:CB   | 1:F:169:THR:HG22 | 2.40                     | 0.47              |
| 2:M:4:DC:H2"     | 2:M:5:DA:OP2     | 2.15                     | 0.47              |
| 1:C:195:ALA:O    | 1:C:198:VAL:HG22 | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:166:ILE:CG1  | 1:E:167:ALA:N    | 2.60                     | 0.47              |
| 1:H:166:ILE:CG1  | 1:H:167:ALA:H    | 2.02                     | 0.47              |
| 1:H:176:VAL:HG21 | 1:H:251:TYR:OH   | 2.15                     | 0.47              |
| 1:A:166:ILE:HG23 | 1:A:167:ALA:H    | 1.80                     | 0.47              |
| 1:A:210:LEU:C    | 1:A:212:ARG:H    | 2.18                     | 0.47              |
| 1:D:318:ASP:O    | 1:D:319:SER:C    | 2.52                     | 0.47              |
| 1:G:166:ILE:HG23 | 1:G:167:ALA:H    | 1.78                     | 0.47              |
| 2:P:2:DA:H2"     | 2:P:3:DA:OP2     | 2.14                     | 0.47              |
| 1:A:210:LEU:C    | 1:A:212:ARG:N    | 2.68                     | 0.47              |
| 1:B:140:VAL:HG12 | 1:B:174:ILE:CD1  | 2.44                     | 0.47              |
| 1:D:220:ALA:HA   | 1:D:236:TYR:CD1  | 2.50                     | 0.47              |
| 1:E:195:ALA:O    | 1:E:198:VAL:HG22 | 2.15                     | 0.47              |
| 1:E:271:SER:O    | 1:E:272:SER:HB3  | 2.15                     | 0.47              |
| 1:G:318:ASP:O    | 1:G:319:SER:C    | 2.53                     | 0.47              |
| 1:C:280:ARG:O    | 1:C:281:PRO:C    | 2.54                     | 0.46              |
| 1:E:158:GLU:H    | 1:E:158:GLU:CD   | 2.18                     | 0.46              |
| 1:E:165:GLN:HG2  | 1:E:307:ALA:O    | 2.16                     | 0.46              |
| 1:E:216:GLU:HB2  | 1:H:264:LEU:CD1  | 2.45                     | 0.46              |
| 1:E:320:ILE:CG1  | 1:E:321:ARG:N    | 2.75                     | 0.46              |
| 1:F:159:LEU:C    | 1:F:161:LYS:N    | 2.67                     | 0.46              |
| 1:F:140:VAL:HG12 | 1:F:174:ILE:CD1  | 2.45                     | 0.46              |
| 1:G:271:SER:O    | 1:G:272:SER:HB3  | 2.15                     | 0.46              |
| 1:H:195:ALA:O    | 1:H:198:VAL:HG22 | 2.15                     | 0.46              |
| 1:H:238:GLU:CG   | 1:H:245:GLN:HG2  | 2.30                     | 0.46              |
| 1:H:269:CYS:O    | 1:H:305:ILE:CD1  | 2.62                     | 0.46              |
| 2:J:4:DC:H2"     | 2:J:5:DA:OP2     | 2.15                     | 0.46              |
| 1:B:305:ILE:O    | 1:B:305:ILE:CG1  | 2.63                     | 0.46              |
| 1:F:210:LEU:C    | 1:F:212:ARG:H    | 2.19                     | 0.46              |
| 1:F:210:LEU:C    | 1:F:212:ARG:N    | 2.69                     | 0.46              |
| 1:G:210:LEU:C    | 1:G:212:ARG:N    | 2.69                     | 0.46              |
| 1:H:210:LEU:C    | 1:H:212:ARG:N    | 2.68                     | 0.46              |
| 1:B:195:ALA:O    | 1:B:198:VAL:HG22 | 2.15                     | 0.46              |
| 1:C:159:LEU:C    | 1:C:161:LYS:N    | 2.68                     | 0.46              |
| 1:E:166:ILE:CG1  | 1:E:167:ALA:H    | 2.03                     | 0.46              |
| 2:N:1:DA:H2"     | 2:N:2:DA:O5'     | 2.15                     | 0.46              |
| 1:C:221:PRO:HB2  | 1:C:224:HIS:CD2  | 2.51                     | 0.46              |
| 1:D:142:PHE:CZ   | 1:D:162:LEU:HD12 | 2.49                     | 0.46              |
| 1:E:220:ALA:HA   | 1:E:236:TYR:CD1  | 2.50                     | 0.46              |
| 1:G:158:GLU:H    | 1:G:158:GLU:CD   | 2.18                     | 0.46              |
| 1:H:138:PHE:O    | 1:H:299:ARG:HD3  | 2.16                     | 0.46              |
| 1:H:212:ARG:NE   | 1:H:212:ARG:HA   | 2.21                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:210:LEU:C    | 1:H:212:ARG:H    | 2.18                     | 0.46              |
| 1:A:278:ASN:O    | 1:A:280:ARG:N    | 2.49                     | 0.46              |
| 1:B:220:ALA:HA   | 1:B:236:TYR:CD1  | 2.51                     | 0.46              |
| 1:D:158:GLU:CD   | 1:D:158:GLU:H    | 2.18                     | 0.46              |
| 1:D:159:LEU:C    | 1:D:161:LYS:N    | 2.67                     | 0.46              |
| 1:F:195:ALA:O    | 1:F:198:VAL:HG22 | 2.14                     | 0.46              |
| 1:G:210:LEU:C    | 1:G:212:ARG:H    | 2.19                     | 0.46              |
| 2:I:1:DA:H2''    | 2:I:2:DA:O5'     | 2.15                     | 0.46              |
| 1:B:166:ILE:HG23 | 1:B:167:ALA:H    | 1.80                     | 0.46              |
| 1:B:210:LEU:C    | 1:B:212:ARG:N    | 2.69                     | 0.46              |
| 1:C:196:GLU:CD   | 1:C:196:GLU:H    | 2.17                     | 0.46              |
| 1:D:271:SER:O    | 1:D:272:SER:HB3  | 2.16                     | 0.46              |
| 1:E:135:PRO:HD2  | 1:E:296:LEU:O    | 2.16                     | 0.46              |
| 1:E:241:ILE:HG23 | 1:E:242:THR:N    | 2.31                     | 0.46              |
| 1:E:277:MET:O    | 1:E:278:ASN:C    | 2.54                     | 0.46              |
| 1:A:244:ARG:NH1  | 1:A:244:ARG:HG2  | 2.31                     | 0.46              |
| 1:C:220:ALA:HA   | 1:C:236:TYR:CD1  | 2.50                     | 0.46              |
| 1:E:201:VAL:HG12 | 1:E:244:ARG:HG2  | 1.98                     | 0.46              |
| 1:F:220:ALA:HA   | 1:F:236:TYR:CD1  | 2.51                     | 0.46              |
| 1:F:277:MET:O    | 1:F:278:ASN:C    | 2.54                     | 0.46              |
| 1:G:220:ALA:HA   | 1:G:236:TYR:CD1  | 2.51                     | 0.46              |
| 2:K:1:DA:H2''    | 2:K:2:DA:O5'     | 2.16                     | 0.46              |
| 2:M:3:DA:C1'     | 2:M:4:DC:H5'     | 2.39                     | 0.46              |
| 1:D:143:GLN:HG2  | 1:D:144:GLN:N    | 2.29                     | 0.46              |
| 1:E:204:ARG:HH12 | 1:E:208:HIS:HB3  | 1.81                     | 0.46              |
| 1:F:183:GLY:HA2  | 1:F:291:ARG:HE   | 1.81                     | 0.46              |
| 1:F:244:ARG:HG2  | 1:F:244:ARG:HH11 | 1.80                     | 0.46              |
| 1:G:142:PHE:CZ   | 1:G:162:LEU:HD12 | 2.50                     | 0.46              |
| 1:A:159:LEU:C    | 1:A:161:LYS:N    | 2.67                     | 0.46              |
| 1:C:142:PHE:CZ   | 1:C:162:LEU:HD12 | 2.50                     | 0.46              |
| 1:C:244:ARG:NH1  | 1:C:244:ARG:HG2  | 2.31                     | 0.46              |
| 1:D:280:ARG:O    | 1:D:281:PRO:C    | 2.54                     | 0.46              |
| 1:E:305:ILE:CG1  | 1:E:305:ILE:O    | 2.64                     | 0.46              |
| 1:H:290:THR:HB   | 1:H:296:LEU:CD2  | 2.41                     | 0.46              |
| 1:A:264:LEU:CD1  | 1:D:216:GLU:CB   | 2.86                     | 0.46              |
| 1:E:220:ALA:HB2  | 1:E:236:TYR:HE1  | 1.81                     | 0.46              |
| 1:F:241:ILE:HG23 | 1:F:242:THR:N    | 2.31                     | 0.46              |
| 1:F:278:ASN:O    | 1:F:280:ARG:N    | 2.49                     | 0.46              |
| 1:A:220:ALA:HA   | 1:A:236:TYR:CD1  | 2.51                     | 0.45              |
| 1:A:241:ILE:HG23 | 1:A:242:THR:N    | 2.31                     | 0.45              |
| 1:C:176:VAL:HG21 | 1:C:251:TYR:OH   | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:238:GLU:CG   | 1:F:245:GLN:HG2  | 2.30                     | 0.45              |
| 1:H:158:GLU:H    | 1:H:158:GLU:CD   | 2.19                     | 0.45              |
| 1:H:241:ILE:HG23 | 1:H:242:THR:N    | 2.32                     | 0.45              |
| 1:A:138:PHE:O    | 1:A:299:ARG:HD3  | 2.16                     | 0.45              |
| 1:A:165:GLN:HG2  | 1:A:307:ALA:O    | 2.16                     | 0.45              |
| 1:B:189:MET:HE3  | 1:B:246:SER:HB2  | 1.98                     | 0.45              |
| 1:D:183:GLY:HA2  | 1:D:291:ARG:HE   | 1.81                     | 0.45              |
| 1:D:278:ASN:O    | 1:D:280:ARG:N    | 2.49                     | 0.45              |
| 1:D:305:ILE:CG1  | 1:D:305:ILE:O    | 2.64                     | 0.45              |
| 1:H:290:THR:OG1  | 1:H:291:ARG:N    | 2.50                     | 0.45              |
| 2:O:4:DC:H2''    | 2:O:5:DA:OP2     | 2.17                     | 0.45              |
| 1:B:278:ASN:O    | 1:B:280:ARG:N    | 2.48                     | 0.45              |
| 1:D:140:VAL:O    | 1:D:141:SER:HB3  | 2.16                     | 0.45              |
| 1:E:176:VAL:HG21 | 1:E:251:TYR:OH   | 2.16                     | 0.45              |
| 1:G:190:PRO:HG2  | 1:G:202:VAL:HG23 | 1.94                     | 0.45              |
| 1:A:224:HIS:HA   | 1:A:245:GLN:NE2  | 2.32                     | 0.45              |
| 1:C:210:LEU:C    | 1:C:212:ARG:H    | 2.20                     | 0.45              |
| 1:C:305:ILE:CG1  | 1:C:305:ILE:O    | 2.64                     | 0.45              |
| 1:F:175:LYS:HG2  | 1:F:176:VAL:N    | 2.31                     | 0.45              |
| 1:G:238:GLU:CG   | 1:G:245:GLN:HG2  | 2.30                     | 0.45              |
| 1:H:244:ARG:HH11 | 1:H:244:ARG:HG2  | 1.81                     | 0.45              |
| 1:H:271:SER:O    | 1:H:272:SER:HB3  | 2.15                     | 0.45              |
| 1:H:280:ARG:O    | 1:H:281:PRO:C    | 2.55                     | 0.45              |
| 1:A:183:GLY:HA2  | 1:A:291:ARG:HE   | 1.81                     | 0.45              |
| 1:B:241:ILE:HG23 | 1:B:242:THR:N    | 2.32                     | 0.45              |
| 1:B:176:VAL:HG21 | 1:B:251:TYR:OH   | 2.16                     | 0.45              |
| 1:B:318:ASP:O    | 1:B:320:ILE:N    | 2.50                     | 0.45              |
| 1:C:210:LEU:C    | 1:C:212:ARG:N    | 2.70                     | 0.45              |
| 1:D:210:LEU:C    | 1:D:212:ARG:H    | 2.20                     | 0.45              |
| 1:E:241:ILE:HG23 | 1:E:242:THR:CG2  | 2.41                     | 0.45              |
| 1:E:244:ARG:NH1  | 1:E:244:ARG:HG2  | 2.31                     | 0.45              |
| 1:F:165:GLN:HG2  | 1:F:307:ALA:O    | 2.16                     | 0.45              |
| 1:G:305:ILE:O    | 1:G:305:ILE:CG1  | 2.64                     | 0.45              |
| 2:L:9:DT:H5'     | 2:L:9:DT:H6      | 1.81                     | 0.45              |
| 1:A:280:ARG:O    | 1:A:281:PRO:C    | 2.54                     | 0.45              |
| 1:B:165:GLN:HG2  | 1:B:307:ALA:O    | 2.16                     | 0.45              |
| 1:C:220:ALA:HB2  | 1:C:236:TYR:HE1  | 1.82                     | 0.45              |
| 1:C:278:ASN:O    | 1:C:280:ARG:N    | 2.49                     | 0.45              |
| 1:C:304:ARG:HG2  | 1:C:304:ARG:O    | 2.15                     | 0.45              |
| 1:D:128:SER:HB2  | 1:F:255:GLN:HB3  | 1.98                     | 0.45              |
| 1:D:165:GLN:HG2  | 1:D:307:ALA:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:220:ALA:CB   | 1:E:236:TYR:CE1  | 3.00                     | 0.45              |
| 1:F:244:ARG:HG2  | 1:F:244:ARG:NH1  | 2.32                     | 0.45              |
| 1:F:280:ARG:O    | 1:F:281:PRO:C    | 2.54                     | 0.45              |
| 1:F:305:ILE:CG1  | 1:F:305:ILE:O    | 2.64                     | 0.45              |
| 1:A:176:VAL:HG21 | 1:A:251:TYR:OH   | 2.17                     | 0.45              |
| 1:A:305:ILE:O    | 1:A:305:ILE:CG1  | 2.65                     | 0.45              |
| 1:C:138:PHE:O    | 1:C:299:ARG:HD3  | 2.17                     | 0.45              |
| 1:D:196:GLU:HA   | 1:F:169:THR:CG2  | 2.45                     | 0.45              |
| 1:G:138:PHE:O    | 1:G:299:ARG:HD3  | 2.17                     | 0.45              |
| 1:G:159:LEU:C    | 1:G:161:LYS:N    | 2.66                     | 0.45              |
| 1:G:165:GLN:HG2  | 1:G:307:ALA:O    | 2.17                     | 0.45              |
| 1:G:183:GLY:HA2  | 1:G:291:ARG:HE   | 1.81                     | 0.45              |
| 2:M:10:DT:H2''   | 2:O:2:DA:H5'     | 1.97                     | 0.45              |
| 1:B:244:ARG:HH11 | 1:B:244:ARG:HG2  | 1.81                     | 0.45              |
| 1:C:313:ARG:HG3  | 1:C:313:ARG:HH11 | 1.82                     | 0.45              |
| 1:D:238:GLU:CG   | 1:D:245:GLN:HG2  | 2.30                     | 0.45              |
| 1:E:210:LEU:C    | 1:E:212:ARG:N    | 2.70                     | 0.45              |
| 1:G:176:VAL:HG21 | 1:G:251:TYR:OH   | 2.17                     | 0.45              |
| 1:C:207:ASN:ND2  | 1:D:274:VAL:C    | 2.67                     | 0.45              |
| 1:D:241:ILE:HG23 | 1:D:242:THR:N    | 2.32                     | 0.45              |
| 1:E:221:PRO:HB2  | 1:E:224:HIS:CD2  | 2.52                     | 0.45              |
| 1:E:290:THR:HB   | 1:E:296:LEU:CD2  | 2.40                     | 0.45              |
| 1:A:232:SER:HB2  | 1:D:232:SER:CB   | 2.47                     | 0.44              |
| 1:B:183:GLY:HA2  | 1:B:291:ARG:HE   | 1.81                     | 0.44              |
| 1:B:210:LEU:C    | 1:B:212:ARG:H    | 2.19                     | 0.44              |
| 1:C:241:ILE:HG23 | 1:C:242:THR:N    | 2.32                     | 0.44              |
| 1:D:184:ALA:HB1  | 1:D:251:TYR:HB3  | 1.99                     | 0.44              |
| 1:E:206:PRO:HD2  | 1:F:207:ASN:ND2  | 2.32                     | 0.44              |
| 1:F:220:ALA:HB2  | 1:F:236:TYR:HE1  | 1.82                     | 0.44              |
| 2:J:1:DA:H2''    | 2:J:2:DA:O5'     | 2.17                     | 0.44              |
| 1:B:313:ARG:HH11 | 1:B:313:ARG:HG3  | 1.83                     | 0.44              |
| 1:E:217:GLY:C    | 1:E:219:ILE:H    | 2.21                     | 0.44              |
| 1:G:220:ALA:HB2  | 1:G:236:TYR:HE1  | 1.82                     | 0.44              |
| 1:G:244:ARG:HH11 | 1:G:244:ARG:HG2  | 1.81                     | 0.44              |
| 1:H:165:GLN:HG2  | 1:H:307:ALA:O    | 2.17                     | 0.44              |
| 1:B:140:VAL:O    | 1:B:141:SER:HB3  | 2.17                     | 0.44              |
| 1:E:138:PHE:O    | 1:E:299:ARG:HD3  | 2.18                     | 0.44              |
| 1:E:210:LEU:C    | 1:E:212:ARG:H    | 2.20                     | 0.44              |
| 1:G:277:MET:O    | 1:G:278:ASN:C    | 2.55                     | 0.44              |
| 1:H:175:LYS:HG2  | 1:H:176:VAL:N    | 2.33                     | 0.44              |
| 1:H:264:LEU:N    | 1:H:264:LEU:CD1  | 2.80                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:183:GLY:HA2  | 1:H:291:ARG:HE   | 1.82                     | 0.44              |
| 2:M:9:DT:H6      | 2:M:9:DT:H5'     | 1.82                     | 0.44              |
| 1:B:244:ARG:HG2  | 1:B:244:ARG:NH1  | 2.33                     | 0.44              |
| 1:E:183:GLY:HA2  | 1:E:291:ARG:HE   | 1.81                     | 0.44              |
| 1:F:201:VAL:HG12 | 1:F:244:ARG:HG2  | 2.00                     | 0.44              |
| 1:F:271:SER:O    | 1:F:272:SER:HB3  | 2.17                     | 0.44              |
| 1:G:204:ARG:HH12 | 1:G:208:HIS:HB3  | 1.80                     | 0.44              |
| 1:G:224:HIS:HA   | 1:G:245:GLN:NE2  | 2.32                     | 0.44              |
| 2:M:5:DA:H1'     | 2:M:6:DT:H5'     | 1.99                     | 0.44              |
| 1:A:158:GLU:CD   | 1:A:158:GLU:H    | 2.19                     | 0.44              |
| 1:A:191:VAL:HG11 | 1:A:285:ILE:HD11 | 1.99                     | 0.44              |
| 1:A:271:SER:O    | 1:A:272:SER:HB3  | 2.17                     | 0.44              |
| 1:B:221:PRO:HB2  | 1:B:224:HIS:CD2  | 2.52                     | 0.44              |
| 1:C:183:GLY:HA2  | 1:C:291:ARG:HE   | 1.82                     | 0.44              |
| 1:D:138:PHE:O    | 1:D:299:ARG:HD3  | 2.18                     | 0.44              |
| 1:F:204:ARG:HH12 | 1:F:208:HIS:HB3  | 1.82                     | 0.44              |
| 1:F:221:PRO:HB2  | 1:F:224:HIS:CD2  | 2.52                     | 0.44              |
| 1:G:220:ALA:CB   | 1:G:236:TYR:CE1  | 3.01                     | 0.44              |
| 2:M:10:DT:H2''   | 2:O:1:DA:C1'     | 2.48                     | 0.44              |
| 2:N:6:DT:H1'     | 2:N:7:DG:C8      | 2.53                     | 0.44              |
| 1:B:158:GLU:H    | 1:B:158:GLU:CD   | 2.19                     | 0.44              |
| 1:C:271:SER:O    | 1:C:272:SER:HB3  | 2.17                     | 0.44              |
| 1:C:277:MET:O    | 1:C:278:ASN:C    | 2.55                     | 0.44              |
| 1:D:277:MET:O    | 1:D:278:ASN:C    | 2.55                     | 0.44              |
| 1:E:140:VAL:O    | 1:E:141:SER:HB3  | 2.18                     | 0.44              |
| 1:E:184:ALA:HB1  | 1:E:251:TYR:HB3  | 2.00                     | 0.44              |
| 2:L:5:DA:H1'     | 2:L:6:DT:H5'     | 2.00                     | 0.44              |
| 1:B:277:MET:O    | 1:B:278:ASN:C    | 2.55                     | 0.44              |
| 1:D:176:VAL:HG21 | 1:D:251:TYR:OH   | 2.17                     | 0.44              |
| 1:D:196:GLU:OE1  | 1:F:152:THR:HG21 | 2.17                     | 0.44              |
| 1:D:210:LEU:C    | 1:D:212:ARG:N    | 2.70                     | 0.44              |
| 1:G:140:VAL:O    | 1:G:141:SER:HB3  | 2.18                     | 0.44              |
| 1:G:241:ILE:HG23 | 1:G:242:THR:N    | 2.32                     | 0.44              |
| 1:H:184:ALA:HB1  | 1:H:251:TYR:HB3  | 2.00                     | 0.44              |
| 1:H:220:ALA:HB2  | 1:H:236:TYR:HE1  | 1.82                     | 0.44              |
| 1:H:313:ARG:HG3  | 1:H:313:ARG:HH11 | 1.83                     | 0.44              |
| 1:A:201:VAL:HG12 | 1:A:244:ARG:HG2  | 1.99                     | 0.44              |
| 1:A:277:MET:O    | 1:A:278:ASN:C    | 2.55                     | 0.44              |
| 1:C:255:GLN:CD   | 1:E:128:SER:HB2  | 2.37                     | 0.44              |
| 1:D:244:ARG:HH11 | 1:D:244:ARG:HG2  | 1.81                     | 0.44              |
| 1:F:290:THR:HB   | 1:F:296:LEU:CD2  | 2.41                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:288:LEU:O    | 1:G:296:LEU:HB2  | 2.18                     | 0.44              |
| 1:H:140:VAL:O    | 1:H:141:SER:HB3  | 2.17                     | 0.44              |
| 1:H:305:ILE:O    | 1:H:305:ILE:CG1  | 2.65                     | 0.44              |
| 2:L:1:DA:H2''    | 2:L:2:DA:O5'     | 2.18                     | 0.44              |
| 1:B:201:VAL:HG12 | 1:B:244:ARG:HG2  | 1.99                     | 0.44              |
| 1:C:290:THR:OG1  | 1:C:291:ARG:N    | 2.51                     | 0.44              |
| 1:D:196:GLU:CB   | 1:F:169:THR:CG2  | 2.95                     | 0.44              |
| 1:E:209:GLU:HB2  | 1:E:222:PRO:O    | 2.18                     | 0.44              |
| 1:F:140:VAL:O    | 1:F:141:SER:HB3  | 2.18                     | 0.44              |
| 1:G:175:LYS:HG2  | 1:G:176:VAL:N    | 2.33                     | 0.44              |
| 1:H:201:VAL:HG12 | 1:H:244:ARG:HG2  | 2.00                     | 0.44              |
| 1:H:209:GLU:HB2  | 1:H:222:PRO:O    | 2.18                     | 0.44              |
| 1:A:184:ALA:HB1  | 1:A:251:TYR:HB3  | 2.00                     | 0.43              |
| 1:B:138:PHE:O    | 1:B:299:ARG:HD3  | 2.18                     | 0.43              |
| 1:C:217:GLY:C    | 1:C:219:ILE:H    | 2.21                     | 0.43              |
| 1:D:220:ALA:HB2  | 1:D:236:TYR:HE1  | 1.83                     | 0.43              |
| 1:G:244:ARG:HG2  | 1:G:244:ARG:NH1  | 2.33                     | 0.43              |
| 1:G:313:ARG:HG3  | 1:G:313:ARG:HH11 | 1.82                     | 0.43              |
| 2:O:9:DT:H5'     | 2:O:9:DT:H6      | 1.83                     | 0.43              |
| 1:A:221:PRO:HB2  | 1:A:224:HIS:CD2  | 2.52                     | 0.43              |
| 1:A:290:THR:OG1  | 1:A:291:ARG:N    | 2.51                     | 0.43              |
| 1:B:280:ARG:O    | 1:B:281:PRO:C    | 2.55                     | 0.43              |
| 1:E:159:LEU:C    | 1:E:161:LYS:N    | 2.67                     | 0.43              |
| 1:E:313:ARG:HH11 | 1:E:313:ARG:HG3  | 1.83                     | 0.43              |
| 1:G:290:THR:HB   | 1:G:296:LEU:CD2  | 2.40                     | 0.43              |
| 1:H:221:PRO:HB2  | 1:H:224:HIS:CD2  | 2.53                     | 0.43              |
| 1:H:224:HIS:HA   | 1:H:245:GLN:NE2  | 2.33                     | 0.43              |
| 1:A:313:ARG:HH11 | 1:A:313:ARG:HG3  | 1.83                     | 0.43              |
| 1:B:209:GLU:HB2  | 1:B:222:PRO:O    | 2.18                     | 0.43              |
| 1:D:220:ALA:CB   | 1:D:236:TYR:CE1  | 3.02                     | 0.43              |
| 1:D:290:THR:HB   | 1:D:296:LEU:CD2  | 2.41                     | 0.43              |
| 2:J:3:DA:C1'     | 2:J:4:DC:H5'     | 2.40                     | 0.43              |
| 2:N:5:DA:H1'     | 2:N:6:DT:H5''    | 2.00                     | 0.43              |
| 1:F:158:GLU:CD   | 1:F:159:LEU:N    | 2.69                     | 0.43              |
| 1:F:212:ARG:HA   | 1:F:212:ARG:NE   | 2.21                     | 0.43              |
| 1:F:290:THR:OG1  | 1:F:291:ARG:N    | 2.52                     | 0.43              |
| 1:A:220:ALA:CB   | 1:A:236:TYR:CE1  | 3.01                     | 0.43              |
| 1:B:217:GLY:C    | 1:B:219:ILE:H    | 2.21                     | 0.43              |
| 1:B:184:ALA:HB1  | 1:B:251:TYR:HB3  | 2.00                     | 0.43              |
| 1:C:148:ALA:O    | 1:C:150:SER:N    | 2.46                     | 0.43              |
| 1:C:165:GLN:HG2  | 1:C:307:ALA:O    | 2.17                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:201:VAL:HG12 | 1:C:244:ARG:HG2  | 1.99                     | 0.43              |
| 1:C:220:ALA:CB   | 1:C:236:TYR:CE1  | 3.01                     | 0.43              |
| 1:D:221:PRO:HB2  | 1:D:224:HIS:CD2  | 2.54                     | 0.43              |
| 1:D:290:THR:OG1  | 1:D:291:ARG:N    | 2.52                     | 0.43              |
| 1:E:175:LYS:HG2  | 1:E:176:VAL:N    | 2.33                     | 0.43              |
| 1:G:217:GLY:C    | 1:G:219:ILE:H    | 2.20                     | 0.43              |
| 1:G:221:PRO:HB2  | 1:G:224:HIS:CD2  | 2.53                     | 0.43              |
| 2:J:5:DA:H1'     | 2:J:6:DT:H5'     | 2.01                     | 0.43              |
| 1:A:220:ALA:HB2  | 1:A:236:TYR:HE1  | 1.83                     | 0.43              |
| 1:C:175:LYS:HG2  | 1:C:176:VAL:N    | 2.33                     | 0.43              |
| 1:C:184:ALA:HB1  | 1:C:251:TYR:HB3  | 2.00                     | 0.43              |
| 1:H:191:VAL:HG11 | 1:H:285:ILE:HD11 | 2.00                     | 0.43              |
| 1:A:140:VAL:O    | 1:A:141:SER:HB3  | 2.19                     | 0.43              |
| 1:B:224:HIS:HA   | 1:B:245:GLN:NE2  | 2.33                     | 0.43              |
| 1:C:239:ASP:OD1  | 1:C:240:PRO:HD2  | 2.19                     | 0.43              |
| 1:D:244:ARG:NH1  | 1:D:244:ARG:HG2  | 2.33                     | 0.43              |
| 1:D:224:HIS:HA   | 1:D:245:GLN:NE2  | 2.33                     | 0.43              |
| 1:E:224:HIS:HA   | 1:E:245:GLN:NE2  | 2.34                     | 0.43              |
| 1:F:209:GLU:HB2  | 1:F:222:PRO:O    | 2.18                     | 0.43              |
| 1:G:295:VAL:HG22 | 1:G:296:LEU:N    | 2.34                     | 0.43              |
| 1:H:220:ALA:CB   | 1:H:236:TYR:CE1  | 3.00                     | 0.43              |
| 1:H:244:ARG:NH1  | 1:H:244:ARG:HG2  | 2.33                     | 0.43              |
| 1:A:209:GLU:HB2  | 1:A:222:PRO:O    | 2.19                     | 0.43              |
| 1:F:220:ALA:CB   | 1:F:236:TYR:CE1  | 3.02                     | 0.43              |
| 1:G:201:VAL:HG12 | 1:G:244:ARG:HG2  | 1.99                     | 0.43              |
| 2:J:9:DT:H1'     | 2:J:10:DT:C5'    | 2.49                     | 0.43              |
| 1:A:175:LYS:HG2  | 1:A:176:VAL:N    | 2.33                     | 0.43              |
| 1:D:313:ARG:HH11 | 1:D:313:ARG:HG3  | 1.84                     | 0.43              |
| 1:E:239:ASP:OD1  | 1:E:240:PRO:HD2  | 2.19                     | 0.43              |
| 1:F:217:GLY:C    | 1:F:219:ILE:H    | 2.22                     | 0.43              |
| 1:F:224:HIS:HA   | 1:F:245:GLN:NE2  | 2.33                     | 0.43              |
| 1:B:220:ALA:CB   | 1:B:236:TYR:CE1  | 3.02                     | 0.43              |
| 1:D:201:VAL:HG12 | 1:D:244:ARG:HG2  | 1.99                     | 0.43              |
| 1:F:176:VAL:HG21 | 1:F:251:TYR:OH   | 2.18                     | 0.43              |
| 1:G:209:GLU:HB2  | 1:G:222:PRO:O    | 2.19                     | 0.43              |
| 2:I:5:DA:H1'     | 2:I:6:DT:H5''    | 2.01                     | 0.43              |
| 2:I:5:DA:C2'     | 2:I:6:DT:H5'     | 2.48                     | 0.43              |
| 1:D:175:LYS:HG2  | 1:D:176:VAL:N    | 2.33                     | 0.42              |
| 1:D:217:GLY:C    | 1:D:219:ILE:H    | 2.22                     | 0.42              |
| 1:C:169:THR:CG2  | 1:E:196:GLU:CD   | 2.87                     | 0.42              |
| 1:E:278:ASN:O    | 1:E:280:ARG:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:138:PHE:O    | 1:F:299:ARG:HD3  | 2.18                     | 0.42              |
| 1:H:278:ASN:HA   | 1:H:279:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:217:GLY:C    | 1:A:219:ILE:H    | 2.20                     | 0.42              |
| 1:B:220:ALA:HB2  | 1:B:236:TYR:HE1  | 1.83                     | 0.42              |
| 1:C:158:GLU:CD   | 1:C:159:LEU:N    | 2.71                     | 0.42              |
| 1:C:158:GLU:N    | 1:C:158:GLU:CD   | 2.73                     | 0.42              |
| 1:H:217:GLY:C    | 1:H:219:ILE:H    | 2.22                     | 0.42              |
| 2:O:5:DA:H1'     | 2:O:6:DT:H5'     | 2.01                     | 0.42              |
| 1:B:278:ASN:HA   | 1:B:279:ARG:HH12 | 1.84                     | 0.42              |
| 1:B:191:VAL:HG11 | 1:B:285:ILE:HD11 | 2.00                     | 0.42              |
| 1:E:212:ARG:HA   | 1:E:212:ARG:NE   | 2.22                     | 0.42              |
| 1:F:184:ALA:HB1  | 1:F:251:TYR:HB3  | 2.00                     | 0.42              |
| 1:G:184:ALA:HB1  | 1:G:251:TYR:HB3  | 2.01                     | 0.42              |
| 1:B:311:ARG:NH2  | 2:J:7:DG:N7      | 2.45                     | 0.42              |
| 1:A:201:VAL:HA   | 1:A:244:ARG:HH12 | 1.85                     | 0.42              |
| 1:B:175:LYS:HG2  | 1:B:176:VAL:N    | 2.33                     | 0.42              |
| 1:D:209:GLU:HB2  | 1:D:222:PRO:O    | 2.18                     | 0.42              |
| 1:F:288:LEU:O    | 1:F:296:LEU:HB2  | 2.19                     | 0.42              |
| 1:G:158:GLU:N    | 1:G:158:GLU:CD   | 2.73                     | 0.42              |
| 2:J:9:DT:H5'     | 2:J:9:DT:H6      | 1.84                     | 0.42              |
| 1:B:290:THR:OG1  | 1:B:291:ARG:N    | 2.53                     | 0.42              |
| 1:C:140:VAL:O    | 1:C:141:SER:HB3  | 2.19                     | 0.42              |
| 1:F:136:HIS:HB3  | 1:F:178:THR:O    | 2.20                     | 0.42              |
| 1:G:279:ARG:CB   | 2:O:6:DT:OP1     | 2.67                     | 0.42              |
| 1:G:191:VAL:HG11 | 1:G:285:ILE:HD11 | 2.01                     | 0.42              |
| 1:G:290:THR:OG1  | 1:G:291:ARG:N    | 2.53                     | 0.42              |
| 1:B:288:LEU:O    | 1:B:296:LEU:HB2  | 2.19                     | 0.42              |
| 1:E:280:ARG:O    | 1:E:281:PRO:C    | 2.56                     | 0.42              |
| 1:F:166:ILE:CG1  | 1:F:167:ALA:N    | 2.60                     | 0.42              |
| 1:G:159:LEU:O    | 1:G:160:LYS:C    | 2.58                     | 0.42              |
| 1:G:264:LEU:N    | 1:G:264:LEU:CD1  | 2.82                     | 0.42              |
| 1:H:239:ASP:OD1  | 1:H:240:PRO:HD2  | 2.19                     | 0.42              |
| 1:H:288:LEU:O    | 1:H:296:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:136:HIS:HB3  | 1:A:178:THR:O    | 2.20                     | 0.42              |
| 1:C:290:THR:HG23 | 1:C:293:GLY:H    | 1.85                     | 0.42              |
| 1:C:169:THR:CB   | 1:E:196:GLU:HB3  | 2.49                     | 0.42              |
| 1:F:213:GLU:O    | 1:F:214:PHE:CB   | 2.67                     | 0.42              |
| 1:F:239:ASP:OD1  | 1:F:240:PRO:HD2  | 2.20                     | 0.42              |
| 1:G:136:HIS:HB3  | 1:G:178:THR:O    | 2.19                     | 0.42              |
| 1:H:277:MET:O    | 1:H:278:ASN:C    | 2.56                     | 0.42              |
| 1:H:295:VAL:HG22 | 1:H:296:LEU:N    | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:9:DT:H1'     | 2:L:10:DT:C5'    | 2.50                     | 0.42              |
| 2:M:1:DA:H2''    | 2:M:2:DA:O5'     | 2.19                     | 0.42              |
| 1:C:136:HIS:HB3  | 1:C:178:THR:O    | 2.19                     | 0.42              |
| 1:C:304:ARG:HH11 | 1:C:304:ARG:HG3  | 1.84                     | 0.42              |
| 1:E:288:LEU:O    | 1:E:296:LEU:HB2  | 2.19                     | 0.42              |
| 1:F:158:GLU:OE2  | 1:F:159:LEU:HG   | 2.20                     | 0.42              |
| 1:H:213:GLU:O    | 1:H:214:PHE:CB   | 2.68                     | 0.42              |
| 1:H:241:ILE:HG23 | 1:H:242:THR:CG2  | 2.43                     | 0.42              |
| 1:A:158:GLU:OE2  | 1:A:159:LEU:HG   | 2.20                     | 0.42              |
| 1:A:187:ARG:HG3  | 1:A:246:SER:OG   | 2.20                     | 0.42              |
| 1:A:264:LEU:N    | 1:A:264:LEU:CD1  | 2.83                     | 0.42              |
| 1:B:204:ARG:HH12 | 1:B:208:HIS:HB3  | 1.81                     | 0.42              |
| 2:I:3:DA:H1'     | 2:I:4:DC:H5'     | 2.01                     | 0.42              |
| 1:B:215:ASN:HD22 | 1:B:215:ASN:N    | 2.18                     | 0.42              |
| 1:C:213:GLU:O    | 1:C:214:PHE:CB   | 2.68                     | 0.42              |
| 1:D:158:GLU:CD   | 1:D:158:GLU:N    | 2.73                     | 0.42              |
| 1:D:239:ASP:OD1  | 1:D:240:PRO:HD2  | 2.20                     | 0.42              |
| 1:E:158:GLU:CD   | 1:E:158:GLU:N    | 2.73                     | 0.42              |
| 1:F:158:GLU:N    | 1:F:158:GLU:CD   | 2.73                     | 0.42              |
| 2:O:1:DA:H2''    | 2:O:2:DA:O5'     | 2.19                     | 0.42              |
| 2:P:5:DA:C2'     | 2:P:6:DT:H5'     | 2.48                     | 0.42              |
| 2:P:6:DT:H1'     | 2:P:7:DG:C8      | 2.55                     | 0.42              |
| 1:D:213:GLU:O    | 1:D:214:PHE:CB   | 2.66                     | 0.41              |
| 1:E:308:CYS:O    | 1:E:310:GLY:N    | 2.53                     | 0.41              |
| 1:F:264:LEU:N    | 1:F:264:LEU:CD1  | 2.83                     | 0.41              |
| 2:P:5:DA:H1'     | 2:P:6:DT:H5''    | 2.01                     | 0.41              |
| 1:A:148:ALA:O    | 1:A:150:SER:N    | 2.48                     | 0.41              |
| 1:B:136:HIS:HB3  | 1:B:178:THR:O    | 2.20                     | 0.41              |
| 1:B:213:GLU:O    | 1:B:214:PHE:CB   | 2.68                     | 0.41              |
| 1:C:221:PRO:HB2  | 1:C:224:HIS:HD2  | 1.84                     | 0.41              |
| 1:D:304:ARG:HH11 | 1:D:304:ARG:HG3  | 1.85                     | 0.41              |
| 1:F:304:ARG:HG3  | 1:F:304:ARG:HH11 | 1.85                     | 0.41              |
| 2:I:7:DG:H1'     | 2:I:8:DT:H5'     | 2.02                     | 0.41              |
| 1:B:201:VAL:HA   | 1:B:244:ARG:HH12 | 1.85                     | 0.41              |
| 1:B:221:PRO:HB2  | 1:B:224:HIS:HD2  | 1.85                     | 0.41              |
| 1:B:187:ARG:HG3  | 1:B:246:SER:OG   | 2.20                     | 0.41              |
| 1:C:169:THR:HB   | 1:E:196:GLU:HB3  | 2.01                     | 0.41              |
| 1:D:278:ASN:HA   | 1:D:279:ARG:HH12 | 1.85                     | 0.41              |
| 1:E:278:ASN:HA   | 1:E:279:ARG:HH12 | 1.84                     | 0.41              |
| 1:E:290:THR:OG1  | 1:E:291:ARG:N    | 2.53                     | 0.41              |
| 1:H:201:VAL:HA   | 1:H:244:ARG:HH12 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:5:DA:H1'     | 2:K:6:DT:H5''    | 2.00                     | 0.41              |
| 2:P:7:DG:H1'     | 2:P:8:DT:H5'     | 2.02                     | 0.41              |
| 1:A:290:THR:HB   | 1:A:296:LEU:CD2  | 2.41                     | 0.41              |
| 1:B:158:GLU:CD   | 1:B:159:LEU:N    | 2.72                     | 0.41              |
| 1:E:148:ALA:O    | 1:E:150:SER:N    | 2.46                     | 0.41              |
| 1:E:213:GLU:O    | 1:E:214:PHE:CB   | 2.68                     | 0.41              |
| 1:E:320:ILE:HG13 | 1:E:321:ARG:H    | 1.81                     | 0.41              |
| 1:F:148:ALA:O    | 1:F:150:SER:N    | 2.47                     | 0.41              |
| 1:F:295:VAL:HG22 | 1:F:297:GLY:H    | 1.84                     | 0.41              |
| 2:M:9:DT:H1'     | 2:M:10:DT:C5'    | 2.51                     | 0.41              |
| 1:B:158:GLU:N    | 1:B:158:GLU:CD   | 2.74                     | 0.41              |
| 1:B:318:ASP:O    | 1:B:319:SER:C    | 2.59                     | 0.41              |
| 1:C:255:GLN:NE2  | 1:E:128:SER:HB2  | 2.36                     | 0.41              |
| 1:C:308:CYS:O    | 1:C:310:GLY:N    | 2.54                     | 0.41              |
| 1:D:241:ILE:HG23 | 1:D:242:THR:CG2  | 2.43                     | 0.41              |
| 1:D:264:LEU:CD1  | 1:D:264:LEU:N    | 2.83                     | 0.41              |
| 1:D:295:VAL:HG22 | 1:D:296:LEU:N    | 2.35                     | 0.41              |
| 1:D:308:CYS:O    | 1:D:310:GLY:N    | 2.53                     | 0.41              |
| 1:G:187:ARG:HG3  | 1:G:246:SER:OG   | 2.21                     | 0.41              |
| 1:H:158:GLU:OE2  | 1:H:159:LEU:HG   | 2.19                     | 0.41              |
| 2:O:3:DA:C1'     | 2:O:4:DC:H5'     | 2.39                     | 0.41              |
| 1:A:158:GLU:CD   | 1:A:159:LEU:N    | 2.69                     | 0.41              |
| 1:A:215:ASN:N    | 1:A:215:ASN:HD22 | 2.18                     | 0.41              |
| 1:B:159:LEU:O    | 1:B:160:LYS:C    | 2.58                     | 0.41              |
| 1:C:209:GLU:HB2  | 1:C:222:PRO:O    | 2.20                     | 0.41              |
| 1:D:215:ASN:N    | 1:D:215:ASN:HD22 | 2.16                     | 0.41              |
| 1:E:318:ASP:O    | 1:E:321:ARG:N    | 2.53                     | 0.41              |
| 1:F:295:VAL:HG22 | 1:F:296:LEU:N    | 2.36                     | 0.41              |
| 1:G:213:GLU:O    | 1:G:214:PHE:CB   | 2.68                     | 0.41              |
| 1:A:221:PRO:HB2  | 1:A:224:HIS:HD2  | 1.86                     | 0.41              |
| 1:B:279:ARG:HB2  | 2:J:6:DT:OP1     | 2.21                     | 0.41              |
| 1:C:191:VAL:HG11 | 1:C:285:ILE:HD11 | 2.01                     | 0.41              |
| 1:C:224:HIS:HA   | 1:C:245:GLN:NE2  | 2.36                     | 0.41              |
| 1:C:187:ARG:HG3  | 1:C:246:SER:OG   | 2.21                     | 0.41              |
| 1:C:288:LEU:O    | 1:C:296:LEU:HB2  | 2.21                     | 0.41              |
| 1:D:136:HIS:HB3  | 1:D:178:THR:O    | 2.20                     | 0.41              |
| 1:D:187:ARG:HG3  | 1:D:246:SER:OG   | 2.21                     | 0.41              |
| 1:E:201:VAL:HA   | 1:E:244:ARG:HH12 | 1.85                     | 0.41              |
| 1:A:278:ASN:HA   | 1:A:279:ARG:HH12 | 1.86                     | 0.41              |
| 1:C:210:LEU:CD1  | 1:D:206:PRO:HB3  | 2.51                     | 0.41              |
| 1:E:215:ASN:N    | 1:E:215:ASN:HD22 | 2.19                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:221:PRO:HB2  | 1:E:224:HIS:HD2  | 1.86                     | 0.41              |
| 1:E:304:ARG:HG3  | 1:E:304:ARG:HH11 | 1.85                     | 0.41              |
| 1:D:191:VAL:HG11 | 1:D:285:ILE:HD11 | 2.01                     | 0.41              |
| 1:E:187:ARG:HG3  | 1:E:246:SER:OG   | 2.20                     | 0.41              |
| 1:F:255:GLN:O    | 1:F:256:VAL:C    | 2.59                     | 0.41              |
| 1:G:226:ILE:HG12 | 1:G:267:PHE:CE2  | 2.56                     | 0.41              |
| 1:H:158:GLU:CD   | 1:H:159:LEU:N    | 2.70                     | 0.41              |
| 2:K:3:DA:H1'     | 2:K:4:DC:H5'     | 2.02                     | 0.41              |
| 1:A:290:THR:HG23 | 1:A:293:GLY:H    | 1.86                     | 0.41              |
| 1:C:201:VAL:HA   | 1:C:244:ARG:HH12 | 1.86                     | 0.41              |
| 1:G:295:VAL:HG22 | 1:G:297:GLY:H    | 1.86                     | 0.41              |
| 1:H:158:GLU:N    | 1:H:158:GLU:CD   | 2.74                     | 0.41              |
| 2:K:6:DT:H1'     | 2:K:7:DG:C8      | 2.56                     | 0.41              |
| 1:D:158:GLU:OE2  | 1:D:159:LEU:HG   | 2.21                     | 0.41              |
| 1:D:163:TYR:HD1  | 1:D:163:TYR:N    | 2.19                     | 0.41              |
| 1:H:215:ASN:HD22 | 1:H:215:ASN:N    | 2.19                     | 0.41              |
| 1:H:255:GLN:O    | 1:H:256:VAL:C    | 2.60                     | 0.41              |
| 2:N:3:DA:H1'     | 2:N:4:DC:H5'     | 2.03                     | 0.41              |
| 1:A:239:ASP:OD1  | 1:A:240:PRO:HD2  | 2.21                     | 0.40              |
| 1:A:304:ARG:HH11 | 1:A:304:ARG:HG3  | 1.87                     | 0.40              |
| 1:B:255:GLN:O    | 1:B:256:VAL:C    | 2.59                     | 0.40              |
| 1:B:295:VAL:HG22 | 1:B:296:LEU:N    | 2.36                     | 0.40              |
| 1:B:304:ARG:HG3  | 1:B:304:ARG:HH11 | 1.86                     | 0.40              |
| 1:C:166:ILE:CG2  | 1:C:167:ALA:H    | 2.34                     | 0.40              |
| 1:D:288:LEU:O    | 1:D:296:LEU:HB2  | 2.20                     | 0.40              |
| 1:E:264:LEU:CD1  | 1:E:264:LEU:N    | 2.83                     | 0.40              |
| 1:F:187:ARG:HG3  | 1:F:246:SER:OG   | 2.20                     | 0.40              |
| 1:G:163:TYR:N    | 1:G:163:TYR:HD1  | 2.19                     | 0.40              |
| 1:G:183:GLY:HA3  | 1:G:291:ARG:HB2  | 2.03                     | 0.40              |
| 2:N:6:DT:H2''    | 2:N:7:DG:C8      | 2.56                     | 0.40              |
| 1:A:232:SER:HB2  | 1:D:232:SER:HB3  | 2.01                     | 0.40              |
| 1:D:221:PRO:HB2  | 1:D:224:HIS:HD2  | 1.87                     | 0.40              |
| 1:E:189:MET:HG3  | 1:E:190:PRO:HD2  | 2.02                     | 0.40              |
| 1:F:278:ASN:HA   | 1:F:279:ARG:HH12 | 1.86                     | 0.40              |
| 1:H:136:HIS:HB3  | 1:H:178:THR:O    | 2.21                     | 0.40              |
| 1:H:226:ILE:HG12 | 1:H:267:PHE:CE2  | 2.56                     | 0.40              |
| 1:D:166:ILE:CG2  | 1:D:167:ALA:H    | 2.35                     | 0.40              |
| 1:E:192:TYR:OH   | 1:E:280:ARG:NH2  | 2.54                     | 0.40              |
| 1:F:166:ILE:CG2  | 1:F:167:ALA:H    | 2.34                     | 0.40              |
| 1:F:191:VAL:HG11 | 1:F:285:ILE:HD11 | 2.02                     | 0.40              |
| 1:B:279:ARG:CB   | 2:J:6:DT:OP1     | 2.69                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:213:GLU:O    | 1:A:214:PHE:CB   | 2.69                     | 0.40              |
| 1:B:264:LEU:N    | 1:B:264:LEU:CD1  | 2.83                     | 0.40              |
| 1:C:290:THR:HB   | 1:C:296:LEU:CD2  | 2.42                     | 0.40              |
| 1:E:159:LEU:O    | 1:E:160:LYS:C    | 2.59                     | 0.40              |
| 1:E:255:GLN:O    | 1:E:256:VAL:C    | 2.60                     | 0.40              |
| 1:H:308:CYS:O    | 1:H:310:GLY:N    | 2.54                     | 0.40              |
| 1:D:159:LEU:O    | 1:D:160:LYS:C    | 2.59                     | 0.40              |
| 1:E:158:GLU:OE2  | 1:E:159:LEU:HG   | 2.21                     | 0.40              |
| 1:E:191:VAL:HG11 | 1:E:285:ILE:HD11 | 2.03                     | 0.40              |
| 1:F:159:LEU:O    | 1:F:160:LYS:C    | 2.59                     | 0.40              |
| 1:F:290:THR:HG23 | 1:F:293:GLY:H    | 1.87                     | 0.40              |
| 1:G:158:GLU:CD   | 1:G:159:LEU:N    | 2.70                     | 0.40              |
| 1:H:159:LEU:O    | 1:H:160:LYS:C    | 2.58                     | 0.40              |
| 1:H:192:TYR:OH   | 1:H:280:ARG:NH2  | 2.55                     | 0.40              |
| 1:H:290:THR:HG23 | 1:H:293:GLY:H    | 1.87                     | 0.40              |
| 2:O:9:DT:H1'     | 2:O:10:DT:C5'    | 2.51                     | 0.40              |

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:C:291:ARG:NH1 | 1:E:239:ASP:OD1[2_555] | 1.98                     | 0.22              |
| 1:C:233:HIS:CE1 | 1:C:233:HIS:CE1[2_555] | 2.02                     | 0.18              |
| 1:H:132:TYR:OH  | 1:H:132:TYR:OH[2_455]  | 2.05                     | 0.15              |
| 1:C:235:GLN:OE1 | 1:E:240:PRO:O[2_555]   | 2.07                     | 0.13              |

## 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     | 188/203 (93%) | 131 (70%) | 39 (21%) | 18 (10%) | <b>0</b> <b>3</b> |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|-----------|----------|-------------|---|
| 1   | B     | 187/203 (92%)   | 131 (70%)  | 39 (21%)  | 17 (9%)  | 1           | 3 |
| 1   | C     | 193/203 (95%)   | 132 (68%)  | 43 (22%)  | 18 (9%)  | 0           | 3 |
| 1   | D     | 194/203 (96%)   | 134 (69%)  | 42 (22%)  | 18 (9%)  | 0           | 3 |
| 1   | E     | 195/203 (96%)   | 135 (69%)  | 42 (22%)  | 18 (9%)  | 1           | 3 |
| 1   | F     | 193/203 (95%)   | 133 (69%)  | 42 (22%)  | 18 (9%)  | 0           | 3 |
| 1   | G     | 186/203 (92%)   | 129 (69%)  | 40 (22%)  | 17 (9%)  | 1           | 3 |
| 1   | H     | 185/203 (91%)   | 130 (70%)  | 38 (20%)  | 17 (9%)  | 1           | 3 |
| All | All   | 1521/1624 (94%) | 1055 (69%) | 325 (21%) | 141 (9%) | 0           | 3 |

All (141) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 148 | ALA  |
| 1   | A     | 166 | ILE  |
| 1   | A     | 172 | ILE  |
| 1   | A     | 256 | VAL  |
| 1   | A     | 272 | SER  |
| 1   | A     | 279 | ARG  |
| 1   | A     | 319 | SER  |
| 1   | B     | 166 | ILE  |
| 1   | B     | 172 | ILE  |
| 1   | B     | 181 | PRO  |
| 1   | B     | 256 | VAL  |
| 1   | B     | 272 | SER  |
| 1   | B     | 279 | ARG  |
| 1   | B     | 319 | SER  |
| 1   | C     | 148 | ALA  |
| 1   | C     | 166 | ILE  |
| 1   | C     | 172 | ILE  |
| 1   | C     | 256 | VAL  |
| 1   | C     | 272 | SER  |
| 1   | C     | 279 | ARG  |
| 1   | C     | 319 | SER  |
| 1   | D     | 148 | ALA  |
| 1   | D     | 166 | ILE  |
| 1   | D     | 172 | ILE  |
| 1   | D     | 256 | VAL  |
| 1   | D     | 272 | SER  |
| 1   | D     | 279 | ARG  |
| 1   | D     | 319 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 148 | ALA  |
| 1   | E     | 166 | ILE  |
| 1   | E     | 172 | ILE  |
| 1   | E     | 181 | PRO  |
| 1   | E     | 256 | VAL  |
| 1   | E     | 272 | SER  |
| 1   | E     | 279 | ARG  |
| 1   | E     | 319 | SER  |
| 1   | F     | 148 | ALA  |
| 1   | F     | 166 | ILE  |
| 1   | F     | 172 | ILE  |
| 1   | F     | 256 | VAL  |
| 1   | F     | 272 | SER  |
| 1   | F     | 279 | ARG  |
| 1   | F     | 319 | SER  |
| 1   | G     | 166 | ILE  |
| 1   | G     | 172 | ILE  |
| 1   | G     | 181 | PRO  |
| 1   | G     | 256 | VAL  |
| 1   | G     | 272 | SER  |
| 1   | G     | 279 | ARG  |
| 1   | G     | 319 | SER  |
| 1   | H     | 165 | GLN  |
| 1   | H     | 166 | ILE  |
| 1   | H     | 172 | ILE  |
| 1   | H     | 256 | VAL  |
| 1   | H     | 272 | SER  |
| 1   | H     | 279 | ARG  |
| 1   | H     | 319 | SER  |
| 1   | A     | 165 | GLN  |
| 1   | A     | 181 | PRO  |
| 1   | A     | 184 | ALA  |
| 1   | A     | 191 | VAL  |
| 1   | A     | 196 | GLU  |
| 1   | A     | 211 | SER  |
| 1   | B     | 165 | GLN  |
| 1   | B     | 184 | ALA  |
| 1   | B     | 191 | VAL  |
| 1   | B     | 196 | GLU  |
| 1   | B     | 211 | SER  |
| 1   | C     | 165 | GLN  |
| 1   | C     | 181 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 184 | ALA  |
| 1   | C     | 196 | GLU  |
| 1   | C     | 211 | SER  |
| 1   | D     | 165 | GLN  |
| 1   | D     | 181 | PRO  |
| 1   | D     | 184 | ALA  |
| 1   | D     | 196 | GLU  |
| 1   | D     | 211 | SER  |
| 1   | E     | 165 | GLN  |
| 1   | E     | 184 | ALA  |
| 1   | E     | 191 | VAL  |
| 1   | E     | 196 | GLU  |
| 1   | E     | 211 | SER  |
| 1   | F     | 165 | GLN  |
| 1   | F     | 181 | PRO  |
| 1   | F     | 184 | ALA  |
| 1   | F     | 191 | VAL  |
| 1   | F     | 196 | GLU  |
| 1   | F     | 211 | SER  |
| 1   | G     | 165 | GLN  |
| 1   | G     | 184 | ALA  |
| 1   | G     | 191 | VAL  |
| 1   | G     | 196 | GLU  |
| 1   | G     | 211 | SER  |
| 1   | H     | 181 | PRO  |
| 1   | H     | 184 | ALA  |
| 1   | H     | 191 | VAL  |
| 1   | H     | 196 | GLU  |
| 1   | H     | 211 | SER  |
| 1   | A     | 210 | LEU  |
| 1   | A     | 318 | ASP  |
| 1   | B     | 210 | LEU  |
| 1   | B     | 318 | ASP  |
| 1   | C     | 191 | VAL  |
| 1   | C     | 210 | LEU  |
| 1   | C     | 318 | ASP  |
| 1   | D     | 191 | VAL  |
| 1   | D     | 210 | LEU  |
| 1   | E     | 210 | LEU  |
| 1   | E     | 318 | ASP  |
| 1   | F     | 210 | LEU  |
| 1   | G     | 210 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 210 | LEU  |
| 1   | D     | 318 | ASP  |
| 1   | F     | 312 | ASP  |
| 1   | F     | 318 | ASP  |
| 1   | G     | 318 | ASP  |
| 1   | H     | 318 | ASP  |
| 1   | A     | 312 | ASP  |
| 1   | B     | 312 | ASP  |
| 1   | C     | 312 | ASP  |
| 1   | D     | 312 | ASP  |
| 1   | E     | 312 | ASP  |
| 1   | G     | 312 | ASP  |
| 1   | H     | 312 | ASP  |
| 1   | B     | 171 | PRO  |
| 1   | C     | 171 | PRO  |
| 1   | D     | 171 | PRO  |
| 1   | D     | 276 | GLY  |
| 1   | F     | 171 | PRO  |
| 1   | H     | 171 | PRO  |
| 1   | A     | 171 | PRO  |
| 1   | A     | 276 | GLY  |
| 1   | B     | 276 | GLY  |
| 1   | C     | 276 | GLY  |
| 1   | E     | 171 | PRO  |
| 1   | E     | 276 | GLY  |
| 1   | F     | 276 | GLY  |
| 1   | G     | 171 | PRO  |
| 1   | G     | 276 | GLY  |
| 1   | H     | 276 | GLY  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |
|-----|-------|---------------|-----------|----------|-------------|
| 1   | A     | 169/179 (94%) | 148 (88%) | 21 (12%) | 4 21        |
| 1   | B     | 170/179 (95%) | 149 (88%) | 21 (12%) | 4 21        |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | C     | 172/179 (96%)   | 150 (87%)  | 22 (13%)  | 4           | 20 |
| 1   | D     | 172/179 (96%)   | 151 (88%)  | 21 (12%)  | 5           | 22 |
| 1   | E     | 173/179 (97%)   | 150 (87%)  | 23 (13%)  | 4           | 18 |
| 1   | F     | 172/179 (96%)   | 150 (87%)  | 22 (13%)  | 4           | 20 |
| 1   | G     | 168/179 (94%)   | 146 (87%)  | 22 (13%)  | 4           | 19 |
| 1   | H     | 168/179 (94%)   | 146 (87%)  | 22 (13%)  | 4           | 19 |
| All | All   | 1364/1432 (95%) | 1190 (87%) | 174 (13%) | 4           | 20 |

All (174) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 158 | GLU  |
| 1   | A     | 163 | TYR  |
| 1   | A     | 164 | CYS  |
| 1   | A     | 176 | VAL  |
| 1   | A     | 177 | MET  |
| 1   | A     | 178 | THR  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 202 | VAL  |
| 1   | A     | 204 | ARG  |
| 1   | A     | 212 | ARG  |
| 1   | A     | 216 | GLU  |
| 1   | A     | 249 | VAL  |
| 1   | A     | 259 | GLU  |
| 1   | A     | 269 | CYS  |
| 1   | A     | 279 | ARG  |
| 1   | A     | 282 | ILE  |
| 1   | A     | 283 | LEU  |
| 1   | A     | 287 | THR  |
| 1   | A     | 305 | ILE  |
| 1   | A     | 312 | ASP  |
| 1   | A     | 313 | ARG  |
| 1   | B     | 144 | GLN  |
| 1   | B     | 158 | GLU  |
| 1   | B     | 163 | TYR  |
| 1   | B     | 164 | CYS  |
| 1   | B     | 176 | VAL  |
| 1   | B     | 177 | MET  |
| 1   | B     | 178 | THR  |
| 1   | B     | 182 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 202 | VAL  |
| 1   | B     | 204 | ARG  |
| 1   | B     | 212 | ARG  |
| 1   | B     | 216 | GLU  |
| 1   | B     | 259 | GLU  |
| 1   | B     | 269 | CYS  |
| 1   | B     | 279 | ARG  |
| 1   | B     | 282 | ILE  |
| 1   | B     | 283 | LEU  |
| 1   | B     | 287 | THR  |
| 1   | B     | 305 | ILE  |
| 1   | B     | 312 | ASP  |
| 1   | B     | 313 | ARG  |
| 1   | C     | 132 | TYR  |
| 1   | C     | 144 | GLN  |
| 1   | C     | 158 | GLU  |
| 1   | C     | 163 | TYR  |
| 1   | C     | 164 | CYS  |
| 1   | C     | 176 | VAL  |
| 1   | C     | 177 | MET  |
| 1   | C     | 178 | THR  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 202 | VAL  |
| 1   | C     | 204 | ARG  |
| 1   | C     | 212 | ARG  |
| 1   | C     | 216 | GLU  |
| 1   | C     | 259 | GLU  |
| 1   | C     | 269 | CYS  |
| 1   | C     | 279 | ARG  |
| 1   | C     | 282 | ILE  |
| 1   | C     | 283 | LEU  |
| 1   | C     | 287 | THR  |
| 1   | C     | 305 | ILE  |
| 1   | C     | 312 | ASP  |
| 1   | C     | 313 | ARG  |
| 1   | D     | 144 | GLN  |
| 1   | D     | 158 | GLU  |
| 1   | D     | 163 | TYR  |
| 1   | D     | 164 | CYS  |
| 1   | D     | 176 | VAL  |
| 1   | D     | 177 | MET  |
| 1   | D     | 178 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 182 | GLN  |
| 1   | D     | 202 | VAL  |
| 1   | D     | 204 | ARG  |
| 1   | D     | 212 | ARG  |
| 1   | D     | 216 | GLU  |
| 1   | D     | 259 | GLU  |
| 1   | D     | 269 | CYS  |
| 1   | D     | 279 | ARG  |
| 1   | D     | 282 | ILE  |
| 1   | D     | 283 | LEU  |
| 1   | D     | 287 | THR  |
| 1   | D     | 305 | ILE  |
| 1   | D     | 312 | ASP  |
| 1   | D     | 313 | ARG  |
| 1   | E     | 132 | TYR  |
| 1   | E     | 144 | GLN  |
| 1   | E     | 158 | GLU  |
| 1   | E     | 163 | TYR  |
| 1   | E     | 164 | CYS  |
| 1   | E     | 176 | VAL  |
| 1   | E     | 177 | MET  |
| 1   | E     | 178 | THR  |
| 1   | E     | 182 | GLN  |
| 1   | E     | 202 | VAL  |
| 1   | E     | 204 | ARG  |
| 1   | E     | 212 | ARG  |
| 1   | E     | 216 | GLU  |
| 1   | E     | 249 | VAL  |
| 1   | E     | 259 | GLU  |
| 1   | E     | 269 | CYS  |
| 1   | E     | 279 | ARG  |
| 1   | E     | 282 | ILE  |
| 1   | E     | 283 | LEU  |
| 1   | E     | 287 | THR  |
| 1   | E     | 305 | ILE  |
| 1   | E     | 312 | ASP  |
| 1   | E     | 313 | ARG  |
| 1   | F     | 144 | GLN  |
| 1   | F     | 158 | GLU  |
| 1   | F     | 163 | TYR  |
| 1   | F     | 164 | CYS  |
| 1   | F     | 176 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 177 | MET  |
| 1   | F     | 178 | THR  |
| 1   | F     | 182 | GLN  |
| 1   | F     | 202 | VAL  |
| 1   | F     | 204 | ARG  |
| 1   | F     | 212 | ARG  |
| 1   | F     | 216 | GLU  |
| 1   | F     | 249 | VAL  |
| 1   | F     | 259 | GLU  |
| 1   | F     | 269 | CYS  |
| 1   | F     | 279 | ARG  |
| 1   | F     | 282 | ILE  |
| 1   | F     | 283 | LEU  |
| 1   | F     | 287 | THR  |
| 1   | F     | 305 | ILE  |
| 1   | F     | 312 | ASP  |
| 1   | F     | 313 | ARG  |
| 1   | G     | 144 | GLN  |
| 1   | G     | 158 | GLU  |
| 1   | G     | 163 | TYR  |
| 1   | G     | 164 | CYS  |
| 1   | G     | 176 | VAL  |
| 1   | G     | 177 | MET  |
| 1   | G     | 178 | THR  |
| 1   | G     | 182 | GLN  |
| 1   | G     | 202 | VAL  |
| 1   | G     | 204 | ARG  |
| 1   | G     | 212 | ARG  |
| 1   | G     | 216 | GLU  |
| 1   | G     | 249 | VAL  |
| 1   | G     | 259 | GLU  |
| 1   | G     | 269 | CYS  |
| 1   | G     | 279 | ARG  |
| 1   | G     | 282 | ILE  |
| 1   | G     | 283 | LEU  |
| 1   | G     | 287 | THR  |
| 1   | G     | 305 | ILE  |
| 1   | G     | 312 | ASP  |
| 1   | G     | 313 | ARG  |
| 1   | H     | 144 | GLN  |
| 1   | H     | 158 | GLU  |
| 1   | H     | 163 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 164 | CYS  |
| 1   | H     | 176 | VAL  |
| 1   | H     | 177 | MET  |
| 1   | H     | 178 | THR  |
| 1   | H     | 182 | GLN  |
| 1   | H     | 202 | VAL  |
| 1   | H     | 204 | ARG  |
| 1   | H     | 212 | ARG  |
| 1   | H     | 216 | GLU  |
| 1   | H     | 249 | VAL  |
| 1   | H     | 259 | GLU  |
| 1   | H     | 269 | CYS  |
| 1   | H     | 279 | ARG  |
| 1   | H     | 282 | ILE  |
| 1   | H     | 283 | LEU  |
| 1   | H     | 287 | THR  |
| 1   | H     | 305 | ILE  |
| 1   | H     | 312 | ASP  |
| 1   | H     | 313 | ARG  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 207 | ASN  |
| 1   | A     | 215 | ASN  |
| 1   | A     | 218 | GLN  |
| 1   | A     | 224 | HIS  |
| 1   | A     | 266 | ASN  |
| 1   | A     | 278 | ASN  |
| 1   | B     | 207 | ASN  |
| 1   | B     | 215 | ASN  |
| 1   | B     | 218 | GLN  |
| 1   | B     | 224 | HIS  |
| 1   | B     | 266 | ASN  |
| 1   | B     | 278 | ASN  |
| 1   | C     | 207 | ASN  |
| 1   | C     | 215 | ASN  |
| 1   | C     | 218 | GLN  |
| 1   | C     | 224 | HIS  |
| 1   | C     | 255 | GLN  |
| 1   | C     | 266 | ASN  |
| 1   | C     | 278 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 207 | ASN  |
| 1   | D     | 215 | ASN  |
| 1   | D     | 218 | GLN  |
| 1   | D     | 224 | HIS  |
| 1   | D     | 266 | ASN  |
| 1   | D     | 278 | ASN  |
| 1   | E     | 215 | ASN  |
| 1   | E     | 218 | GLN  |
| 1   | E     | 224 | HIS  |
| 1   | E     | 266 | ASN  |
| 1   | E     | 278 | ASN  |
| 1   | F     | 215 | ASN  |
| 1   | F     | 218 | GLN  |
| 1   | F     | 224 | HIS  |
| 1   | F     | 266 | ASN  |
| 1   | F     | 278 | ASN  |
| 1   | G     | 207 | ASN  |
| 1   | G     | 215 | ASN  |
| 1   | G     | 218 | GLN  |
| 1   | G     | 224 | HIS  |
| 1   | G     | 266 | ASN  |
| 1   | G     | 278 | ASN  |
| 1   | H     | 207 | ASN  |
| 1   | H     | 215 | ASN  |
| 1   | H     | 218 | GLN  |
| 1   | H     | 224 | HIS  |
| 1   | H     | 266 | ASN  |
| 1   | H     | 278 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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     | 192/203 (94%)   | -0.01  | 7 (3%) 42 27  | 99, 154, 212, 235     | 0     |
| 1   | B     | 191/203 (94%)   | -0.04  | 7 (3%) 41 26  | 104, 156, 215, 247    | 0     |
| 1   | C     | 195/203 (96%)   | -0.19  | 0 100 100     | 66, 118, 175, 218     | 0     |
| 1   | D     | 196/203 (96%)   | -0.17  | 2 (1%) 82 72  | 83, 137, 204, 237     | 0     |
| 1   | E     | 197/203 (97%)   | -0.18  | 2 (1%) 82 72  | 76, 123, 197, 244     | 0     |
| 1   | F     | 195/203 (96%)   | -0.17  | 3 (1%) 73 61  | 81, 130, 193, 218     | 0     |
| 1   | G     | 190/203 (93%)   | -0.06  | 4 (2%) 63 49  | 90, 140, 202, 227     | 0     |
| 1   | H     | 189/203 (93%)   | -0.09  | 3 (1%) 72 59  | 81, 141, 196, 233     | 0     |
| 2   | I     | 10/10 (100%)    | -0.69  | 0 100 100     | 93, 112, 127, 128     | 0     |
| 2   | J     | 10/10 (100%)    | -0.63  | 0 100 100     | 97, 110, 118, 118     | 0     |
| 2   | K     | 10/10 (100%)    | -0.64  | 0 100 100     | 75, 100, 119, 120     | 0     |
| 2   | L     | 10/10 (100%)    | -0.52  | 0 100 100     | 89, 98, 114, 117      | 0     |
| 2   | M     | 10/10 (100%)    | -0.66  | 0 100 100     | 82, 94, 101, 111      | 0     |
| 2   | N     | 10/10 (100%)    | -0.60  | 0 100 100     | 79, 98, 120, 120      | 0     |
| 2   | O     | 10/10 (100%)    | -0.55  | 0 100 100     | 93, 104, 110, 115     | 0     |
| 2   | P     | 10/10 (100%)    | -0.57  | 0 100 100     | 79, 95, 112, 114      | 0     |
| All | All   | 1625/1704 (95%) | -0.14  | 28 (1%) 70 57 | 66, 137, 205, 247     | 0     |

All (28) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 144 | GLN  | 5.6  |
| 1   | A     | 239 | ASP  | 4.1  |
| 1   | G     | 182 | GLN  | 3.2  |
| 1   | D     | 177 | MET  | 3.0  |
| 1   | A     | 240 | PRO  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 292 | ASP  | 2.8  |
| 1   | A     | 147 | THR  | 2.7  |
| 1   | H     | 150 | SER  | 2.7  |
| 1   | F     | 238 | GLU  | 2.7  |
| 1   | A     | 238 | GLU  | 2.7  |
| 1   | H     | 238 | GLU  | 2.7  |
| 1   | F     | 292 | ASP  | 2.7  |
| 1   | G     | 292 | ASP  | 2.6  |
| 1   | D     | 148 | ALA  | 2.5  |
| 1   | H     | 218 | GLN  | 2.5  |
| 1   | F     | 138 | PHE  | 2.5  |
| 1   | A     | 218 | GLN  | 2.4  |
| 1   | G     | 229 | GLU  | 2.4  |
| 1   | A     | 243 | GLY  | 2.3  |
| 1   | E     | 148 | ALA  | 2.2  |
| 1   | B     | 159 | LEU  | 2.2  |
| 1   | B     | 218 | GLN  | 2.2  |
| 1   | E     | 151 | ALA  | 2.2  |
| 1   | A     | 150 | SER  | 2.2  |
| 1   | B     | 259 | GLU  | 2.1  |
| 1   | B     | 187 | ARG  | 2.1  |
| 1   | B     | 194 | LYS  | 2.0  |
| 1   | B     | 256 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|
|-----|------|-------|-----|-------|------|-----|-----------------------------|-------|

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | ZN   | D     | 901 | 1/1   | 0.92 | 0.22 | 116,116,116,116             | 0     |
| 3   | ZN   | B     | 901 | 1/1   | 0.96 | 0.17 | 132,132,132,132             | 0     |
| 3   | ZN   | G     | 901 | 1/1   | 0.97 | 0.19 | 140,140,140,140             | 0     |
| 3   | ZN   | E     | 901 | 1/1   | 0.97 | 0.20 | 126,126,126,126             | 0     |
| 3   | ZN   | A     | 901 | 1/1   | 0.98 | 0.15 | 155,155,155,155             | 0     |
| 3   | ZN   | F     | 901 | 1/1   | 0.98 | 0.17 | 112,112,112,112             | 0     |
| 3   | ZN   | H     | 901 | 1/1   | 0.99 | 0.20 | 140,140,140,140             | 0     |
| 3   | ZN   | C     | 901 | 1/1   | 1.00 | 0.15 | 99,99,99,99                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.