



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:51 AM UTC

PDB ID : 2EL9 / pdb\_00002el9  
Title : Crystal structure of E.coli Histidyl-tRNA synthetase complexed with a histidyl-adenylate analogue  
Authors : Yanagisawa, T.; Si, S.Y.; Matsuno, M.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-03-27  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

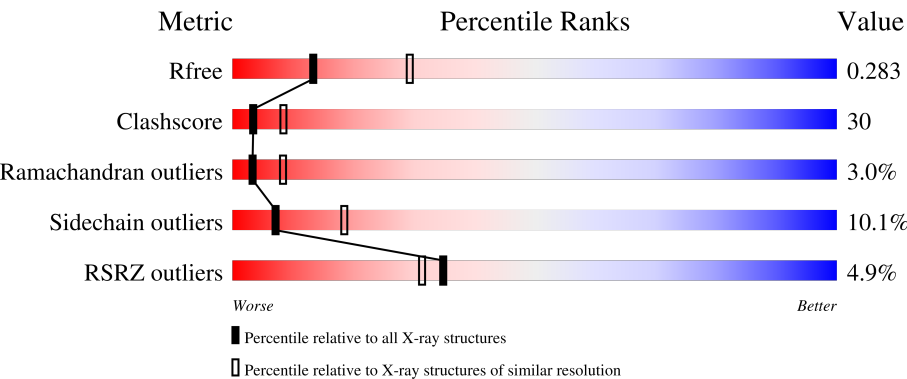
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 3538 (2.70-2.70)                                      |
| Clashscore            | 190562                      | 3843 (2.70-2.70)                                      |
| Ramachandran outliers | 187476                      | 3778 (2.70-2.70)                                      |
| Sidechain outliers    | 187428                      | 3778 (2.70-2.70)                                      |
| RSRZ outliers         | 180081                      | 3538 (2.70-2.70)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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     | 431    | <div><div>4%</div><div><div></div><div>39%</div><div>39%</div><div>8%</div><div>14%</div></div></div> |
| 1   | B     | 431    | <div><div>3%</div><div><div></div><div>48%</div><div>33%</div><div>5%</div><div>13%</div></div></div> |
| 1   | C     | 431    | <div><div>5%</div><div><div></div><div>43%</div><div>36%</div><div>7%</div><div>14%</div></div></div> |
| 1   | D     | 431    | <div><div>4%</div><div><div></div><div>46%</div><div>35%</div><div>7%</div><div>11%</div></div></div> |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | HSS  | C     | 710 | -         | -        | X       | -                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12050 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 Histidyl-tRNA synthetase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 372      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2903  | 1826 | 521 | 545 | 11 |         |         |       |
| 1   | B     | 376      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2923  | 1837 | 525 | 550 | 11 |         |         |       |
| 1   | C     | 372      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2899  | 1822 | 521 | 545 | 11 |         |         |       |
| 1   | D     | 385      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2993  | 1883 | 535 | 564 | 11 |         |         |       |

There are 28 discrepancies between the modelled and reference sequences:

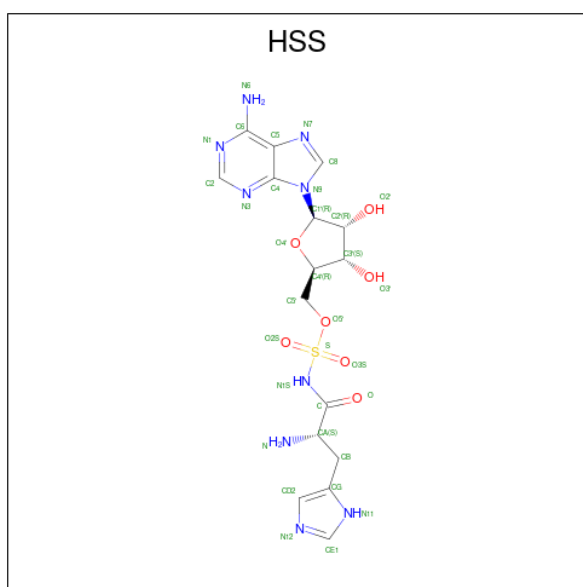
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -6      | GLY      | -      | expression tag | UNP P60906 |
| A     | -5      | PRO      | -      | expression tag | UNP P60906 |
| A     | -4      | GLY      | -      | expression tag | UNP P60906 |
| A     | -3      | TYR      | -      | expression tag | UNP P60906 |
| A     | -2      | GLN      | -      | expression tag | UNP P60906 |
| A     | -1      | ASP      | -      | expression tag | UNP P60906 |
| A     | 0       | PRO      | -      | expression tag | UNP P60906 |
| B     | -6      | GLY      | -      | expression tag | UNP P60906 |
| B     | -5      | PRO      | -      | expression tag | UNP P60906 |
| B     | -4      | GLY      | -      | expression tag | UNP P60906 |
| B     | -3      | TYR      | -      | expression tag | UNP P60906 |
| B     | -2      | GLN      | -      | expression tag | UNP P60906 |
| B     | -1      | ASP      | -      | expression tag | UNP P60906 |
| B     | 0       | PRO      | -      | expression tag | UNP P60906 |
| C     | -6      | GLY      | -      | expression tag | UNP P60906 |
| C     | -5      | PRO      | -      | expression tag | UNP P60906 |
| C     | -4      | GLY      | -      | expression tag | UNP P60906 |
| C     | -3      | TYR      | -      | expression tag | UNP P60906 |
| C     | -2      | GLN      | -      | expression tag | UNP P60906 |
| C     | -1      | ASP      | -      | expression tag | UNP P60906 |
| C     | 0       | PRO      | -      | expression tag | UNP P60906 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -6      | GLY      | -      | expression tag | UNP P60906 |
| D     | -5      | PRO      | -      | expression tag | UNP P60906 |
| D     | -4      | GLY      | -      | expression tag | UNP P60906 |
| D     | -3      | TYR      | -      | expression tag | UNP P60906 |
| D     | -2      | GLN      | -      | expression tag | UNP P60906 |
| D     | -1      | ASP      | -      | expression tag | UNP P60906 |
| D     | 0       | PRO      | -      | expression tag | UNP P60906 |

- Molecule 2 is 5'-O-[(L-HISTIDYLAMINO)SULFONYL]ADENOSINE (CCD ID: HSS) (formula: C<sub>16</sub>H<sub>21</sub>N<sub>9</sub>O<sub>7</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 33    | 16 | 9 | 7 | 1 |         |         |
| 2   | B     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 33    | 16 | 9 | 7 | 1 |         |         |
| 2   | C     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 33    | 16 | 9 | 7 | 1 |         |         |
| 2   | D     | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 33    | 16 | 9 | 7 | 1 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |

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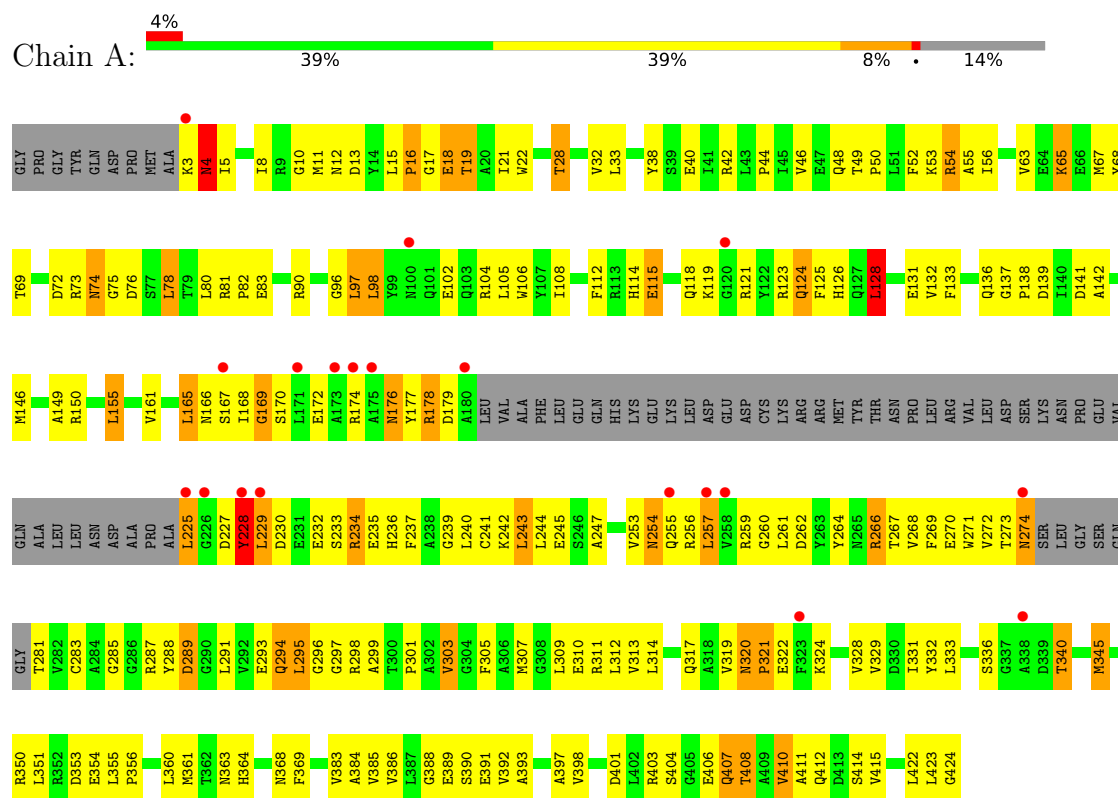
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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | B     | 49       | Total<br>49 | O<br>49 | 0       | 0       |
| 3   | C     | 45       | Total<br>45 | O<br>45 | 0       | 0       |
| 3   | D     | 66       | Total<br>66 | O<br>66 | 0       | 0       |

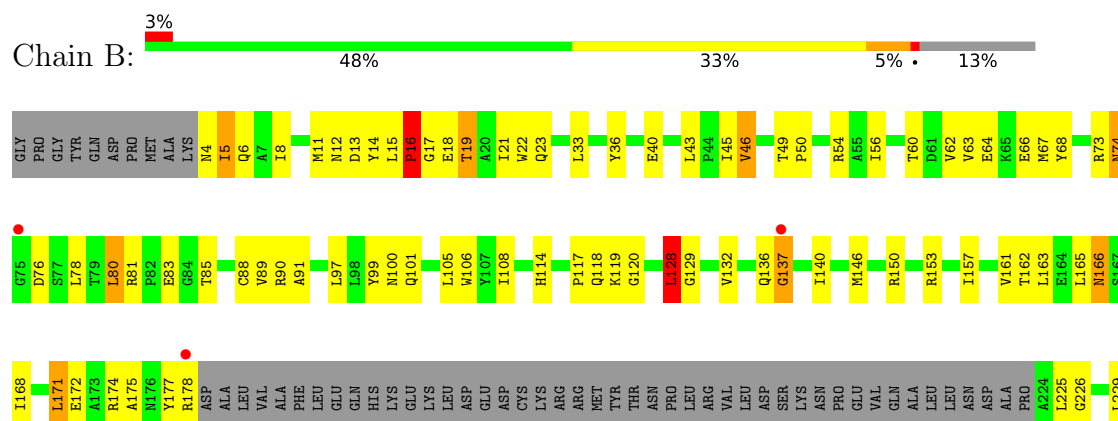
### 3 Residue-property plots

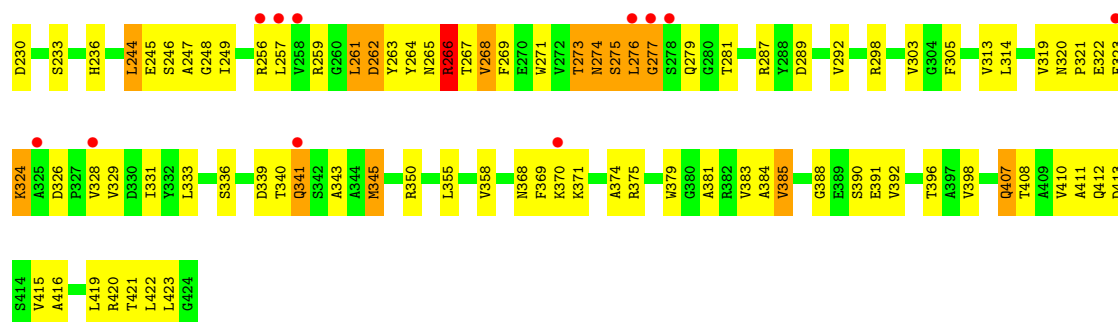
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Histidyl-tRNA synthetase

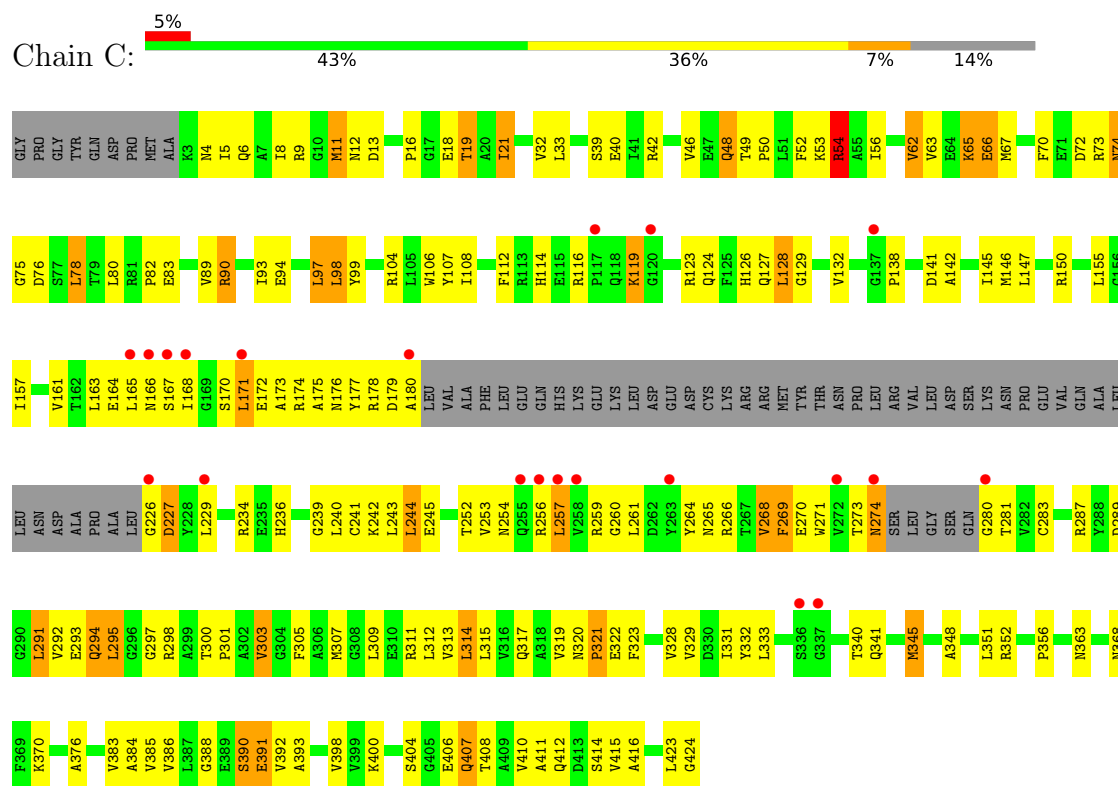


#### • Molecule 1: Histidyl-tRNA synthetase

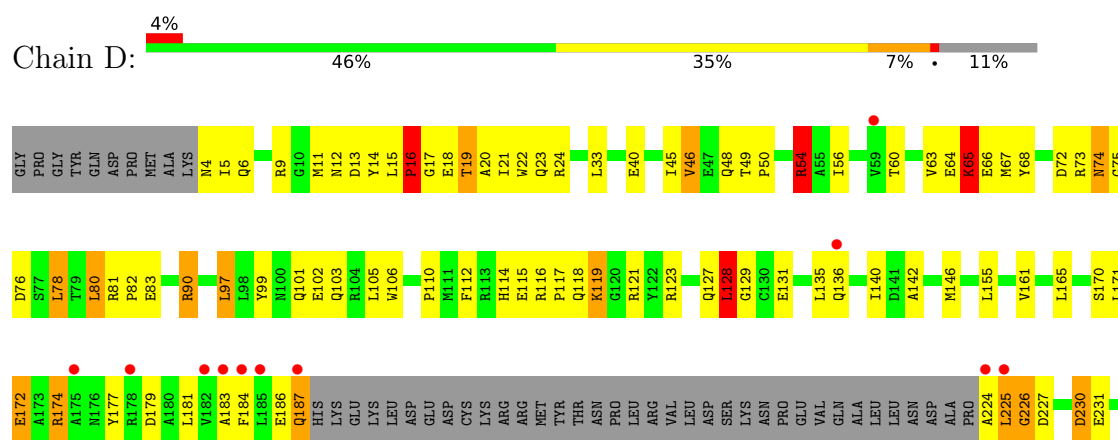




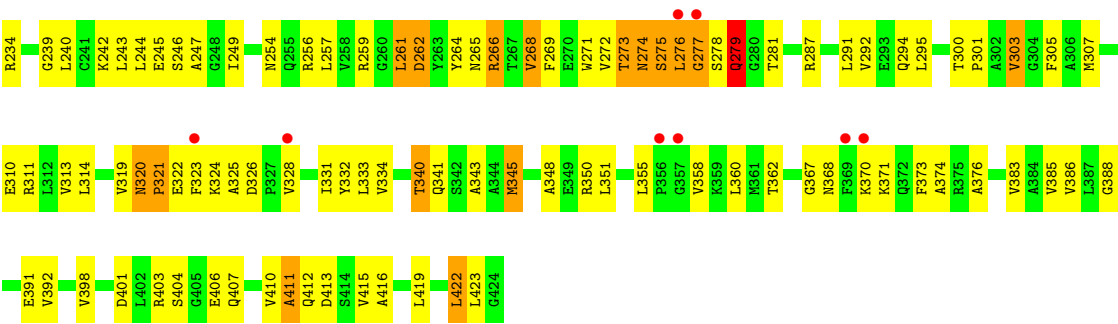
• Molecule 1: Histidyl-tRNA synthetase



• Molecule 1: Histidyl-tRNA synthetase







## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 60.11Å 108.34Å 193.65Å<br>90.00° 98.21° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 48.80 – 2.70<br>48.80 – 2.70                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.3 (48.80-2.70)<br>95.4 (48.80-2.70)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.11 (at 2.69Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.285<br>0.224 , 0.283                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 6521 reflections (10.11%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.335                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 77.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$ | Xtriage          |
| Estimated twinning fraction                                             | 0.000 for h,-k,-h-l                                         | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 12050                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8788e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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     | 0.57         | 0/2955      | 1.09        | 21/3995 (0.5%)  |
| 1   | B     | 0.62         | 0/2976      | 1.08        | 18/4025 (0.4%)  |
| 1   | C     | 0.54         | 0/2951      | 1.02        | 11/3989 (0.3%)  |
| 1   | D     | 0.61         | 0/3047      | 1.10        | 14/4122 (0.3%)  |
| All | All   | 0.59         | 0/11929     | 1.07        | 64/16131 (0.4%) |

There are no bond length outliers.

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | D     | 340 | THR  | N-CA-C  | -10.86 | 100.17      | 113.41   |
| 1   | A     | 340 | THR  | N-CA-C  | -8.86  | 102.48      | 113.38   |
| 1   | B     | 12  | ASN  | N-CA-C  | 8.49   | 122.01      | 110.55   |
| 1   | D     | 291 | LEU  | N-CA-C  | -7.42  | 104.20      | 113.55   |
| 1   | D     | 269 | PHE  | N-CA-C  | 7.39   | 120.30      | 109.07   |
| 1   | A     | 355 | LEU  | CA-C-N  | -6.99  | 112.79      | 119.85   |
| 1   | A     | 355 | LEU  | C-N-CA  | -6.99  | 112.79      | 119.85   |
| 1   | A     | 410 | VAL  | N-CA-C  | 6.88   | 118.72      | 108.46   |
| 1   | C     | 97  | LEU  | N-CA-C  | -6.86  | 104.58      | 114.12   |
| 1   | B     | 340 | THR  | N-CA-C  | -6.67  | 105.01      | 113.01   |
| 1   | C     | 66  | GLU  | N-CA-C  | 6.60   | 122.83      | 114.31   |
| 1   | C     | 94  | GLU  | N-CA-C  | 6.50   | 119.19      | 111.33   |
| 1   | D     | 12  | ASN  | N-CA-C  | 6.45   | 120.06      | 110.52   |
| 1   | D     | 367 | GLY  | N-CA-C  | -6.37  | 105.54      | 112.04   |
| 1   | B     | 266 | ARG  | CB-CA-C | -6.34  | 109.25      | 116.54   |
| 1   | C     | 356 | PRO  | N-CA-C  | -6.24  | 101.47      | 111.38   |
| 1   | B     | 85  | THR  | N-CA-C  | 6.23   | 117.74      | 111.07   |
| 1   | A     | 12  | ASN  | N-CA-C  | 6.18   | 120.00      | 110.42   |
| 1   | B     | 5   | ILE  | N-CA-C  | 6.08   | 117.89      | 109.80   |
| 1   | C     | 128 | LEU  | CA-C-N  | -6.03  | 118.02      | 122.18   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 128 | LEU  | C-N-CA  | -6.03 | 118.02      | 122.18   |
| 1   | A     | 53  | LYS  | N-CA-C  | -6.01 | 104.07      | 111.40   |
| 1   | B     | 137 | GLY  | CA-C-N  | 5.98  | 125.60      | 119.56   |
| 1   | B     | 137 | GLY  | C-N-CA  | 5.98  | 125.60      | 119.56   |
| 1   | D     | 266 | ARG  | CB-CA-C | -5.95 | 109.14      | 117.23   |
| 1   | D     | 65  | LYS  | N-CA-C  | 5.94  | 120.38      | 112.30   |
| 1   | D     | 128 | LEU  | N-CA-C  | -5.91 | 97.50       | 108.02   |
| 1   | C     | 269 | PHE  | N-CA-C  | 5.88  | 118.00      | 109.07   |
| 1   | A     | 176 | ASN  | N-CA-C  | -5.85 | 107.13      | 114.56   |
| 1   | A     | 4   | ASN  | N-CA-C  | 5.81  | 123.18      | 110.80   |
| 1   | D     | 66  | GLU  | N-CA-C  | 5.81  | 121.80      | 114.31   |
| 1   | C     | 128 | LEU  | N-CA-C  | -5.68 | 97.91       | 108.02   |
| 1   | A     | 128 | LEU  | N-CA-C  | -5.67 | 98.09       | 108.02   |
| 1   | B     | 263 | TYR  | N-CA-C  | 5.67  | 119.89      | 112.92   |
| 1   | C     | 12  | ASN  | N-CA-C  | 5.60  | 118.81      | 110.52   |
| 1   | A     | 126 | HIS  | N-CA-C  | 5.60  | 118.52      | 109.40   |
| 1   | D     | 411 | ALA  | N-CA-C  | -5.51 | 102.13      | 110.28   |
| 1   | D     | 81  | ARG  | N-CA-C  | 5.50  | 117.52      | 109.71   |
| 1   | B     | 105 | LEU  | N-CA-C  | 5.42  | 118.54      | 110.14   |
| 1   | A     | 289 | ASP  | N-CA-C  | 5.41  | 118.09      | 111.82   |
| 1   | A     | 115 | GLU  | N-CA-C  | -5.40 | 102.02      | 110.17   |
| 1   | B     | 128 | LEU  | N-CA-C  | -5.39 | 98.43       | 108.02   |
| 1   | B     | 45  | ILE  | N-CA-C  | -5.38 | 105.47      | 110.53   |
| 1   | B     | 269 | PHE  | N-CA-C  | 5.34  | 116.91      | 108.96   |
| 1   | B     | 248 | GLY  | CA-C-N  | -5.28 | 116.15      | 122.90   |
| 1   | B     | 248 | GLY  | C-N-CA  | -5.28 | 116.15      | 122.90   |
| 1   | A     | 128 | LEU  | CA-C-N  | -5.25 | 118.56      | 122.18   |
| 1   | A     | 128 | LEU  | C-N-CA  | -5.25 | 118.56      | 122.18   |
| 1   | A     | 356 | PRO  | N-CA-C  | -5.24 | 103.06      | 111.38   |
| 1   | A     | 124 | GLN  | N-CA-C  | -5.23 | 98.87       | 108.02   |
| 1   | A     | 262 | ASP  | N-CA-C  | 5.22  | 117.23      | 110.65   |
| 1   | B     | 324 | LYS  | N-CA-C  | 5.20  | 116.57      | 109.18   |
| 1   | A     | 81  | ARG  | CA-C-N  | 5.17  | 127.15      | 120.89   |
| 1   | A     | 81  | ARG  | C-N-CA  | 5.17  | 127.15      | 120.89   |
| 1   | A     | 97  | LEU  | N-CA-C  | -5.16 | 105.33      | 113.02   |
| 1   | B     | 267 | THR  | N-CA-C  | 5.13  | 117.91      | 110.42   |
| 1   | C     | 126 | HIS  | N-CA-C  | 5.12  | 117.75      | 109.40   |
| 1   | B     | 262 | ASP  | N-CA-C  | 5.11  | 119.23      | 113.15   |
| 1   | D     | 54  | ARG  | N-CA-C  | 5.05  | 116.64      | 111.03   |
| 1   | C     | 340 | THR  | N-CA-C  | -5.05 | 106.38      | 112.54   |
| 1   | D     | 174 | ARG  | N-CA-C  | -5.04 | 105.69      | 111.14   |
| 1   | D     | 97  | LEU  | N-CA-C  | -5.01 | 107.56      | 113.97   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 81  | ARG  | N-CA-C | 5.00  | 115.73      | 109.57   |
| 1   | A     | 234 | ARG  | N-CA-C | -5.00 | 106.69      | 112.89   |

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     | 2903  | 0        | 2869     | 212     | 0            |
| 1   | B     | 2923  | 0        | 2888     | 154     | 0            |
| 1   | C     | 2899  | 0        | 2861     | 205     | 0            |
| 1   | D     | 2993  | 0        | 2956     | 195     | 0            |
| 2   | A     | 33    | 0        | 21       | 4       | 0            |
| 2   | B     | 33    | 0        | 21       | 2       | 0            |
| 2   | C     | 33    | 0        | 21       | 9       | 0            |
| 2   | D     | 33    | 0        | 21       | 5       | 0            |
| 3   | A     | 40    | 0        | 0        | 2       | 0            |
| 3   | B     | 49    | 0        | 0        | 2       | 0            |
| 3   | C     | 45    | 0        | 0        | 1       | 0            |
| 3   | D     | 66    | 0        | 0        | 4       | 0            |
| All | All   | 12050 | 0        | 11658    | 707     | 0            |

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

All (707) 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:287:ARG:HG2  | 1:A:303:VAL:HG13 | 1.32                     | 1.06              |
| 1:C:127:GLN:HE22 | 2:C:710:HSS:H5'2 | 1.25                     | 1.01              |
| 1:A:320:ASN:N    | 1:A:320:ASN:HD22 | 1.55                     | 1.00              |
| 1:C:127:GLN:NE2  | 2:C:710:HSS:H5'2 | 1.79                     | 0.97              |
| 1:C:74:ASN:ND2   | 1:C:76:ASP:H     | 1.60                     | 0.97              |
| 1:A:4:ASN:HD22   | 1:A:4:ASN:H      | 0.99                     | 0.96              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:ARG:NH2  | 2:C:710:HSS:HN1S | 1.64                     | 0.94              |
| 1:A:168:ILE:HD12 | 1:A:174:ARG:NH2  | 1.83                     | 0.94              |
| 1:C:40:GLU:O     | 1:D:19:THR:HG21  | 1.69                     | 0.93              |
| 1:C:311:ARG:NH1  | 2:C:710:HSS:H2'  | 1.84                     | 0.93              |
| 1:D:127:GLN:NE2  | 2:D:810:HSS:H5'2 | 1.83                     | 0.92              |
| 1:A:8:ILE:HD12   | 1:B:46:VAL:HG23  | 1.48                     | 0.91              |
| 1:D:274:ASN:HD22 | 1:D:276:LEU:HD21 | 1.34                     | 0.91              |
| 1:A:4:ASN:H      | 1:A:4:ASN:ND2    | 1.59                     | 0.89              |
| 1:C:74:ASN:HD21  | 1:C:76:ASP:H     | 1.21                     | 0.89              |
| 1:C:170:SER:O    | 1:C:174:ARG:HG3  | 1.72                     | 0.89              |
| 1:B:171:LEU:HA   | 1:B:174:ARG:HH12 | 1.39                     | 0.88              |
| 1:C:287:ARG:HG2  | 1:C:303:VAL:HG13 | 1.57                     | 0.87              |
| 1:D:127:GLN:HE21 | 2:D:810:HSS:H5'2 | 1.38                     | 0.86              |
| 1:C:93:ILE:HD12  | 1:C:297:GLY:HA3  | 1.57                     | 0.86              |
| 1:B:171:LEU:HA   | 1:B:174:ARG:NH1  | 1.91                     | 0.85              |
| 1:D:63:VAL:HA    | 1:D:67:MET:HE2   | 1.58                     | 0.85              |
| 1:A:146:MET:HE1  | 1:B:345:MET:HE3  | 1.57                     | 0.84              |
| 1:A:320:ASN:HD22 | 1:A:320:ASN:H    | 1.23                     | 0.83              |
| 1:A:178:ARG:HG2  | 1:A:179:ASP:N    | 1.94                     | 0.82              |
| 1:D:97:LEU:HB3   | 1:D:103:GLN:HE21 | 1.45                     | 0.81              |
| 1:A:320:ASN:N    | 1:A:320:ASN:ND2  | 2.28                     | 0.79              |
| 1:C:333:LEU:HG   | 1:C:385:VAL:HG23 | 1.64                     | 0.79              |
| 1:C:171:LEU:HD13 | 1:C:172:GLU:H    | 1.48                     | 0.79              |
| 1:A:176:ASN:HB3  | 1:A:228:TYR:CZ   | 2.17                     | 0.78              |
| 1:B:319:VAL:C    | 1:B:320:ASN:HD22 | 1.91                     | 0.78              |
| 1:C:345:MET:HE3  | 1:D:146:MET:HE1  | 1.66                     | 0.78              |
| 1:C:259:ARG:HH22 | 2:C:710:HSS:HN1S | 1.28                     | 0.78              |
| 1:B:171:LEU:H    | 1:B:171:LEU:HD22 | 1.49                     | 0.77              |
| 1:B:388:GLY:O    | 1:B:392:VAL:HG23 | 1.85                     | 0.77              |
| 1:D:172:GLU:CD   | 1:D:172:GLU:H    | 1.90                     | 0.77              |
| 1:D:287:ARG:HG2  | 1:D:303:VAL:CG1  | 2.15                     | 0.77              |
| 1:D:319:VAL:C    | 1:D:320:ASN:HD22 | 1.93                     | 0.77              |
| 1:B:99:TYR:O     | 1:B:101:GLN:HG3  | 1.83                     | 0.77              |
| 1:C:328:VAL:HG23 | 1:C:329:VAL:HG23 | 1.67                     | 0.76              |
| 1:A:40:GLU:O     | 1:B:19:THR:HG21  | 1.85                     | 0.76              |
| 1:A:333:LEU:HG   | 1:A:385:VAL:CG2  | 2.16                     | 0.76              |
| 2:D:810:HSS:H5'1 | 2:D:810:HSS:H8   | 1.67                     | 0.75              |
| 1:A:391:GLU:CD   | 1:A:391:GLU:H    | 1.94                     | 0.75              |
| 1:C:168:ILE:HG13 | 1:C:265:ASN:O    | 1.86                     | 0.75              |
| 1:C:259:ARG:NH2  | 2:C:710:HSS:N1S  | 2.35                     | 0.75              |
| 1:A:13:ASP:CG    | 1:B:90:ARG:HH22  | 1.95                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:5:ILE:HD12   | 1:D:5:ILE:H      | 1.52                     | 0.75              |
| 1:D:368:ASN:OD1  | 1:D:370:LYS:HB3  | 1.86                     | 0.75              |
| 1:C:74:ASN:HD22  | 1:C:75:GLY:N     | 1.84                     | 0.74              |
| 1:B:355:LEU:O    | 1:B:358:VAL:HG22 | 1.88                     | 0.74              |
| 1:A:404:SER:OG   | 1:A:406:GLU:HG2  | 1.87                     | 0.74              |
| 1:D:310:GLU:O    | 1:D:314:LEU:HD13 | 1.87                     | 0.74              |
| 1:A:161:VAL:HG12 | 1:A:271:TRP:CE3  | 2.24                     | 0.73              |
| 1:A:328:VAL:HG23 | 1:A:329:VAL:HG23 | 1.69                     | 0.73              |
| 1:C:119:LYS:HE2  | 1:C:314:LEU:HD21 | 1.71                     | 0.73              |
| 1:C:142:ALA:HB1  | 1:C:146:MET:HE3  | 1.69                     | 0.73              |
| 1:C:171:LEU:HD22 | 1:C:172:GLU:N    | 2.03                     | 0.73              |
| 1:C:345:MET:HE3  | 1:D:146:MET:CE   | 2.18                     | 0.73              |
| 1:A:46:VAL:HG12  | 1:A:80:LEU:HD12  | 1.70                     | 0.73              |
| 1:C:72:ASP:HB2   | 1:C:78:LEU:CD2   | 2.19                     | 0.72              |
| 1:C:309:LEU:O    | 1:C:313:VAL:HG23 | 1.88                     | 0.72              |
| 1:A:293:GLU:HA   | 1:A:297:GLY:O    | 1.90                     | 0.72              |
| 1:D:102:GLU:OE1  | 1:D:135:LEU:HD21 | 1.89                     | 0.72              |
| 1:D:412:GLN:O    | 1:D:415:VAL:HG22 | 1.89                     | 0.72              |
| 1:D:273:THR:HG23 | 1:D:276:LEU:HD23 | 1.71                     | 0.72              |
| 1:A:264:TYR:HA   | 1:A:287:ARG:O    | 1.89                     | 0.71              |
| 1:C:127:GLN:NE2  | 2:C:710:HSS:C5'  | 2.52                     | 0.71              |
| 1:B:117:PRO:O    | 1:B:118:GLN:HG2  | 1.91                     | 0.71              |
| 1:C:21:ILE:HD12  | 1:C:21:ILE:H     | 1.55                     | 0.71              |
| 1:D:230:ASP:O    | 1:D:234:ARG:HG3  | 1.91                     | 0.71              |
| 1:B:412:GLN:O    | 1:B:415:VAL:HG22 | 1.90                     | 0.71              |
| 1:A:345:MET:HE3  | 1:B:146:MET:HE3  | 1.71                     | 0.70              |
| 1:D:265:ASN:O    | 1:D:287:ARG:HB2  | 1.91                     | 0.70              |
| 1:C:49:THR:N     | 1:C:50:PRO:HD2   | 2.07                     | 0.70              |
| 1:A:46:VAL:HG23  | 1:B:8:ILE:HD12   | 1.73                     | 0.70              |
| 1:A:54:ARG:HH22  | 1:B:4:ASN:HA     | 1.55                     | 0.70              |
| 1:C:13:ASP:CG    | 1:D:90:ARG:HH22  | 1.99                     | 0.70              |
| 1:B:16:PRO:O     | 1:B:19:THR:HG22  | 1.92                     | 0.70              |
| 1:C:264:TYR:HA   | 1:C:287:ARG:O    | 1.91                     | 0.70              |
| 1:A:97:LEU:C     | 1:A:98:LEU:HD23  | 2.17                     | 0.69              |
| 1:C:175:ALA:O    | 1:C:178:ARG:HG2  | 1.92                     | 0.69              |
| 1:C:146:MET:HE1  | 1:D:345:MET:HE3  | 1.75                     | 0.69              |
| 1:C:404:SER:OG   | 1:C:406:GLU:HG2  | 1.93                     | 0.68              |
| 1:C:260:GLY:C    | 1:C:261:LEU:HD22 | 2.18                     | 0.68              |
| 1:A:168:ILE:HD12 | 1:A:174:ARG:HH21 | 1.58                     | 0.68              |
| 1:C:21:ILE:HD12  | 1:C:21:ILE:N     | 2.07                     | 0.68              |
| 1:A:388:GLY:O    | 1:A:392:VAL:HG23 | 1.93                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:161:VAL:HG12 | 1:A:271:TRP:HE3  | 1.56                     | 0.68              |
| 1:A:391:GLU:OE1  | 1:A:391:GLU:N    | 2.24                     | 0.68              |
| 1:A:4:ASN:HD22   | 1:A:4:ASN:N      | 1.83                     | 0.67              |
| 1:C:391:GLU:OE1  | 1:C:391:GLU:N    | 2.26                     | 0.67              |
| 1:B:40:GLU:HB2   | 1:B:106:TRP:CZ2  | 2.30                     | 0.67              |
| 1:C:273:THR:HG22 | 1:C:280:GLY:O    | 1.94                     | 0.67              |
| 1:B:319:VAL:HG12 | 1:B:320:ASN:ND2  | 2.09                     | 0.67              |
| 1:B:391:GLU:H    | 1:B:391:GLU:CD   | 2.02                     | 0.67              |
| 1:D:264:TYR:HA   | 1:D:287:ARG:O    | 1.95                     | 0.67              |
| 1:D:74:ASN:C     | 1:D:74:ASN:HD22  | 2.02                     | 0.67              |
| 1:D:287:ARG:HG2  | 1:D:303:VAL:HG13 | 1.75                     | 0.66              |
| 1:A:333:LEU:HG   | 1:A:385:VAL:HG23 | 1.75                     | 0.66              |
| 1:C:239:GLY:O    | 1:C:243:LEU:HD13 | 1.96                     | 0.66              |
| 1:C:333:LEU:HG   | 1:C:385:VAL:CG2  | 2.25                     | 0.66              |
| 1:D:355:LEU:O    | 1:D:358:VAL:HG22 | 1.95                     | 0.66              |
| 1:C:46:VAL:HG12  | 1:C:80:LEU:HD12  | 1.76                     | 0.66              |
| 1:B:172:GLU:CD   | 1:B:172:GLU:H    | 2.03                     | 0.65              |
| 1:A:336:SER:HG   | 1:A:369:PHE:HZ   | 1.44                     | 0.65              |
| 1:A:345:MET:HE3  | 1:B:146:MET:CE   | 2.26                     | 0.65              |
| 1:C:9:ARG:HH21   | 1:C:123:ARG:NH2  | 1.94                     | 0.65              |
| 1:D:350:ARG:NH2  | 1:D:413:ASP:HA   | 2.11                     | 0.65              |
| 1:B:74:ASN:C     | 1:B:74:ASN:HD22  | 2.03                     | 0.65              |
| 1:C:259:ARG:HG3  | 1:C:259:ARG:HH11 | 1.62                     | 0.65              |
| 1:D:273:THR:CG2  | 1:D:276:LEU:HD23 | 2.26                     | 0.65              |
| 1:C:147:LEU:HD23 | 1:C:147:LEU:C    | 2.22                     | 0.65              |
| 1:A:319:VAL:C    | 1:A:321:PRO:HD3  | 2.22                     | 0.65              |
| 1:C:72:ASP:HB2   | 1:C:78:LEU:HD22  | 1.78                     | 0.65              |
| 1:C:226:GLY:O    | 1:C:229:LEU:HG   | 1.97                     | 0.64              |
| 1:C:127:GLN:HE22 | 2:C:710:HSS:C5'  | 2.08                     | 0.64              |
| 1:A:293:GLU:HB2  | 1:A:299:ALA:HB2  | 1.79                     | 0.64              |
| 1:C:19:THR:HG21  | 1:D:40:GLU:O     | 1.97                     | 0.64              |
| 1:D:5:ILE:HG22   | 1:D:6:GLN:N      | 2.12                     | 0.64              |
| 1:A:49:THR:N     | 1:A:50:PRO:HD2   | 2.12                     | 0.63              |
| 1:A:74:ASN:C     | 1:A:74:ASN:ND2   | 2.55                     | 0.63              |
| 1:A:97:LEU:HD11  | 1:B:15:LEU:HD13  | 1.80                     | 0.63              |
| 1:A:287:ARG:HG2  | 1:A:303:VAL:CG1  | 2.17                     | 0.63              |
| 1:C:54:ARG:HH22  | 1:D:4:ASN:HA     | 1.61                     | 0.63              |
| 1:C:165:LEU:HD11 | 1:C:244:LEU:CD2  | 2.28                     | 0.63              |
| 1:D:19:THR:O     | 1:D:23:GLN:HG3   | 1.97                     | 0.63              |
| 1:B:165:LEU:O    | 1:B:166:ASN:HB2  | 1.99                     | 0.63              |
| 1:B:333:LEU:HG   | 1:B:385:VAL:HG22 | 1.81                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:60:THR:O     | 1:B:64:GLU:HB2   | 1.99                     | 0.63              |
| 1:B:171:LEU:H    | 1:B:171:LEU:CD2  | 2.11                     | 0.63              |
| 1:A:141:ASP:HB2  | 1:A:240:LEU:HD13 | 1.80                     | 0.63              |
| 1:A:336:SER:O    | 1:A:340:THR:HG21 | 1.99                     | 0.62              |
| 1:A:353:ASP:OD1  | 1:B:153:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:74:ASN:C     | 1:A:74:ASN:HD22  | 2.06                     | 0.62              |
| 1:A:138:PRO:HB2  | 1:A:240:LEU:HB2  | 1.81                     | 0.62              |
| 1:B:22:TRP:CE2   | 1:B:313:VAL:HG21 | 2.34                     | 0.62              |
| 1:C:319:VAL:C    | 1:C:321:PRO:HD3  | 2.24                     | 0.62              |
| 1:C:256:ARG:HG2  | 1:C:256:ARG:HH11 | 1.65                     | 0.62              |
| 1:C:74:ASN:ND2   | 1:C:74:ASN:C     | 2.54                     | 0.62              |
| 1:C:128:LEU:HB2  | 1:C:309:LEU:HD21 | 1.81                     | 0.62              |
| 1:C:40:GLU:HB2   | 1:C:106:TRP:CZ2  | 2.35                     | 0.61              |
| 1:D:117:PRO:O    | 1:D:118:GLN:HG2  | 1.99                     | 0.61              |
| 1:D:391:GLU:H    | 1:D:391:GLU:CD   | 2.08                     | 0.61              |
| 1:A:68:TYR:HB2   | 1:A:80:LEU:HB2   | 1.82                     | 0.61              |
| 1:C:146:MET:CE   | 1:D:345:MET:HE3  | 2.29                     | 0.61              |
| 1:C:5:ILE:HG22   | 1:C:6:GLN:N      | 2.14                     | 0.61              |
| 1:C:46:VAL:CG2   | 1:D:11:MET:SD    | 2.89                     | 0.61              |
| 1:A:33:LEU:HD11  | 1:A:128:LEU:HD11 | 1.81                     | 0.61              |
| 1:C:241:CYS:O    | 1:C:245:GLU:HG3  | 2.00                     | 0.61              |
| 1:D:350:ARG:HH22 | 1:D:413:ASP:HA   | 1.66                     | 0.61              |
| 1:A:241:CYS:O    | 1:A:245:GLU:HG3  | 2.00                     | 0.61              |
| 1:A:13:ASP:OD2   | 1:B:90:ARG:NH2   | 2.34                     | 0.61              |
| 1:C:33:LEU:HD13  | 1:C:106:TRP:CG   | 2.36                     | 0.61              |
| 1:C:311:ARG:HH12 | 2:C:710:HSS:H2'  | 1.66                     | 0.61              |
| 2:A:510:HSS:O3S  | 2:A:510:HSS:O    | 2.13                     | 0.60              |
| 1:B:89:VAL:HG13  | 1:B:292:VAL:HG22 | 1.84                     | 0.60              |
| 1:B:277:GLY:HA2  | 3:B:650:HOH:O    | 2.01                     | 0.60              |
| 1:D:74:ASN:ND2   | 1:D:76:ASP:H     | 1.99                     | 0.60              |
| 1:D:239:GLY:O    | 1:D:242:LYS:HG2  | 2.01                     | 0.60              |
| 1:C:141:ASP:HB2  | 1:C:240:LEU:HD13 | 1.84                     | 0.60              |
| 1:D:320:ASN:HD22 | 1:D:320:ASN:N    | 1.99                     | 0.60              |
| 1:A:54:ARG:NH2   | 1:B:4:ASN:HA     | 2.16                     | 0.60              |
| 1:C:74:ASN:HD22  | 1:C:74:ASN:C     | 2.06                     | 0.60              |
| 1:D:274:ASN:HB2  | 1:D:276:LEU:CD2  | 2.31                     | 0.60              |
| 1:A:19:THR:HG21  | 1:B:40:GLU:O     | 2.02                     | 0.60              |
| 1:D:261:LEU:N    | 1:D:261:LEU:HD22 | 2.16                     | 0.60              |
| 1:C:33:LEU:HD23  | 1:C:147:LEU:HD11 | 1.84                     | 0.59              |
| 1:A:353:ASP:CG   | 1:B:153:ARG:HH12 | 2.09                     | 0.59              |
| 1:C:391:GLU:CD   | 1:C:391:GLU:H    | 2.10                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:239:GLY:O    | 1:A:242:LYS:HG2  | 2.03                     | 0.59              |
| 1:D:161:VAL:HG12 | 1:D:271:TRP:HE3  | 1.66                     | 0.59              |
| 1:A:136:GLN:O    | 1:A:236:HIS:HE1  | 1.85                     | 0.59              |
| 1:B:21:ILE:H     | 1:B:21:ILE:HD12  | 1.68                     | 0.59              |
| 1:D:351:LEU:HD21 | 1:D:415:VAL:HG23 | 1.84                     | 0.59              |
| 1:A:242:LYS:HG3  | 1:A:243:LEU:N    | 2.18                     | 0.59              |
| 1:A:4:ASN:ND2    | 1:A:4:ASN:N      | 2.38                     | 0.59              |
| 1:C:72:ASP:HB2   | 1:C:78:LEU:HD21  | 1.84                     | 0.59              |
| 1:C:56:ILE:HG23  | 1:C:261:LEU:HD12 | 1.84                     | 0.59              |
| 1:A:313:VAL:O    | 1:A:317:GLN:HG3  | 2.02                     | 0.58              |
| 1:C:348:ALA:O    | 1:C:352:ARG:HG3  | 2.03                     | 0.58              |
| 1:B:165:LEU:HD11 | 1:B:244:LEU:HD23 | 1.85                     | 0.58              |
| 1:A:166:ASN:OD1  | 1:A:255:GLN:HA   | 2.04                     | 0.58              |
| 1:C:332:TYR:CE2  | 1:C:363:ASN:HB2  | 2.38                     | 0.58              |
| 1:D:401:ASP:OD1  | 1:D:403:ARG:HB2  | 2.03                     | 0.58              |
| 1:A:178:ARG:CG   | 1:A:179:ASP:N    | 2.67                     | 0.58              |
| 1:A:412:GLN:O    | 1:A:415:VAL:HG22 | 2.04                     | 0.58              |
| 1:B:120:GLY:H    | 1:B:279:GLN:HE21 | 1.52                     | 0.58              |
| 1:A:176:ASN:HB3  | 1:A:228:TYR:CE1  | 2.39                     | 0.58              |
| 1:C:170:SER:H    | 1:C:173:ALA:HB3  | 1.68                     | 0.58              |
| 1:C:175:ALA:C    | 1:C:177:TYR:H    | 2.12                     | 0.58              |
| 1:C:388:GLY:O    | 1:C:392:VAL:HG23 | 2.04                     | 0.58              |
| 1:D:259:ARG:CG   | 1:D:268:VAL:HG22 | 2.34                     | 0.58              |
| 1:B:74:ASN:ND2   | 1:B:76:ASP:H     | 2.02                     | 0.58              |
| 1:C:21:ILE:H     | 1:C:21:ILE:CD1   | 2.16                     | 0.58              |
| 1:B:171:LEU:CA   | 1:B:174:ARG:HH12 | 2.13                     | 0.57              |
| 1:B:168:ILE:HD12 | 1:B:174:ARG:HE   | 1.68                     | 0.57              |
| 1:B:171:LEU:HD22 | 1:B:171:LEU:N    | 2.19                     | 0.57              |
| 1:B:391:GLU:HB3  | 1:B:396:THR:O    | 2.05                     | 0.57              |
| 1:D:165:LEU:HD11 | 1:D:244:LEU:CD2  | 2.33                     | 0.57              |
| 1:C:175:ALA:O    | 1:C:177:TYR:N    | 2.38                     | 0.57              |
| 1:D:99:TYR:O     | 1:D:101:GLN:HG3  | 2.03                     | 0.57              |
| 1:A:139:ASP:HA   | 1:A:243:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:150:ARG:HG3  | 1:A:150:ARG:HH11 | 1.70                     | 0.57              |
| 1:C:171:LEU:HD22 | 1:C:172:GLU:HG2  | 1.86                     | 0.57              |
| 1:C:411:ALA:O    | 1:C:414:SER:N    | 2.34                     | 0.57              |
| 1:D:410:VAL:CG1  | 1:D:415:VAL:HG12 | 2.34                     | 0.57              |
| 1:A:108:ILE:HD12 | 1:A:128:LEU:HD23 | 1.87                     | 0.57              |
| 1:A:139:ASP:O    | 1:A:142:ALA:HB3  | 2.04                     | 0.57              |
| 1:A:74:ASN:ND2   | 1:A:76:ASP:H     | 2.02                     | 0.57              |
| 1:A:115:GLU:OE1  | 1:A:121:ARG:HD3  | 2.05                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:419:LEU:HA   | 1:D:422:LEU:HD11 | 1.87                     | 0.57              |
| 1:A:74:ASN:HD22  | 1:A:75:GLY:N     | 2.03                     | 0.56              |
| 1:C:331:ILE:HD11 | 1:C:423:LEU:HD11 | 1.88                     | 0.56              |
| 1:A:55:ALA:HB2   | 1:A:295:LEU:HD11 | 1.86                     | 0.56              |
| 1:B:5:ILE:HG22   | 1:B:6:GLN:N      | 2.18                     | 0.56              |
| 1:B:174:ARG:HH21 | 1:B:265:ASN:HA   | 1.69                     | 0.56              |
| 1:D:46:VAL:CG1   | 1:D:80:LEU:HD12  | 2.36                     | 0.56              |
| 1:A:242:LYS:HG3  | 1:A:243:LEU:HD13 | 1.86                     | 0.56              |
| 1:C:257:LEU:HD12 | 1:C:268:VAL:CG1  | 2.35                     | 0.56              |
| 1:C:97:LEU:HD21  | 1:D:15:LEU:HD13  | 1.86                     | 0.56              |
| 1:B:331:ILE:HD11 | 1:B:423:LEU:HD11 | 1.87                     | 0.56              |
| 1:D:272:VAL:HG12 | 1:D:273:THR:N    | 2.21                     | 0.56              |
| 1:B:19:THR:O     | 1:B:23:GLN:HG3   | 2.05                     | 0.56              |
| 1:D:334:VAL:HG21 | 1:D:373:PHE:CE1  | 2.41                     | 0.56              |
| 1:A:5:ILE:HD11   | 1:B:54:ARG:HH21  | 1.71                     | 0.56              |
| 1:C:400:LYS:HE2  | 1:C:407:GLN:NE2  | 2.20                     | 0.56              |
| 1:B:21:ILE:HD12  | 1:B:21:ILE:N     | 2.22                     | 0.55              |
| 1:C:70:PHE:CE2   | 1:C:78:LEU:HD23  | 2.41                     | 0.55              |
| 1:C:138:PRO:HD3  | 1:C:236:HIS:CD2  | 2.41                     | 0.55              |
| 1:C:320:ASN:C    | 1:C:322:GLU:H    | 2.13                     | 0.55              |
| 1:D:46:VAL:HG13  | 1:D:80:LEU:HD12  | 1.88                     | 0.55              |
| 1:D:305:PHE:CD1  | 1:D:305:PHE:C    | 2.83                     | 0.55              |
| 1:B:411:ALA:O    | 1:B:415:VAL:HG13 | 2.06                     | 0.55              |
| 1:D:225:LEU:O    | 1:D:227:ASP:N    | 2.39                     | 0.55              |
| 1:A:8:ILE:HD12   | 1:B:46:VAL:CG2   | 2.30                     | 0.55              |
| 1:A:82:PRO:HA    | 1:A:112:PHE:O    | 2.06                     | 0.55              |
| 1:C:63:VAL:HG12  | 1:C:63:VAL:O     | 2.06                     | 0.55              |
| 1:D:74:ASN:C     | 1:D:74:ASN:ND2   | 2.65                     | 0.55              |
| 1:D:415:VAL:HG23 | 1:D:416:ALA:N    | 2.22                     | 0.55              |
| 1:B:74:ASN:C     | 1:B:74:ASN:ND2   | 2.65                     | 0.55              |
| 1:A:386:VAL:HB   | 1:A:398:VAL:HB   | 1.87                     | 0.55              |
| 1:C:138:PRO:HD3  | 1:C:236:HIS:HD2  | 1.72                     | 0.55              |
| 1:C:345:MET:CE   | 1:D:146:MET:HE1  | 2.36                     | 0.55              |
| 1:D:172:GLU:CD   | 1:D:172:GLU:N    | 2.62                     | 0.55              |
| 1:D:183:ALA:HB3  | 3:D:837:HOH:O    | 2.07                     | 0.55              |
| 1:B:117:PRO:C    | 1:B:118:GLN:HG2  | 2.32                     | 0.55              |
| 1:D:16:PRO:O     | 1:D:19:THR:HG22  | 2.07                     | 0.55              |
| 1:A:52:PHE:CE1   | 1:A:82:PRO:HD2   | 2.42                     | 0.55              |
| 1:C:239:GLY:O    | 1:C:242:LYS:HG2  | 2.07                     | 0.55              |
| 1:A:309:LEU:O    | 1:A:313:VAL:HG23 | 2.07                     | 0.54              |
| 1:C:62:VAL:HA    | 1:C:66:GLU:HB2   | 1.90                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:72:ASP:HB2   | 1:D:78:LEU:HD22  | 1.90                     | 0.54              |
| 1:A:33:LEU:HD13  | 1:A:106:TRP:CG   | 2.41                     | 0.54              |
| 1:B:261:LEU:N    | 1:B:261:LEU:HD22 | 2.21                     | 0.54              |
| 1:B:410:VAL:HB   | 1:B:415:VAL:HG12 | 1.89                     | 0.54              |
| 1:C:114:HIS:ND1  | 1:D:73:ARG:HD2   | 2.22                     | 0.54              |
| 1:D:334:VAL:HG21 | 1:D:373:PHE:HE1  | 1.73                     | 0.54              |
| 1:C:179:ASP:O    | 1:C:180:ALA:HB2  | 2.08                     | 0.54              |
| 1:D:278:SER:O    | 1:D:279:GLN:NE2  | 2.41                     | 0.54              |
| 1:C:383:VAL:HG12 | 1:C:384:ALA:N    | 2.21                     | 0.54              |
| 1:B:273:THR:HG23 | 1:B:274:ASN:N    | 2.22                     | 0.54              |
| 1:B:136:GLN:O    | 1:B:236:HIS:HE1  | 1.91                     | 0.54              |
| 1:D:225:LEU:O    | 1:D:226:GLY:C    | 2.51                     | 0.54              |
| 1:A:401:ASP:OD1  | 1:A:403:ARG:HB2  | 2.08                     | 0.54              |
| 1:D:172:GLU:N    | 1:D:172:GLU:OE2  | 2.41                     | 0.54              |
| 1:D:333:LEU:CD1  | 1:D:348:ALA:HB2  | 2.38                     | 0.54              |
| 1:A:11:MET:SD    | 1:B:46:VAL:HG22  | 2.48                     | 0.53              |
| 1:B:100:ASN:C    | 1:B:101:GLN:HG3  | 2.32                     | 0.53              |
| 1:C:97:LEU:C     | 1:C:98:LEU:HD23  | 2.34                     | 0.53              |
| 1:C:147:LEU:HD23 | 1:C:147:LEU:O    | 2.08                     | 0.53              |
| 1:A:72:ASP:HB2   | 1:A:78:LEU:HD22  | 1.90                     | 0.53              |
| 1:B:273:THR:O    | 1:B:275:SER:N    | 2.41                     | 0.53              |
| 1:C:48:GLN:C     | 1:C:50:PRO:HD2   | 2.34                     | 0.53              |
| 1:C:307:MET:SD   | 1:C:312:LEU:HD22 | 2.48                     | 0.53              |
| 1:D:388:GLY:O    | 1:D:392:VAL:HG23 | 2.09                     | 0.53              |
| 1:C:90:ARG:NH2   | 1:D:13:ASP:OD2   | 2.39                     | 0.53              |
| 1:D:121:ARG:HG2  | 1:D:311:ARG:HH21 | 1.72                     | 0.53              |
| 1:A:225:LEU:N    | 1:A:225:LEU:HD12 | 2.23                     | 0.53              |
| 1:D:5:ILE:CG2    | 1:D:6:GLN:N      | 2.71                     | 0.53              |
| 1:D:161:VAL:HG12 | 1:D:271:TRP:CE3  | 2.43                     | 0.53              |
| 1:A:11:MET:HG2   | 1:A:124:GLN:HB2  | 1.91                     | 0.53              |
| 1:C:400:LYS:HE2  | 1:C:407:GLN:HE22 | 1.74                     | 0.53              |
| 1:D:245:GLU:C    | 1:D:247:ALA:H    | 2.17                     | 0.53              |
| 1:D:278:SER:C    | 1:D:279:GLN:HG2  | 2.33                     | 0.53              |
| 1:A:410:VAL:HG12 | 1:A:411:ALA:O    | 2.09                     | 0.53              |
| 1:C:97:LEU:HD11  | 1:D:15:LEU:HD22  | 1.91                     | 0.53              |
| 1:C:5:ILE:CG2    | 1:C:6:GLN:N      | 2.71                     | 0.53              |
| 1:C:9:ARG:HH21   | 1:C:123:ARG:HH22 | 1.56                     | 0.53              |
| 1:C:73:ARG:NH2   | 1:D:67:MET:O     | 2.42                     | 0.53              |
| 1:A:5:ILE:HD11   | 1:B:54:ARG:NH2   | 2.24                     | 0.53              |
| 1:B:322:GLU:O    | 1:B:323:PHE:C    | 2.52                     | 0.52              |
| 1:C:40:GLU:HB2   | 1:C:106:TRP:CE2  | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:131:GLU:OE1  | 2:A:510:HSS:N12  | 2.42                     | 0.52              |
| 1:C:163:LEU:HB2  | 1:C:271:TRP:CZ3  | 2.45                     | 0.52              |
| 1:B:108:ILE:HD12 | 1:B:128:LEU:CD2  | 2.39                     | 0.52              |
| 1:B:256:ARG:HG2  | 1:B:256:ARG:HH11 | 1.74                     | 0.52              |
| 1:B:40:GLU:HB2   | 1:B:106:TRP:CE2  | 2.45                     | 0.52              |
| 1:B:305:PHE:CD1  | 1:B:305:PHE:C    | 2.86                     | 0.52              |
| 1:C:171:LEU:CD2  | 1:C:172:GLU:HG2  | 2.39                     | 0.52              |
| 1:A:32:VAL:HG13  | 1:A:150:ARG:HD2  | 1.91                     | 0.52              |
| 1:C:54:ARG:NH2   | 1:D:4:ASN:HA     | 2.23                     | 0.52              |
| 1:A:272:VAL:HG12 | 1:A:273:THR:N    | 2.25                     | 0.52              |
| 1:C:11:MET:HE2   | 1:C:124:GLN:HB2  | 1.92                     | 0.52              |
| 1:D:245:GLU:C    | 1:D:247:ALA:N    | 2.67                     | 0.52              |
| 1:A:3:LYS:HB2    | 1:A:4:ASN:HD22   | 1.75                     | 0.52              |
| 1:D:259:ARG:HG3  | 1:D:268:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:285:GLY:HA3  | 1:A:305:PHE:HA   | 1.92                     | 0.52              |
| 1:C:56:ILE:HG23  | 1:C:261:LEU:CD1  | 2.40                     | 0.52              |
| 1:C:313:VAL:O    | 1:C:317:GLN:HG3  | 2.08                     | 0.52              |
| 1:D:142:ALA:HB1  | 1:D:146:MET:HE3  | 1.92                     | 0.52              |
| 1:A:21:ILE:N     | 1:A:21:ILE:HD12  | 2.25                     | 0.52              |
| 1:A:150:ARG:HG3  | 1:A:150:ARG:NH1  | 2.25                     | 0.52              |
| 1:B:371:LYS:O    | 1:B:375:ARG:HG3  | 2.09                     | 0.52              |
| 1:C:171:LEU:HD22 | 1:C:172:GLU:H    | 1.74                     | 0.51              |
| 1:C:320:ASN:O    | 1:C:322:GLU:N    | 2.43                     | 0.51              |
| 1:C:46:VAL:HG23  | 1:D:11:MET:SD    | 2.50                     | 0.51              |
| 1:C:259:ARG:HG3  | 1:C:259:ARG:NH1  | 2.24                     | 0.51              |
| 1:C:411:ALA:O    | 1:C:414:SER:HB2  | 2.10                     | 0.51              |
| 1:B:350:ARG:NH2  | 1:B:413:ASP:HA   | 2.26                     | 0.51              |
| 1:C:74:ASN:HD21  | 1:C:76:ASP:N     | 2.01                     | 0.51              |
| 1:A:228:TYR:O    | 1:A:229:LEU:C    | 2.53                     | 0.51              |
| 1:B:287:ARG:HD3  | 1:B:289:ASP:OD2  | 2.11                     | 0.51              |
| 1:C:423:LEU:O    | 1:C:424:GLY:C    | 2.53                     | 0.51              |
| 1:D:273:THR:HG23 | 1:D:274:ASN:N    | 2.26                     | 0.51              |
| 1:D:274:ASN:ND2  | 1:D:276:LEU:HD21 | 2.16                     | 0.51              |
| 1:A:104:ARG:HG2  | 1:A:132:VAL:HG13 | 1.93                     | 0.51              |
| 1:A:229:LEU:O    | 1:A:234:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:257:LEU:HD11 | 1:A:270:GLU:HG3  | 1.93                     | 0.51              |
| 1:A:112:PHE:CE2  | 1:A:124:GLN:HG3  | 2.46                     | 0.51              |
| 1:C:5:ILE:HD12   | 1:C:5:ILE:N      | 2.26                     | 0.51              |
| 1:D:22:TRP:CE2   | 1:D:313:VAL:HG21 | 2.46                     | 0.51              |
| 1:D:239:GLY:O    | 1:D:243:LEU:HD13 | 2.11                     | 0.51              |
| 1:C:52:PHE:CE1   | 1:C:82:PRO:HD2   | 2.46                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:275:SER:OG   | 1:D:276:LEU:N    | 2.44                     | 0.51              |
| 1:B:331:ILE:HD13 | 1:B:419:LEU:HD13 | 1.93                     | 0.50              |
| 1:A:146:MET:CE   | 1:B:345:MET:HE3  | 2.35                     | 0.50              |
| 1:B:319:VAL:C    | 1:B:320:ASN:ND2  | 2.65                     | 0.50              |
| 1:B:161:VAL:HG12 | 1:B:271:TRP:HE3  | 1.76                     | 0.50              |
| 1:B:33:LEU:HD11  | 1:B:128:LEU:HD11 | 1.94                     | 0.50              |
| 1:B:264:TYR:HA   | 1:B:287:ARG:O    | 2.11                     | 0.50              |
| 1:D:117:PRO:C    | 1:D:118:GLN:HG2  | 2.37                     | 0.50              |
| 1:D:410:VAL:HG12 | 1:D:411:ALA:O    | 2.11                     | 0.50              |
| 1:A:28:THR:HG21  | 1:A:155:LEU:HD13 | 1.94                     | 0.50              |
| 1:A:293:GLU:C    | 1:A:295:LEU:H    | 2.20                     | 0.50              |
| 1:B:396:THR:HG22 | 1:B:411:ALA:HA   | 1.93                     | 0.50              |
| 1:C:305:PHE:C    | 1:C:305:PHE:CD1  | 2.90                     | 0.50              |
| 1:A:102:GLU:HA   | 1:A:133:PHE:O    | 2.12                     | 0.49              |
| 1:B:15:LEU:HB3   | 1:B:16:PRO:HD2   | 1.93                     | 0.49              |
| 1:B:355:LEU:HD21 | 1:B:420:ARG:HB2  | 1.93                     | 0.49              |
| 1:D:186:GLU:O    | 1:D:187:GLN:C    | 2.54                     | 0.49              |
| 1:A:146:MET:HE1  | 1:B:345:MET:HG2  | 1.94                     | 0.49              |
| 1:C:150:ARG:HG3  | 1:C:150:ARG:HH11 | 1.77                     | 0.49              |
| 1:C:322:GLU:O    | 1:C:323:PHE:C    | 2.55                     | 0.49              |
| 1:D:146:MET:HG2  | 1:D:249:ILE:HD11 | 1.94                     | 0.49              |
| 1:D:231:GLU:OE2  | 1:D:234:ARG:HD3  | 2.12                     | 0.49              |
| 1:A:345:MET:SD   | 1:A:364:HIS:HE1  | 2.35                     | 0.49              |
| 1:A:383:VAL:HG12 | 1:A:384:ALA:N    | 2.26                     | 0.49              |
| 1:B:161:VAL:HG12 | 1:B:271:TRP:CE3  | 2.48                     | 0.49              |
| 1:C:236:HIS:HD1  | 1:C:266:ARG:HD2  | 1.77                     | 0.49              |
| 1:D:103:GLN:HB3  | 1:D:105:LEU:HD21 | 1.93                     | 0.49              |
| 1:B:63:VAL:HG13  | 1:B:67:MET:HE2   | 1.94                     | 0.49              |
| 1:C:42:ARG:HB2   | 1:D:14:TYR:HB2   | 1.95                     | 0.49              |
| 1:C:73:ARG:HG3   | 1:D:114:HIS:CE1  | 2.48                     | 0.49              |
| 1:C:141:ASP:O    | 1:C:145:ILE:HG13 | 2.12                     | 0.49              |
| 1:C:292:VAL:HG11 | 1:C:300:THR:HG22 | 1.94                     | 0.49              |
| 1:D:18:GLU:HA    | 1:D:21:ILE:HD13  | 1.95                     | 0.49              |
| 1:D:351:LEU:HD13 | 1:D:419:LEU:HD11 | 1.94                     | 0.49              |
| 1:A:245:GLU:C    | 1:A:247:ALA:H    | 2.20                     | 0.49              |
| 1:A:319:VAL:O    | 1:A:321:PRO:HD3  | 2.12                     | 0.49              |
| 1:A:390:SER:O    | 1:A:393:ALA:N    | 2.44                     | 0.49              |
| 1:A:407:GLN:C    | 1:A:408:THR:HG22 | 2.36                     | 0.49              |
| 1:C:150:ARG:HG3  | 1:C:150:ARG:NH1  | 2.28                     | 0.49              |
| 1:D:259:ARG:HH22 | 2:D:810:HSS:HN1S | 1.58                     | 0.49              |
| 1:D:385:VAL:HG23 | 1:D:385:VAL:O    | 2.12                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:319:VAL:HG12 | 1:B:320:ASN:HD21 | 1.77                     | 0.49              |
| 1:C:39:SER:OG    | 1:D:328:VAL:HG11 | 2.13                     | 0.49              |
| 1:B:5:ILE:CG2    | 1:B:6:GLN:N      | 2.76                     | 0.49              |
| 1:C:351:LEU:HD21 | 1:C:415:VAL:HG23 | 1.93                     | 0.49              |
| 1:C:63:VAL:HG13  | 1:C:67:MET:HE2   | 1.94                     | 0.49              |
| 1:D:24:ARG:HD3   | 1:D:323:PHE:CE2  | 2.48                     | 0.49              |
| 1:A:174:ARG:C    | 1:A:176:ASN:H    | 2.20                     | 0.49              |
| 1:C:13:ASP:OD2   | 1:D:90:ARG:NH2   | 2.42                     | 0.49              |
| 1:C:320:ASN:C    | 1:C:322:GLU:N    | 2.71                     | 0.49              |
| 1:A:322:GLU:HB2  | 3:A:524:HOH:O    | 2.12                     | 0.49              |
| 1:C:242:LYS:HG3  | 1:C:243:LEU:N    | 2.28                     | 0.48              |
| 1:D:333:LEU:HG   | 1:D:385:VAL:CG2  | 2.43                     | 0.48              |
| 1:A:69:THR:HA    | 1:A:78:LEU:O     | 2.13                     | 0.48              |
| 1:D:259:ARG:NH1  | 1:D:264:TYR:CZ   | 2.81                     | 0.48              |
| 1:A:118:GLN:HG3  | 1:A:121:ARG:NE   | 2.27                     | 0.48              |
| 1:B:18:GLU:HA    | 1:B:21:ILE:HD13  | 1.95                     | 0.48              |
| 1:C:74:ASN:ND2   | 1:C:75:GLY:N     | 2.55                     | 0.48              |
| 1:A:245:GLU:C    | 1:A:247:ALA:N    | 2.69                     | 0.48              |
| 1:B:33:LEU:HD13  | 1:B:106:TRP:CG   | 2.48                     | 0.48              |
| 1:B:54:ARG:HD2   | 3:B:612:HOH:O    | 2.14                     | 0.48              |
| 1:A:232:GLU:HA   | 1:A:235:GLU:HB3  | 1.96                     | 0.48              |
| 1:C:274:ASN:N    | 1:C:274:ASN:HD22 | 2.11                     | 0.48              |
| 1:C:274:ASN:ND2  | 1:C:274:ASN:H    | 2.10                     | 0.48              |
| 1:D:33:LEU:HD11  | 1:D:128:LEU:HD11 | 1.95                     | 0.48              |
| 1:D:274:ASN:HB2  | 1:D:276:LEU:HD22 | 1.95                     | 0.48              |
| 1:B:165:LEU:HD11 | 1:B:244:LEU:CD2  | 2.44                     | 0.48              |
| 1:B:274:ASN:ND2  | 1:B:276:LEU:HD22 | 2.29                     | 0.48              |
| 1:A:332:TYR:CE2  | 1:A:363:ASN:HB2  | 2.49                     | 0.48              |
| 1:D:332:TYR:CD2  | 1:D:376:ALA:HB2  | 2.49                     | 0.48              |
| 1:C:259:ARG:C    | 1:C:261:LEU:H    | 2.20                     | 0.48              |
| 1:A:411:ALA:O    | 1:A:414:SER:HB2  | 2.14                     | 0.48              |
| 1:B:5:ILE:HD12   | 1:B:5:ILE:H      | 1.79                     | 0.48              |
| 1:C:167:SER:HA   | 1:C:266:ARG:O    | 2.14                     | 0.48              |
| 1:D:351:LEU:HD21 | 1:D:415:VAL:CG2  | 2.44                     | 0.48              |
| 1:A:65:LYS:O     | 1:B:73:ARG:NH1   | 2.38                     | 0.47              |
| 1:A:118:GLN:HG3  | 1:A:121:ARG:HE   | 1.79                     | 0.47              |
| 1:A:178:ARG:HG2  | 1:A:179:ASP:H    | 1.73                     | 0.47              |
| 1:B:166:ASN:O    | 1:B:268:VAL:HG12 | 2.14                     | 0.47              |
| 1:C:293:GLU:C    | 1:C:295:LEU:H    | 2.22                     | 0.47              |
| 1:C:383:VAL:CG1  | 1:C:384:ALA:N    | 2.77                     | 0.47              |
| 1:A:5:ILE:HD12   | 1:A:5:ILE:N      | 2.29                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:229:LEU:CD1  | 1:A:233:SER:HB3  | 2.44                     | 0.47              |
| 1:C:415:VAL:HG23 | 1:C:416:ALA:N    | 2.28                     | 0.47              |
| 1:A:63:VAL:HG13  | 1:A:67:MET:HE2   | 1.96                     | 0.47              |
| 1:A:237:PHE:CE2  | 1:A:241:CYS:SG   | 3.07                     | 0.47              |
| 1:A:311:ARG:NH1  | 2:A:510:HSS:H2'  | 2.29                     | 0.47              |
| 1:C:164:GLU:HA   | 1:C:252:THR:O    | 2.14                     | 0.47              |
| 1:C:390:SER:HB2  | 1:C:391:GLU:OE1  | 2.14                     | 0.47              |
| 1:D:245:GLU:O    | 1:D:247:ALA:N    | 2.47                     | 0.47              |
| 1:D:273:THR:O    | 1:D:274:ASN:C    | 2.58                     | 0.47              |
| 1:A:63:VAL:HA    | 1:A:67:MET:HG3   | 1.97                     | 0.47              |
| 1:C:114:HIS:CE1  | 1:D:73:ARG:HD2   | 2.49                     | 0.47              |
| 1:C:320:ASN:N    | 1:C:321:PRO:HD3  | 2.29                     | 0.47              |
| 1:A:331:ILE:HD11 | 1:A:423:LEU:HD11 | 1.96                     | 0.47              |
| 1:B:276:LEU:O    | 1:B:277:GLY:C    | 2.56                     | 0.47              |
| 1:C:49:THR:N     | 1:C:50:PRO:CD    | 2.76                     | 0.47              |
| 1:A:177:TYR:CG   | 1:A:177:TYR:O    | 2.67                     | 0.47              |
| 1:A:256:ARG:HG2  | 1:A:256:ARG:HH11 | 1.80                     | 0.47              |
| 1:D:5:ILE:HD12   | 1:D:5:ILE:N      | 2.25                     | 0.47              |
| 1:A:48:GLN:C     | 1:A:50:PRO:HD2   | 2.38                     | 0.47              |
| 1:A:229:LEU:HG   | 1:A:233:SER:HB2  | 1.95                     | 0.47              |
| 1:A:329:VAL:HG21 | 1:A:361:MET:HE3  | 1.95                     | 0.47              |
| 1:B:49:THR:N     | 1:B:50:PRO:HD2   | 2.30                     | 0.47              |
| 1:B:245:GLU:C    | 1:B:247:ALA:H    | 2.23                     | 0.47              |
| 1:C:368:ASN:OD1  | 1:C:370:LYS:HB3  | 2.14                     | 0.47              |
| 1:D:127:GLN:HA   | 1:D:307:MET:O    | 2.14                     | 0.47              |
| 1:D:240:LEU:O    | 1:D:244:LEU:HD13 | 2.15                     | 0.47              |
| 1:D:411:ALA:O    | 1:D:415:VAL:HG13 | 2.14                     | 0.47              |
| 1:A:10:GLY:C     | 1:A:11:MET:HG3   | 2.40                     | 0.47              |
| 1:B:333:LEU:HG   | 1:B:385:VAL:CG2  | 2.43                     | 0.47              |
| 1:C:415:VAL:O    | 1:C:416:ALA:C    | 2.58                     | 0.47              |
| 1:D:385:VAL:O    | 1:D:385:VAL:CG2  | 2.63                     | 0.47              |
| 1:C:99:TYR:CE1   | 1:C:298:ARG:NH1  | 2.83                     | 0.47              |
| 1:C:108:ILE:HD12 | 1:C:128:LEU:HD23 | 1.96                     | 0.47              |
| 1:C:171:LEU:CD1  | 1:C:172:GLU:H    | 2.22                     | 0.47              |
| 1:A:260:GLY:C    | 1:A:261:LEU:HD22 | 2.40                     | 0.46              |
| 1:C:65:LYS:H     | 1:C:65:LYS:HG3   | 1.58                     | 0.46              |
| 1:A:96:GLY:O     | 1:A:97:LEU:HD23  | 2.14                     | 0.46              |
| 1:C:93:ILE:CD1   | 1:C:297:GLY:HA3  | 2.38                     | 0.46              |
| 1:C:165:LEU:O    | 1:C:166:ASN:HB2  | 2.15                     | 0.46              |
| 1:A:229:LEU:HG   | 1:A:233:SER:CB   | 2.45                     | 0.46              |
| 1:C:287:ARG:CZ   | 1:C:303:VAL:HG22 | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:293:GLU:HA   | 1:C:297:GLY:O    | 2.15                     | 0.46              |
| 1:A:412:GLN:C    | 1:A:414:SER:H    | 2.23                     | 0.46              |
| 1:D:398:VAL:CG1  | 1:D:407:GLN:HB2  | 2.45                     | 0.46              |
| 1:D:410:VAL:HB   | 1:D:415:VAL:HG12 | 1.97                     | 0.46              |
| 1:A:125:PHE:HA   | 1:A:310:GLU:OE2  | 2.16                     | 0.46              |
| 1:C:146:MET:HE1  | 1:D:345:MET:CE   | 2.44                     | 0.46              |
| 1:C:345:MET:HE3  | 1:D:146:MET:HE3  | 1.96                     | 0.46              |
| 1:D:40:GLU:HB2   | 1:D:106:TRP:CZ2  | 2.50                     | 0.46              |
| 1:D:171:LEU:HB3  | 1:D:172:GLU:OE2  | 2.15                     | 0.46              |
| 1:D:224:ALA:HB3  | 3:D:841:HOH:O    | 2.14                     | 0.46              |
| 1:D:404:SER:OG   | 1:D:406:GLU:HG2  | 2.16                     | 0.46              |
| 1:A:49:THR:O     | 1:A:50:PRO:C     | 2.57                     | 0.46              |
| 1:B:36:TYR:HE1   | 1:B:150:ARG:HD2  | 1.79                     | 0.46              |
| 1:B:174:ARG:O    | 1:B:177:TYR:HB3  | 2.15                     | 0.46              |
| 1:B:368:ASN:OD1  | 1:B:370:LYS:HB3  | 2.15                     | 0.46              |
| 1:D:256:ARG:HH11 | 1:D:256:ARG:HG2  | 1.80                     | 0.46              |
| 1:A:254:ASN:ND2  | 1:A:257:LEU:HB2  | 2.31                     | 0.46              |
| 1:B:175:ALA:C    | 1:B:177:TYR:H    | 2.23                     | 0.46              |
| 1:D:56:ILE:O     | 1:D:262:ASP:HB2  | 2.16                     | 0.46              |
| 1:C:90:ARG:HH22  | 1:D:13:ASP:CG    | 2.22                     | 0.46              |
| 1:A:350:ARG:HD3  | 1:A:354:GLU:OE2  | 2.16                     | 0.46              |
| 1:C:112:PHE:CE2  | 1:C:124:GLN:HG3  | 2.50                     | 0.46              |
| 1:D:170:SER:O    | 1:D:174:ARG:HB2  | 2.16                     | 0.46              |
| 1:D:355:LEU:HB3  | 1:D:358:VAL:CG2  | 2.46                     | 0.46              |
| 1:A:42:ARG:HB2   | 1:B:14:TYR:HB2   | 1.98                     | 0.46              |
| 1:C:291:LEU:HD12 | 1:C:291:LEU:O    | 2.15                     | 0.46              |
| 1:D:45:ILE:HD12  | 1:D:110:PRO:HG2  | 1.97                     | 0.46              |
| 1:A:15:LEU:HD22  | 1:B:97:LEU:HD11  | 1.98                     | 0.45              |
| 1:A:229:LEU:HD11 | 1:A:233:SER:HB3  | 1.98                     | 0.45              |
| 1:A:291:LEU:HD12 | 1:A:291:LEU:O    | 2.16                     | 0.45              |
| 1:B:132:VAL:HG11 | 1:B:140:ILE:HG12 | 1.98                     | 0.45              |
| 1:B:350:ARG:HH22 | 1:B:413:ASP:HA   | 1.81                     | 0.45              |
| 1:C:104:ARG:HG2  | 1:C:132:VAL:HG13 | 1.98                     | 0.45              |
| 1:C:170:SER:O    | 1:C:171:LEU:C    | 2.59                     | 0.45              |
| 1:D:115:GLU:O    | 1:D:117:PRO:HD3  | 2.15                     | 0.45              |
| 1:D:331:ILE:HD11 | 1:D:423:LEU:HD11 | 1.97                     | 0.45              |
| 1:B:163:LEU:HD21 | 1:B:165:LEU:HD21 | 1.98                     | 0.45              |
| 1:D:230:ASP:OD1  | 1:D:230:ASP:N    | 2.46                     | 0.45              |
| 1:B:298:ARG:HE   | 1:B:298:ARG:HB3  | 1.61                     | 0.45              |
| 1:C:259:ARG:NH1  | 1:C:264:TYR:CZ   | 2.84                     | 0.45              |
| 1:A:44:PRO:HD3   | 1:B:13:ASP:OD1   | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:283:CYS:SG   | 1:A:305:PHE:CD1  | 3.09                     | 0.45              |
| 1:C:274:ASN:N    | 1:C:274:ASN:ND2  | 2.63                     | 0.45              |
| 1:D:15:LEU:HB3   | 1:D:16:PRO:HD2   | 1.98                     | 0.45              |
| 1:D:131:GLU:OE1  | 2:D:810:HSS:N12  | 2.49                     | 0.45              |
| 1:D:277:GLY:O    | 1:D:278:SER:HB3  | 2.16                     | 0.45              |
| 1:A:267:THR:HG22 | 1:A:268:VAL:N    | 2.32                     | 0.45              |
| 1:B:90:ARG:NH2   | 1:B:91:ALA:HB2   | 2.32                     | 0.45              |
| 1:B:333:LEU:C    | 1:B:333:LEU:HD23 | 2.41                     | 0.45              |
| 1:B:385:VAL:CG2  | 1:B:385:VAL:O    | 2.65                     | 0.45              |
| 1:C:229:LEU:HB2  | 1:C:234:ARG:NH1  | 2.31                     | 0.45              |
| 1:A:230:ASP:O    | 1:A:233:SER:HB2  | 2.17                     | 0.45              |
| 1:C:141:ASP:CB   | 1:C:240:LEU:HD13 | 2.46                     | 0.45              |
| 1:C:390:SER:O    | 1:C:393:ALA:N    | 2.49                     | 0.45              |
| 1:A:138:PRO:O    | 1:A:240:LEU:HD13 | 2.17                     | 0.45              |
| 1:A:368:ASN:OD1  | 1:A:368:ASN:C    | 2.59                     | 0.45              |
| 1:A:288:TYR:O    | 1:A:288:TYR:CD2  | 2.70                     | 0.45              |
| 1:D:97:LEU:HB3   | 1:D:103:GLN:NE2  | 2.22                     | 0.45              |
| 1:D:322:GLU:O    | 1:D:323:PHE:C    | 2.60                     | 0.45              |
| 1:A:115:GLU:OE1  | 1:A:121:ARG:CD   | 2.64                     | 0.45              |
| 1:C:256:ARG:HG2  | 1:C:256:ARG:NH1  | 2.31                     | 0.45              |
| 1:C:333:LEU:HD23 | 1:C:333:LEU:C    | 2.42                     | 0.45              |
| 1:D:60:THR:O     | 1:D:64:GLU:HB2   | 2.17                     | 0.45              |
| 1:D:68:TYR:OH    | 1:D:123:ARG:HD3  | 2.17                     | 0.45              |
| 1:D:333:LEU:HG   | 1:D:385:VAL:HG22 | 1.99                     | 0.45              |
| 1:A:139:ASP:HA   | 1:A:243:LEU:CD2  | 2.47                     | 0.44              |
| 1:B:383:VAL:HG12 | 1:B:384:ALA:N    | 2.30                     | 0.44              |
| 1:A:146:MET:HE1  | 1:B:345:MET:CE   | 2.39                     | 0.44              |
| 1:A:172:GLU:O    | 1:A:176:ASN:HB2  | 2.17                     | 0.44              |
| 1:A:225:LEU:C    | 1:A:227:ASP:N    | 2.75                     | 0.44              |
| 1:A:146:MET:SD   | 1:B:345:MET:HG2  | 2.58                     | 0.44              |
| 1:A:274:ASN:N    | 1:A:274:ASN:ND2  | 2.64                     | 0.44              |
| 1:A:289:ASP:OD1  | 1:A:301:PRO:HA   | 2.17                     | 0.44              |
| 1:C:147:LEU:C    | 1:C:147:LEU:CD2  | 2.91                     | 0.44              |
| 1:D:73:ARG:C     | 1:D:75:GLY:H     | 2.26                     | 0.44              |
| 1:D:275:SER:C    | 1:D:277:GLY:N    | 2.74                     | 0.44              |
| 1:D:278:SER:HB3  | 1:D:279:GLN:HE21 | 1.82                     | 0.44              |
| 1:B:146:MET:HG2  | 1:B:249:ILE:HD11 | 1.99                     | 0.44              |
| 1:C:21:ILE:N     | 1:C:21:ILE:CD1   | 2.75                     | 0.44              |
| 1:C:412:GLN:C    | 1:C:414:SER:H    | 2.24                     | 0.44              |
| 1:D:49:THR:N     | 1:D:50:PRO:HD2   | 2.33                     | 0.44              |
| 1:D:165:LEU:HD11 | 1:D:244:LEU:HD22 | 1.98                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:16:PRO:O     | 1:D:17:GLY:C     | 2.61                     | 0.44              |
| 1:D:320:ASN:O    | 1:D:322:GLU:N    | 2.51                     | 0.44              |
| 1:A:146:MET:O    | 1:A:149:ALA:HB3  | 2.17                     | 0.44              |
| 1:B:62:VAL:HA    | 1:B:66:GLU:HB2   | 1.99                     | 0.44              |
| 1:C:93:ILE:HD12  | 1:C:297:GLY:CA   | 2.38                     | 0.44              |
| 1:D:179:ASP:C    | 1:D:181:LEU:H    | 2.25                     | 0.44              |
| 1:A:274:ASN:ND2  | 1:A:274:ASN:H    | 2.16                     | 0.44              |
| 1:C:116:ARG:N    | 3:C:732:HOH:O    | 2.50                     | 0.44              |
| 1:D:33:LEU:HD13  | 1:D:106:TRP:CG   | 2.53                     | 0.44              |
| 1:D:259:ARG:CZ   | 1:D:259:ARG:HB3  | 2.48                     | 0.44              |
| 1:A:38:TYR:N     | 1:A:38:TYR:CD1   | 2.86                     | 0.44              |
| 1:A:385:VAL:HG23 | 1:A:385:VAL:O    | 2.16                     | 0.44              |
| 1:B:274:ASN:HD22 | 1:B:276:LEU:HD22 | 1.83                     | 0.44              |
| 1:C:410:VAL:HG12 | 1:C:411:ALA:N    | 2.31                     | 0.44              |
| 1:A:168:ILE:O    | 1:A:169:GLY:C    | 2.61                     | 0.44              |
| 1:A:178:ARG:CG   | 1:A:179:ASP:H    | 2.30                     | 0.44              |
| 1:A:422:LEU:C    | 1:A:424:GLY:H    | 2.25                     | 0.44              |
| 1:C:385:VAL:HG23 | 1:C:385:VAL:O    | 2.18                     | 0.44              |
| 1:D:33:LEU:HD13  | 1:D:106:TRP:CD2  | 2.52                     | 0.44              |
| 1:D:275:SER:O    | 1:D:276:LEU:C    | 2.60                     | 0.44              |
| 1:D:320:ASN:N    | 1:D:320:ASN:ND2  | 2.65                     | 0.43              |
| 1:A:269:PHE:CZ   | 1:A:305:PHE:HB3  | 2.53                     | 0.43              |
| 1:A:307:MET:SD   | 1:A:312:LEU:HD13 | 2.57                     | 0.43              |
| 1:A:412:GLN:C    | 1:A:414:SER:N    | 2.73                     | 0.43              |
| 1:B:264:TYR:OH   | 2:B:610:HSS:N11  | 2.39                     | 0.43              |
| 1:A:56:ILE:HG23  | 1:A:261:LEU:CD1  | 2.49                     | 0.43              |
| 1:A:259:ARG:HH22 | 2:A:510:HSS:HN1S | 1.66                     | 0.43              |
| 1:B:68:TYR:HB2   | 1:B:80:LEU:HB2   | 1.99                     | 0.43              |
| 1:B:336:SER:OG   | 1:B:369:PHE:CZ   | 2.70                     | 0.43              |
| 1:D:74:ASN:ND2   | 1:D:76:ASP:OD2   | 2.51                     | 0.43              |
| 1:A:293:GLU:HB2  | 1:A:299:ALA:CB   | 2.47                     | 0.43              |
| 1:B:245:GLU:C    | 1:B:247:ALA:N    | 2.76                     | 0.43              |
| 1:B:273:THR:O    | 1:B:274:ASN:C    | 2.61                     | 0.43              |
| 1:B:274:ASN:O    | 1:B:275:SER:HB3  | 2.18                     | 0.43              |
| 1:C:106:TRP:HA   | 1:C:129:GLY:O    | 2.17                     | 0.43              |
| 1:D:5:ILE:H      | 1:D:5:ILE:CD1    | 2.26                     | 0.43              |
| 1:D:373:PHE:O    | 1:D:376:ALA:HB3  | 2.18                     | 0.43              |
| 1:A:239:GLY:C    | 1:A:242:LYS:HG2  | 2.43                     | 0.43              |
| 1:A:309:LEU:HD23 | 1:A:309:LEU:HA   | 1.80                     | 0.43              |
| 1:B:106:TRP:HA   | 1:B:129:GLY:O    | 2.18                     | 0.43              |
| 1:D:65:LYS:NZ    | 1:D:65:LYS:HB3   | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:277:GLY:O    | 1:D:278:SER:CB   | 2.67                     | 0.43              |
| 1:A:69:THR:HG23  | 1:A:78:LEU:O     | 2.18                     | 0.43              |
| 1:A:253:VAL:HG12 | 1:A:254:ASN:N    | 2.33                     | 0.43              |
| 1:C:157:ILE:HD12 | 1:C:315:LEU:HD23 | 2.01                     | 0.43              |
| 1:C:170:SER:C    | 1:C:174:ARG:HG3  | 2.43                     | 0.43              |
| 1:C:259:ARG:O    | 1:C:261:LEU:N    | 2.49                     | 0.43              |
| 1:A:167:SER:HA   | 1:A:266:ARG:O    | 2.19                     | 0.43              |
| 1:A:168:ILE:CD1  | 1:A:174:ARG:HH21 | 2.30                     | 0.43              |
| 1:A:176:ASN:HB3  | 1:A:228:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:225:LEU:O    | 1:B:226:GLY:C    | 2.59                     | 0.43              |
| 1:C:48:GLN:HB3   | 1:C:50:PRO:HG2   | 2.01                     | 0.43              |
| 1:C:175:ALA:C    | 1:C:177:TYR:N    | 2.72                     | 0.43              |
| 1:C:293:GLU:O    | 1:C:295:LEU:N    | 2.51                     | 0.43              |
| 1:C:386:VAL:HB   | 1:C:398:VAL:HB   | 2.01                     | 0.43              |
| 1:A:105:LEU:HD22 | 1:B:16:PRO:HG3   | 2.00                     | 0.43              |
| 1:A:298:ARG:HD3  | 1:A:298:ARG:HA   | 1.88                     | 0.43              |
| 1:C:293:GLU:C    | 1:C:295:LEU:N    | 2.75                     | 0.43              |
| 1:A:138:PRO:CB   | 1:A:240:LEU:HB2  | 2.46                     | 0.43              |
| 1:D:172:GLU:C    | 1:D:174:ARG:N    | 2.76                     | 0.43              |
| 1:D:319:VAL:C    | 1:D:321:PRO:HD3  | 2.44                     | 0.43              |
| 1:D:355:LEU:HB3  | 1:D:358:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:118:GLN:HB2  | 1:A:121:ARG:HB2  | 2.01                     | 0.42              |
| 1:A:264:TYR:HD1  | 1:A:287:ARG:O    | 2.02                     | 0.42              |
| 1:D:135:LEU:HD12 | 1:D:140:ILE:HD13 | 2.01                     | 0.42              |
| 1:D:225:LEU:HG   | 1:D:226:GLY:N    | 2.34                     | 0.42              |
| 1:B:43:LEU:HD11  | 1:B:88:CYS:HA    | 2.00                     | 0.42              |
| 1:B:56:ILE:O     | 1:B:262:ASP:HB2  | 2.20                     | 0.42              |
| 1:C:172:GLU:O    | 1:C:173:ALA:C    | 2.62                     | 0.42              |
| 1:C:283:CYS:SG   | 1:C:305:PHE:CD1  | 3.13                     | 0.42              |
| 1:B:371:LYS:O    | 1:B:374:ALA:HB3  | 2.20                     | 0.42              |
| 1:D:21:ILE:HD12  | 1:D:21:ILE:H     | 1.84                     | 0.42              |
| 1:A:17:GLY:O     | 1:A:21:ILE:HD13  | 2.19                     | 0.42              |
| 1:A:296:GLY:HA3  | 1:B:4:ASN:HB3    | 2.02                     | 0.42              |
| 1:B:40:GLU:HA    | 1:B:106:TRP:O    | 2.20                     | 0.42              |
| 1:D:82:PRO:HA    | 1:D:112:PHE:O    | 2.20                     | 0.42              |
| 1:A:73:ARG:HG3   | 3:A:550:HOH:O    | 2.20                     | 0.42              |
| 1:A:294:GLN:O    | 1:A:294:GLN:HG2  | 2.19                     | 0.42              |
| 1:C:410:VAL:CG1  | 1:C:411:ALA:N    | 2.81                     | 0.42              |
| 1:A:114:HIS:CE1  | 1:A:123:ARG:NH1  | 2.87                     | 0.42              |
| 1:D:419:LEU:O    | 1:D:422:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:259:ARG:HG3  | 1:A:264:TYR:CE2  | 2.54                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:33:LEU:HD11  | 1:C:128:LEU:HD11 | 2.01                     | 0.42              |
| 1:A:15:LEU:HB3   | 1:A:16:PRO:HD2   | 2.01                     | 0.42              |
| 1:A:90:ARG:HH22  | 1:B:13:ASP:CG    | 2.27                     | 0.42              |
| 1:A:336:SER:O    | 1:A:340:THR:CG2  | 2.68                     | 0.42              |
| 1:A:360:LEU:HD23 | 1:A:360:LEU:C    | 2.45                     | 0.42              |
| 1:A:391:GLU:CD   | 1:A:391:GLU:N    | 2.68                     | 0.42              |
| 1:B:233:SER:OG   | 1:B:266:ARG:HD3  | 2.20                     | 0.42              |
| 1:B:274:ASN:O    | 1:B:275:SER:CB   | 2.68                     | 0.42              |
| 1:C:8:ILE:O      | 1:C:11:MET:HG3   | 2.20                     | 0.42              |
| 1:C:259:ARG:NH1  | 1:C:264:TYR:CE2  | 2.87                     | 0.42              |
| 1:C:332:TYR:CD2  | 1:C:376:ALA:HB2  | 2.55                     | 0.42              |
| 1:D:174:ARG:O    | 1:D:177:TYR:HB3  | 2.19                     | 0.42              |
| 1:A:46:VAL:HG22  | 1:B:11:MET:SD    | 2.60                     | 0.42              |
| 1:A:274:ASN:N    | 1:A:274:ASN:HD22 | 2.16                     | 0.42              |
| 1:B:320:ASN:O    | 1:B:322:GLU:N    | 2.53                     | 0.42              |
| 1:A:15:LEU:O     | 1:A:16:PRO:C     | 2.62                     | 0.42              |
| 1:A:298:ARG:O    | 1:A:299:ALA:C    | 2.63                     | 0.42              |
| 1:A:351:LEU:HD21 | 1:A:415:VAL:HG23 | 2.02                     | 0.42              |
| 1:D:106:TRP:HA   | 1:D:129:GLY:O    | 2.19                     | 0.42              |
| 1:A:168:ILE:HB   | 1:A:174:ARG:HH21 | 1.85                     | 0.41              |
| 1:A:269:PHE:HZ   | 1:A:305:PHE:HB3  | 1.85                     | 0.41              |
| 1:C:165:LEU:HD23 | 1:C:269:PHE:HB3  | 2.02                     | 0.41              |
| 1:C:171:LEU:HD13 | 1:C:172:GLU:N    | 2.26                     | 0.41              |
| 1:D:350:ARG:NH1  | 1:D:412:GLN:HB3  | 2.35                     | 0.41              |
| 1:D:415:VAL:CG2  | 1:D:416:ALA:N    | 2.83                     | 0.41              |
| 1:B:341:GLN:C    | 1:B:343:ALA:N    | 2.78                     | 0.41              |
| 1:D:17:GLY:O     | 1:D:21:ILE:HD12  | 2.21                     | 0.41              |
| 1:D:24:ARG:HD2   | 1:D:324:LYS:O    | 2.20                     | 0.41              |
| 1:A:108:ILE:HB   | 1:A:128:LEU:HD22 | 2.03                     | 0.41              |
| 1:C:270:GLU:OE1  | 1:C:281:THR:HG21 | 2.21                     | 0.41              |
| 1:D:9:ARG:HG2    | 1:D:117:PRO:HG2  | 2.03                     | 0.41              |
| 1:D:116:ARG:O    | 1:D:117:PRO:C    | 2.63                     | 0.41              |
| 1:D:292:VAL:HG21 | 1:D:300:THR:HG22 | 2.02                     | 0.41              |
| 1:D:360:LEU:C    | 1:D:360:LEU:HD23 | 2.46                     | 0.41              |
| 1:A:5:ILE:CD1    | 1:B:54:ARG:NH2   | 2.84                     | 0.41              |
| 1:A:291:LEU:HD11 | 1:A:295:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:415:VAL:HG23 | 1:B:416:ALA:N    | 2.36                     | 0.41              |
| 1:B:419:LEU:O    | 1:B:422:LEU:N    | 2.49                     | 0.41              |
| 1:D:20:ALA:HB1   | 1:D:325:ALA:HB1  | 2.02                     | 0.41              |
| 1:B:329:VAL:HB   | 1:B:379:TRP:HB3  | 2.02                     | 0.41              |
| 1:B:407:GLN:C    | 1:B:408:THR:HG23 | 2.46                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:89:VAL:O     | 1:C:93:ILE:HG12  | 2.20                     | 0.41              |
| 1:C:114:HIS:CD2  | 1:C:114:HIS:C    | 2.98                     | 0.41              |
| 1:D:54:ARG:CD    | 3:D:870:HOH:O    | 2.68                     | 0.41              |
| 1:D:54:ARG:O     | 1:D:294:GLN:NE2  | 2.53                     | 0.41              |
| 1:D:74:ASN:HD22  | 1:D:75:GLY:N     | 2.18                     | 0.41              |
| 1:D:254:ASN:OD1  | 1:D:254:ASN:C    | 2.63                     | 0.41              |
| 1:A:3:LYS:O      | 1:B:54:ARG:NH2   | 2.54                     | 0.41              |
| 1:A:13:ASP:CG    | 1:B:90:ARG:NH2   | 2.73                     | 0.41              |
| 1:A:242:LYS:HG3  | 1:A:243:LEU:CD1  | 2.49                     | 0.41              |
| 1:B:259:ARG:HH22 | 2:B:610:HSS:HN1S | 1.69                     | 0.41              |
| 1:B:339:ASP:C    | 1:B:341:GLN:N    | 2.78                     | 0.41              |
| 1:D:320:ASN:C    | 1:D:322:GLU:H    | 2.29                     | 0.41              |
| 1:D:333:LEU:HD12 | 1:D:348:ALA:HB2  | 2.02                     | 0.41              |
| 1:D:371:LYS:O    | 1:D:374:ALA:N    | 2.53                     | 0.41              |
| 1:B:257:LEU:HD12 | 1:B:268:VAL:HG13 | 2.03                     | 0.41              |
| 1:B:259:ARG:CG   | 1:B:268:VAL:HG22 | 2.50                     | 0.41              |
| 1:C:289:ASP:OD1  | 1:C:301:PRO:HB3  | 2.21                     | 0.41              |
| 1:A:73:ARG:HG3   | 1:B:114:HIS:CE1  | 2.56                     | 0.41              |
| 1:A:389:GLU:O    | 1:A:392:VAL:HB   | 2.21                     | 0.41              |
| 1:B:17:GLY:O     | 1:B:21:ILE:CD1   | 2.69                     | 0.41              |
| 1:C:56:ILE:HG22  | 1:C:56:ILE:O     | 2.19                     | 0.41              |
| 1:C:107:TYR:CD1  | 1:C:107:TYR:C    | 2.99                     | 0.41              |
| 1:C:161:VAL:HG12 | 1:C:271:TRP:CE3  | 2.56                     | 0.41              |
| 1:C:253:VAL:HG12 | 1:C:254:ASN:N    | 2.35                     | 0.41              |
| 1:D:274:ASN:HD22 | 1:D:276:LEU:CD2  | 2.19                     | 0.41              |
| 1:D:345:MET:O    | 1:D:348:ALA:HB3  | 2.21                     | 0.41              |
| 1:D:383:VAL:HG21 | 1:D:422:LEU:HD13 | 2.02                     | 0.41              |
| 1:B:320:ASN:ND2  | 1:B:320:ASN:N    | 2.69                     | 0.41              |
| 1:B:329:VAL:O    | 1:B:381:ALA:HA   | 2.21                     | 0.41              |
| 1:C:294:GLN:O    | 1:C:294:GLN:HG2  | 2.21                     | 0.41              |
| 1:D:340:THR:O    | 1:D:343:ALA:HB3  | 2.21                     | 0.41              |
| 1:A:18:GLU:O     | 1:A:22:TRP:HD1   | 2.04                     | 0.40              |
| 1:D:136:GLN:HB2  | 1:D:301:PRO:HG2  | 2.04                     | 0.40              |
| 1:C:54:ARG:NH2   | 1:D:5:ILE:HD12   | 2.36                     | 0.40              |
| 1:C:412:GLN:C    | 1:C:414:SER:N    | 2.79                     | 0.40              |
| 1:D:278:SER:C    | 1:D:279:GLN:CG   | 2.92                     | 0.40              |
| 1:A:345:MET:CE   | 1:B:146:MET:HE1  | 2.51                     | 0.40              |
| 1:A:390:SER:O    | 1:A:391:GLU:C    | 2.64                     | 0.40              |
| 1:C:32:VAL:HG13  | 1:C:150:ARG:HD2  | 2.03                     | 0.40              |
| 1:D:54:ARG:HD3   | 3:D:870:HOH:O    | 2.22                     | 0.40              |
| 1:A:165:LEU:HD22 | 1:A:269:PHE:HB3  | 2.04                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:259:ARG:HG2 | 1:B:268:VAL:CG2  | 2.52                     | 0.40              |
| 1:B:398:VAL:CG1 | 1:B:407:GLN:HB2  | 2.51                     | 0.40              |
| 1:C:53:LYS:HA   | 1:C:63:VAL:HG11  | 2.04                     | 0.40              |
| 1:D:242:LYS:HG3 | 1:D:243:LEU:HD12 | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |   |
|-----|-------|-----------------|------------|----------|----------|-------------|---|
| 1   | A     | 366/431 (85%)   | 324 (88%)  | 31 (8%)  | 11 (3%)  | 3           | 8 |
| 1   | B     | 372/431 (86%)   | 343 (92%)  | 18 (5%)  | 11 (3%)  | 3           | 8 |
| 1   | C     | 366/431 (85%)   | 329 (90%)  | 26 (7%)  | 11 (3%)  | 3           | 8 |
| 1   | D     | 381/431 (88%)   | 330 (87%)  | 39 (10%) | 12 (3%)  | 3           | 8 |
| All | All   | 1485/1724 (86%) | 1326 (89%) | 114 (8%) | 45 (3%)  | 3           | 8 |

All (45) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 229 | LEU  |
| 1   | A     | 266 | ARG  |
| 1   | B     | 274 | ASN  |
| 1   | B     | 275 | SER  |
| 1   | C     | 4   | ASN  |
| 1   | C     | 54  | ARG  |
| 1   | D     | 279 | GLN  |
| 1   | A     | 169 | GLY  |
| 1   | B     | 137 | GLY  |
| 1   | B     | 277 | GLY  |
| 1   | B     | 341 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 176 | ASN  |
| 1   | C     | 291 | LEU  |
| 1   | C     | 341 | GLN  |
| 1   | C     | 390 | SER  |
| 1   | D     | 226 | GLY  |
| 1   | D     | 274 | ASN  |
| 1   | D     | 275 | SER  |
| 1   | D     | 277 | GLY  |
| 1   | D     | 341 | GLN  |
| 1   | A     | 294 | GLN  |
| 1   | A     | 397 | ALA  |
| 1   | B     | 166 | ASN  |
| 1   | B     | 390 | SER  |
| 1   | C     | 294 | GLN  |
| 1   | D     | 119 | LYS  |
| 1   | D     | 246 | SER  |
| 1   | D     | 276 | LEU  |
| 1   | A     | 16  | PRO  |
| 1   | A     | 137 | GLY  |
| 1   | B     | 321 | PRO  |
| 1   | C     | 321 | PRO  |
| 1   | A     | 54  | ARG  |
| 1   | A     | 228 | TYR  |
| 1   | B     | 246 | SER  |
| 1   | C     | 227 | ASP  |
| 1   | C     | 391 | GLU  |
| 1   | D     | 16  | PRO  |
| 1   | D     | 225 | LEU  |
| 1   | D     | 321 | PRO  |
| 1   | A     | 170 | SER  |
| 1   | A     | 321 | PRO  |
| 1   | B     | 16  | PRO  |
| 1   | C     | 16  | PRO  |
| 1   | B     | 157 | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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



| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 297/347 (86%)   | 267 (90%)  | 30 (10%)  | 7           | 18 |
| 1   | B     | 299/347 (86%)   | 269 (90%)  | 30 (10%)  | 7           | 19 |
| 1   | C     | 296/347 (85%)   | 269 (91%)  | 27 (9%)   | 9           | 22 |
| 1   | D     | 306/347 (88%)   | 272 (89%)  | 34 (11%)  | 6           | 15 |
| All | All   | 1198/1388 (86%) | 1077 (90%) | 121 (10%) | 7           | 18 |

All (121) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |
| 1   | A     | 18  | GLU  |
| 1   | A     | 19  | THR  |
| 1   | A     | 28  | THR  |
| 1   | A     | 65  | LYS  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 78  | LEU  |
| 1   | A     | 83  | GLU  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 119 | LYS  |
| 1   | A     | 128 | LEU  |
| 1   | A     | 155 | LEU  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 178 | ARG  |
| 1   | A     | 225 | LEU  |
| 1   | A     | 228 | TYR  |
| 1   | A     | 243 | LEU  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 254 | ASN  |
| 1   | A     | 257 | LEU  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 281 | THR  |
| 1   | A     | 295 | LEU  |
| 1   | A     | 303 | VAL  |
| 1   | A     | 314 | LEU  |
| 1   | A     | 320 | ASN  |
| 1   | A     | 324 | LYS  |
| 1   | A     | 345 | MET  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 408 | THR  |
| 1   | B     | 16  | PRO  |
| 1   | B     | 19  | THR  |
| 1   | B     | 46  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 74  | ASN  |
| 1   | B     | 78  | LEU  |
| 1   | B     | 80  | LEU  |
| 1   | B     | 83  | GLU  |
| 1   | B     | 119 | LYS  |
| 1   | B     | 128 | LEU  |
| 1   | B     | 162 | THR  |
| 1   | B     | 171 | LEU  |
| 1   | B     | 178 | ARG  |
| 1   | B     | 229 | LEU  |
| 1   | B     | 230 | ASP  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 266 | ARG  |
| 1   | B     | 268 | VAL  |
| 1   | B     | 273 | THR  |
| 1   | B     | 276 | LEU  |
| 1   | B     | 281 | THR  |
| 1   | B     | 303 | VAL  |
| 1   | B     | 314 | LEU  |
| 1   | B     | 324 | LYS  |
| 1   | B     | 326 | ASP  |
| 1   | B     | 328 | VAL  |
| 1   | B     | 345 | MET  |
| 1   | B     | 385 | VAL  |
| 1   | B     | 407 | GLN  |
| 1   | B     | 421 | THR  |
| 1   | C     | 11  | MET  |
| 1   | C     | 18  | GLU  |
| 1   | C     | 19  | THR  |
| 1   | C     | 21  | ILE  |
| 1   | C     | 48  | GLN  |
| 1   | C     | 54  | ARG  |
| 1   | C     | 62  | VAL  |
| 1   | C     | 65  | LYS  |
| 1   | C     | 74  | ASN  |
| 1   | C     | 78  | LEU  |
| 1   | C     | 83  | GLU  |
| 1   | C     | 90  | ARG  |
| 1   | C     | 98  | LEU  |
| 1   | C     | 119 | LYS  |
| 1   | C     | 155 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 171 | LEU  |
| 1   | C     | 227 | ASP  |
| 1   | C     | 244 | LEU  |
| 1   | C     | 257 | LEU  |
| 1   | C     | 268 | VAL  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 295 | LEU  |
| 1   | C     | 303 | VAL  |
| 1   | C     | 314 | LEU  |
| 1   | C     | 345 | MET  |
| 1   | C     | 407 | GLN  |
| 1   | C     | 408 | THR  |
| 1   | D     | 16  | PRO  |
| 1   | D     | 19  | THR  |
| 1   | D     | 46  | VAL  |
| 1   | D     | 48  | GLN  |
| 1   | D     | 54  | ARG  |
| 1   | D     | 65  | LYS  |
| 1   | D     | 74  | ASN  |
| 1   | D     | 78  | LEU  |
| 1   | D     | 80  | LEU  |
| 1   | D     | 83  | GLU  |
| 1   | D     | 90  | ARG  |
| 1   | D     | 119 | LYS  |
| 1   | D     | 128 | LEU  |
| 1   | D     | 155 | LEU  |
| 1   | D     | 172 | GLU  |
| 1   | D     | 184 | PHE  |
| 1   | D     | 187 | GLN  |
| 1   | D     | 230 | ASP  |
| 1   | D     | 257 | LEU  |
| 1   | D     | 261 | LEU  |
| 1   | D     | 262 | ASP  |
| 1   | D     | 266 | ARG  |
| 1   | D     | 268 | VAL  |
| 1   | D     | 273 | THR  |
| 1   | D     | 279 | GLN  |
| 1   | D     | 281 | THR  |
| 1   | D     | 295 | LEU  |
| 1   | D     | 303 | VAL  |
| 1   | D     | 320 | ASN  |
| 1   | D     | 326 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 345 | MET  |
| 1   | D     | 362 | THR  |
| 1   | D     | 386 | VAL  |
| 1   | D     | 422 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | ASN  |
| 1   | A     | 6   | GLN  |
| 1   | A     | 12  | ASN  |
| 1   | A     | 74  | ASN  |
| 1   | A     | 95  | HIS  |
| 1   | A     | 176 | ASN  |
| 1   | A     | 236 | HIS  |
| 1   | A     | 274 | ASN  |
| 1   | A     | 320 | ASN  |
| 1   | A     | 341 | GLN  |
| 1   | A     | 407 | GLN  |
| 1   | A     | 418 | HIS  |
| 1   | B     | 6   | GLN  |
| 1   | B     | 12  | ASN  |
| 1   | B     | 74  | ASN  |
| 1   | B     | 114 | HIS  |
| 1   | B     | 136 | GLN  |
| 1   | B     | 176 | ASN  |
| 1   | B     | 236 | HIS  |
| 1   | B     | 274 | ASN  |
| 1   | B     | 279 | GLN  |
| 1   | B     | 320 | ASN  |
| 1   | B     | 364 | HIS  |
| 1   | C     | 12  | ASN  |
| 1   | C     | 74  | ASN  |
| 1   | C     | 118 | GLN  |
| 1   | C     | 127 | GLN  |
| 1   | C     | 254 | ASN  |
| 1   | C     | 274 | ASN  |
| 1   | C     | 317 | GLN  |
| 1   | C     | 320 | ASN  |
| 1   | C     | 341 | GLN  |
| 1   | C     | 364 | HIS  |
| 1   | C     | 407 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 6   | GLN  |
| 1   | D     | 12  | ASN  |
| 1   | D     | 74  | ASN  |
| 1   | D     | 103 | GLN  |
| 1   | D     | 114 | HIS  |
| 1   | D     | 236 | HIS  |
| 1   | D     | 274 | ASN  |
| 1   | D     | 294 | GLN  |
| 1   | D     | 320 | ASN  |
| 1   | D     | 364 | HIS  |
| 1   | D     | 368 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | HSS  | D     | 810 | -    | 36,36,36     | 2.83 | 11 (30%)    | 49,53,53    | 1.89 | 14 (28%)    |
| 2   | HSS  | C     | 710 | -    | 36,36,36     | 2.85 | 11 (30%)    | 49,53,53    | 1.88 | 12 (24%)    |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HSS  | B     | 610 | -    | 36,36,36     | 2.84 | 11 (30%) | 49,53,53    | 1.86 | 13 (26%) |
| 2   | HSS  | A     | 510 | -    | 36,36,36     | 2.83 | 11 (30%) | 49,53,53    | 2.21 | 14 (28%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | HSS  | D     | 810 | -    | -       | 5/22/39/39 | 0/4/4/4 |
| 2   | HSS  | C     | 710 | -    | -       | 7/22/39/39 | 0/4/4/4 |
| 2   | HSS  | B     | 610 | -    | -       | 4/22/39/39 | 0/4/4/4 |
| 2   | HSS  | A     | 510 | -    | -       | 2/22/39/39 | 0/4/4/4 |

All (44) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 610 | HSS  | O2S-S   | 9.43  | 1.50        | 1.42     |
| 2   | C     | 710 | HSS  | O2S-S   | 9.25  | 1.50        | 1.42     |
| 2   | D     | 810 | HSS  | O2S-S   | 9.24  | 1.50        | 1.42     |
| 2   | A     | 510 | HSS  | O3S-S   | 9.21  | 1.50        | 1.42     |
| 2   | C     | 710 | HSS  | O3S-S   | 9.06  | 1.50        | 1.42     |
| 2   | A     | 510 | HSS  | O2S-S   | 9.04  | 1.50        | 1.42     |
| 2   | D     | 810 | HSS  | O3S-S   | 9.00  | 1.50        | 1.42     |
| 2   | B     | 610 | HSS  | O3S-S   | 8.88  | 1.50        | 1.42     |
| 2   | C     | 710 | HSS  | O5'-S   | -8.23 | 1.43        | 1.60     |
| 2   | D     | 810 | HSS  | O5'-S   | -8.18 | 1.43        | 1.60     |
| 2   | A     | 510 | HSS  | O5'-S   | -8.16 | 1.43        | 1.60     |
| 2   | B     | 610 | HSS  | O5'-S   | -8.10 | 1.43        | 1.60     |
| 2   | C     | 710 | HSS  | C5-N7   | -3.08 | 1.33        | 1.39     |
| 2   | A     | 510 | HSS  | C5-N7   | -3.07 | 1.33        | 1.39     |
| 2   | B     | 610 | HSS  | C5-N7   | -3.06 | 1.33        | 1.39     |
| 2   | D     | 810 | HSS  | C5-N7   | -3.00 | 1.33        | 1.39     |
| 2   | C     | 710 | HSS  | CB-CG   | 2.58  | 1.53        | 1.49     |
| 2   | B     | 610 | HSS  | S-N1S   | 2.54  | 1.63        | 1.59     |
| 2   | D     | 810 | HSS  | CB-CG   | 2.51  | 1.53        | 1.49     |
| 2   | C     | 710 | HSS  | CG-N11  | -2.50 | 1.33        | 1.37     |
| 2   | A     | 510 | HSS  | CB-CG   | 2.47  | 1.53        | 1.49     |
| 2   | A     | 510 | HSS  | CG-N11  | -2.46 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | S-N1S   | 2.46  | 1.63        | 1.59     |
| 2   | A     | 510 | HSS  | CD2-N12 | -2.45 | 1.33        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 610 | HSS  | CD2-N12 | -2.44 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | CG-N11  | -2.44 | 1.33        | 1.37     |
| 2   | B     | 610 | HSS  | CB-CG   | 2.43  | 1.53        | 1.49     |
| 2   | B     | 610 | HSS  | CG-N11  | -2.42 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | CD2-N12 | -2.42 | 1.33        | 1.37     |
| 2   | C     | 710 | HSS  | CD2-N12 | -2.40 | 1.33        | 1.37     |
| 2   | B     | 610 | HSS  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | C8-N9   | -2.36 | 1.33        | 1.37     |
| 2   | C     | 710 | HSS  | C8-N9   | -2.35 | 1.33        | 1.37     |
| 2   | C     | 710 | HSS  | S-N1S   | 2.34  | 1.63        | 1.59     |
| 2   | C     | 710 | HSS  | C-N1S   | -2.33 | 1.33        | 1.37     |
| 2   | A     | 510 | HSS  | S-N1S   | 2.30  | 1.63        | 1.59     |
| 2   | A     | 510 | HSS  | C8-N9   | -2.28 | 1.33        | 1.37     |
| 2   | A     | 510 | HSS  | C-N1S   | -2.27 | 1.33        | 1.37     |
| 2   | B     | 610 | HSS  | C-N1S   | -2.18 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | C-N1S   | -2.18 | 1.33        | 1.37     |
| 2   | B     | 610 | HSS  | C4-N9   | -2.13 | 1.33        | 1.37     |
| 2   | C     | 710 | HSS  | C4-N9   | -2.07 | 1.33        | 1.37     |
| 2   | A     | 510 | HSS  | C4-N9   | -2.05 | 1.33        | 1.37     |
| 2   | D     | 810 | HSS  | C4-N9   | -2.03 | 1.33        | 1.37     |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2   | A     | 510 | HSS  | O3S-S-O2S | -7.74 | 109.26      | 120.85   |
| 2   | C     | 710 | HSS  | C5-C4-N3  | -5.42 | 119.25      | 126.72   |
| 2   | B     | 610 | HSS  | C5-C4-N3  | -5.25 | 119.49      | 126.72   |
| 2   | A     | 510 | HSS  | C5-C4-N3  | -5.14 | 119.64      | 126.72   |
| 2   | D     | 810 | HSS  | C5-C4-N3  | -4.92 | 119.94      | 126.72   |
| 2   | D     | 810 | HSS  | N3-C2-N1  | -4.82 | 121.29      | 128.58   |
| 2   | C     | 710 | HSS  | N3-C2-N1  | -4.63 | 121.57      | 128.58   |
| 2   | A     | 510 | HSS  | N3-C2-N1  | -4.61 | 121.61      | 128.58   |
| 2   | B     | 610 | HSS  | N3-C2-N1  | -4.54 | 121.71      | 128.58   |
| 2   | C     | 710 | HSS  | N3-C4-N9  | 3.74  | 133.52      | 127.17   |
| 2   | C     | 710 | HSS  | C-N1S-S   | -3.68 | 110.59      | 124.07   |
| 2   | C     | 710 | HSS  | C2-N3-C4  | 3.68  | 120.82      | 111.83   |
| 2   | A     | 510 | HSS  | N3-C4-N9  | 3.66  | 133.40      | 127.17   |
| 2   | B     | 610 | HSS  | N3-C4-N9  | 3.63  | 133.34      | 127.17   |
| 2   | D     | 810 | HSS  | C2-N3-C4  | 3.57  | 120.55      | 111.83   |
| 2   | A     | 510 | HSS  | C2-N3-C4  | 3.53  | 120.45      | 111.83   |
| 2   | B     | 610 | HSS  | C2-N3-C4  | 3.53  | 120.44      | 111.83   |
| 2   | D     | 810 | HSS  | N3-C4-N9  | 3.37  | 132.91      | 127.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 510 | HSS  | C-N1S-S     | -3.37 | 111.73      | 124.07   |
| 2   | B     | 610 | HSS  | O5'-C5'-C4' | 3.33  | 113.51      | 107.57   |
| 2   | D     | 810 | HSS  | N9-C8-N7    | -3.31 | 109.25      | 113.94   |
| 2   | B     | 610 | HSS  | N9-C8-N7    | -3.20 | 109.40      | 113.94   |
| 2   | C     | 710 | HSS  | N9-C8-N7    | -3.18 | 109.42      | 113.94   |
| 2   | A     | 510 | HSS  | N9-C8-N7    | -3.13 | 109.50      | 113.94   |
| 2   | D     | 810 | HSS  | C5-N7-C8    | 3.02  | 108.20      | 103.45   |
| 2   | D     | 810 | HSS  | C4-C5-N7    | -3.02 | 107.13      | 110.58   |
| 2   | C     | 710 | HSS  | C4-C5-N7    | -2.99 | 107.16      | 110.58   |
| 2   | C     | 710 | HSS  | C5-N7-C8    | 2.95  | 108.09      | 103.45   |
| 2   | B     | 610 | HSS  | C4-C5-N7    | -2.95 | 107.21      | 110.58   |
| 2   | B     | 610 | HSS  | C5-N7-C8    | 2.93  | 108.06      | 103.45   |
| 2   | A     | 510 | HSS  | C5-N7-C8    | 2.81  | 107.87      | 103.45   |
| 2   | A     | 510 | HSS  | C4-C5-N7    | -2.72 | 107.48      | 110.58   |
| 2   | D     | 810 | HSS  | C5'-O5'-S   | 2.70  | 122.64      | 116.97   |
| 2   | A     | 510 | HSS  | CA-CB-CG    | -2.66 | 108.81      | 113.23   |
| 2   | D     | 810 | HSS  | C-N1S-S     | -2.64 | 114.43      | 124.07   |
| 2   | D     | 810 | HSS  | O5'-S-O3S   | -2.50 | 97.92       | 105.48   |
| 2   | C     | 710 | HSS  | O5'-C5'-C4' | 2.49  | 112.01      | 107.57   |
| 2   | D     | 810 | HSS  | O5'-S-N1S   | -2.45 | 99.36       | 105.69   |
| 2   | D     | 810 | HSS  | C4-N9-C8    | 2.44  | 108.30      | 105.74   |
| 2   | B     | 610 | HSS  | C4-N9-C8    | 2.40  | 108.26      | 105.74   |
| 2   | A     | 510 | HSS  | O5'-C5'-C4' | 2.39  | 111.82      | 107.57   |
| 2   | A     | 510 | HSS  | C4'-O4'-C1' | -2.35 | 104.27      | 109.47   |
| 2   | A     | 510 | HSS  | C4-N9-C8    | 2.34  | 108.20      | 105.74   |
| 2   | B     | 610 | HSS  | O5'-S-O3S   | -2.25 | 98.68       | 105.48   |
| 2   | C     | 710 | HSS  | C4-N9-C8    | 2.25  | 108.10      | 105.74   |
| 2   | D     | 810 | HSS  | O5'-C5'-C4' | 2.24  | 111.56      | 107.57   |
| 2   | D     | 810 | HSS  | CA-CB-CG    | -2.23 | 109.53      | 113.23   |
| 2   | C     | 710 | HSS  | O5'-S-O3S   | -2.22 | 98.76       | 105.48   |
| 2   | C     | 710 | HSS  | O5'-S-N1S   | -2.13 | 100.17      | 105.69   |
| 2   | B     | 610 | HSS  | C2'-C3'-C4' | -2.06 | 98.62       | 102.61   |
| 2   | B     | 610 | HSS  | C-N1S-S     | -2.03 | 116.66      | 124.07   |
| 2   | A     | 510 | HSS  | O4'-C4'-C3' | -2.03 | 101.13      | 105.15   |
| 2   | B     | 610 | HSS  | CD2-CG-N11  | 2.02  | 108.04      | 105.65   |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | A     | 510 | HSS  | C-N1S-S-O2S |
| 2   | A     | 510 | HSS  | C-N1S-S-O3S |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | D     | 810 | HSS  | C5'-O5'-S-N1S   |
| 2   | D     | 810 | HSS  | C5'-O5'-S-O3S   |
| 2   | D     | 810 | HSS  | O4'-C4'-C5'-O5' |
| 2   | D     | 810 | HSS  | C3'-C4'-C5'-O5' |
| 2   | C     | 710 | HSS  | C5'-O5'-S-O3S   |
| 2   | D     | 810 | HSS  | C5'-O5'-S-O2S   |
| 2   | B     | 610 | HSS  | N1S-C-CA-CB     |
| 2   | C     | 710 | HSS  | C5'-O5'-S-O2S   |
| 2   | B     | 610 | HSS  | O-C-CA-N        |
| 2   | B     | 610 | HSS  | O-C-CA-CB       |
| 2   | C     | 710 | HSS  | O-C-CA-CB       |
| 2   | B     | 610 | HSS  | N1S-C-CA-N      |
| 2   | C     | 710 | HSS  | O-C-CA-N        |
| 2   | C     | 710 | HSS  | N1S-C-CA-N      |
| 2   | C     | 710 | HSS  | C5'-O5'-S-N1S   |
| 2   | C     | 710 | HSS  | O4'-C4'-C5'-O5' |

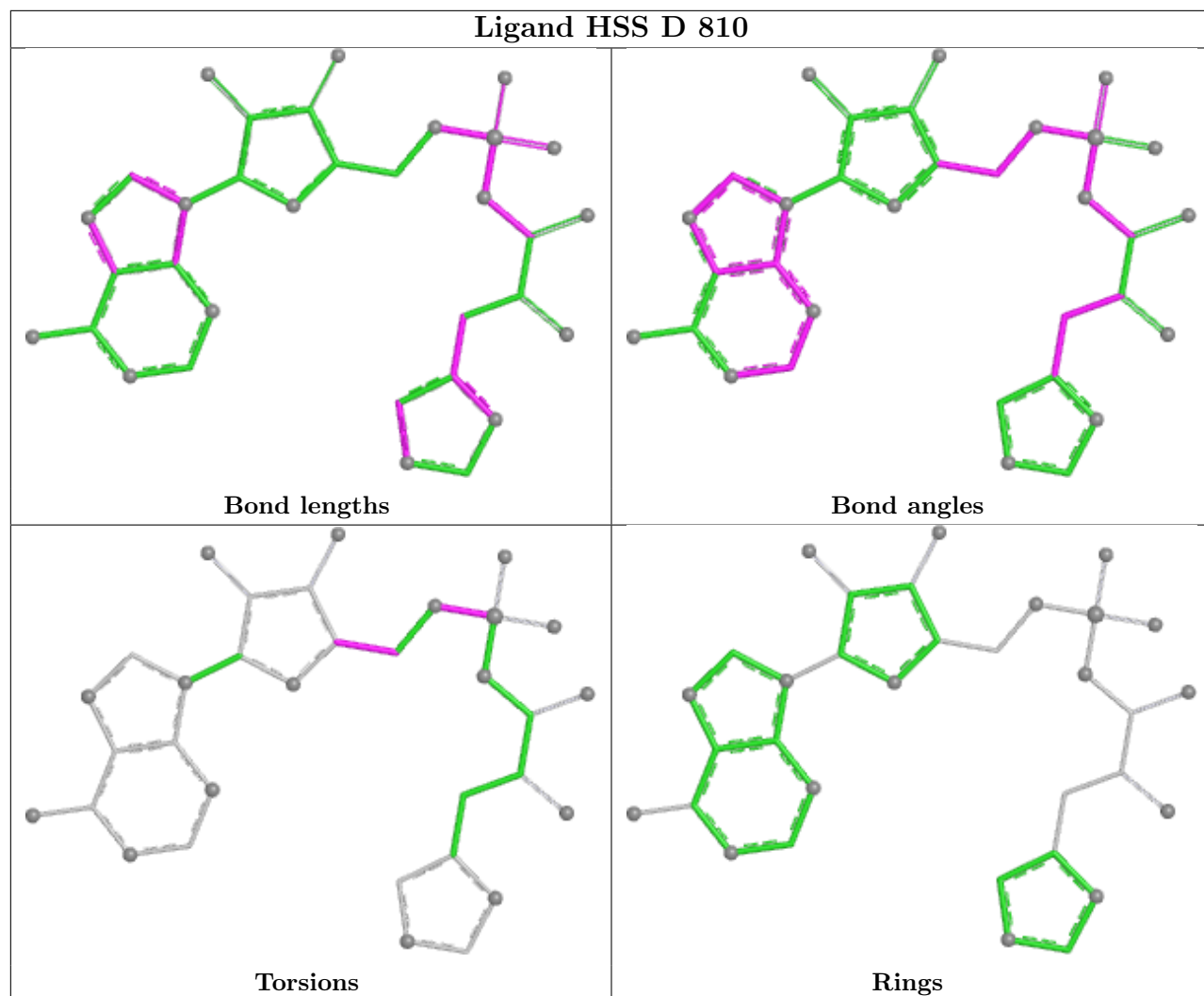
There are no ring outliers.

4 monomers are involved in 20 short contacts:

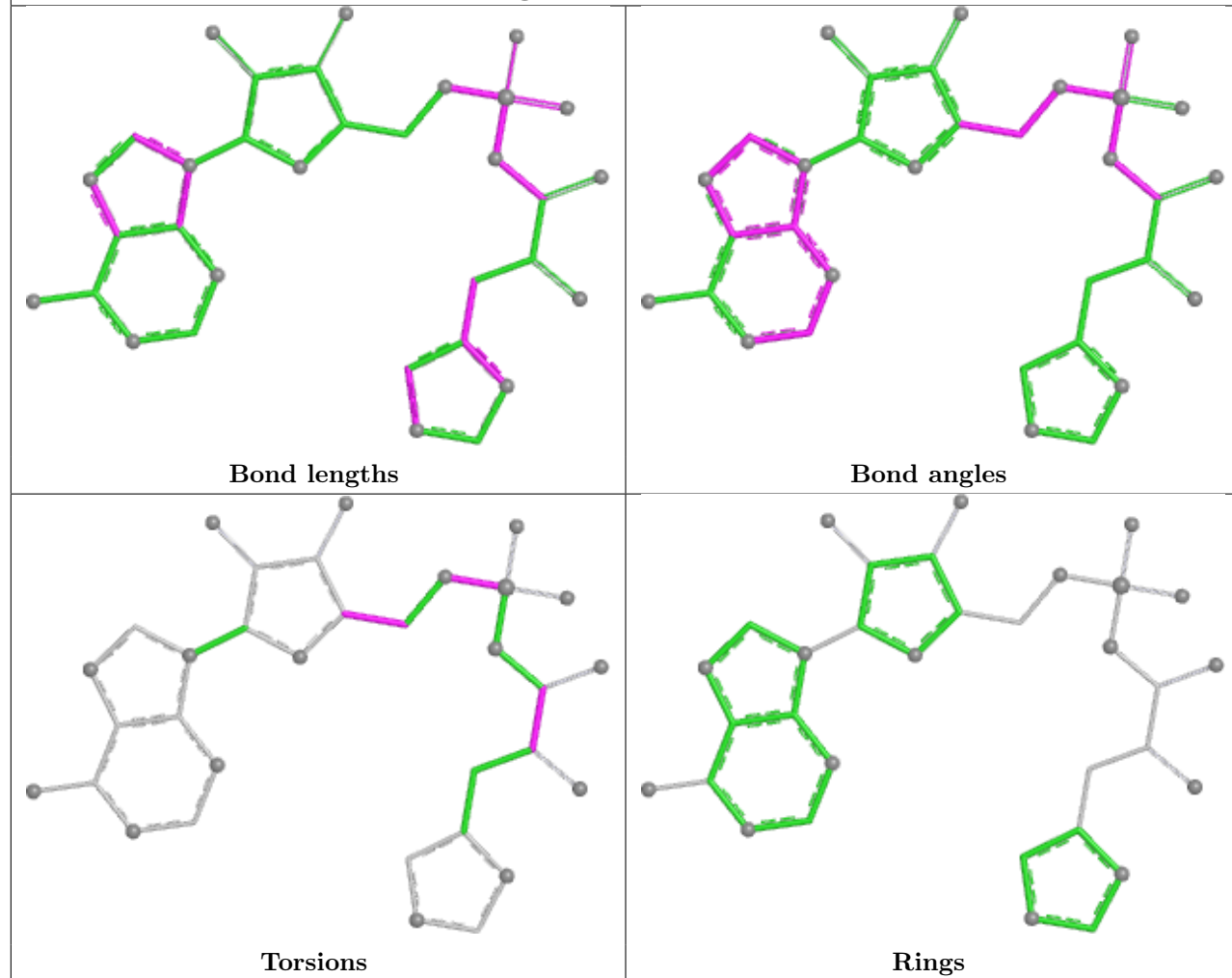
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | D     | 810 | HSS  | 5       | 0            |
| 2   | C     | 710 | HSS  | 9       | 0            |
| 2   | B     | 610 | HSS  | 2       | 0            |
| 2   | A     | 510 | HSS  | 4       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

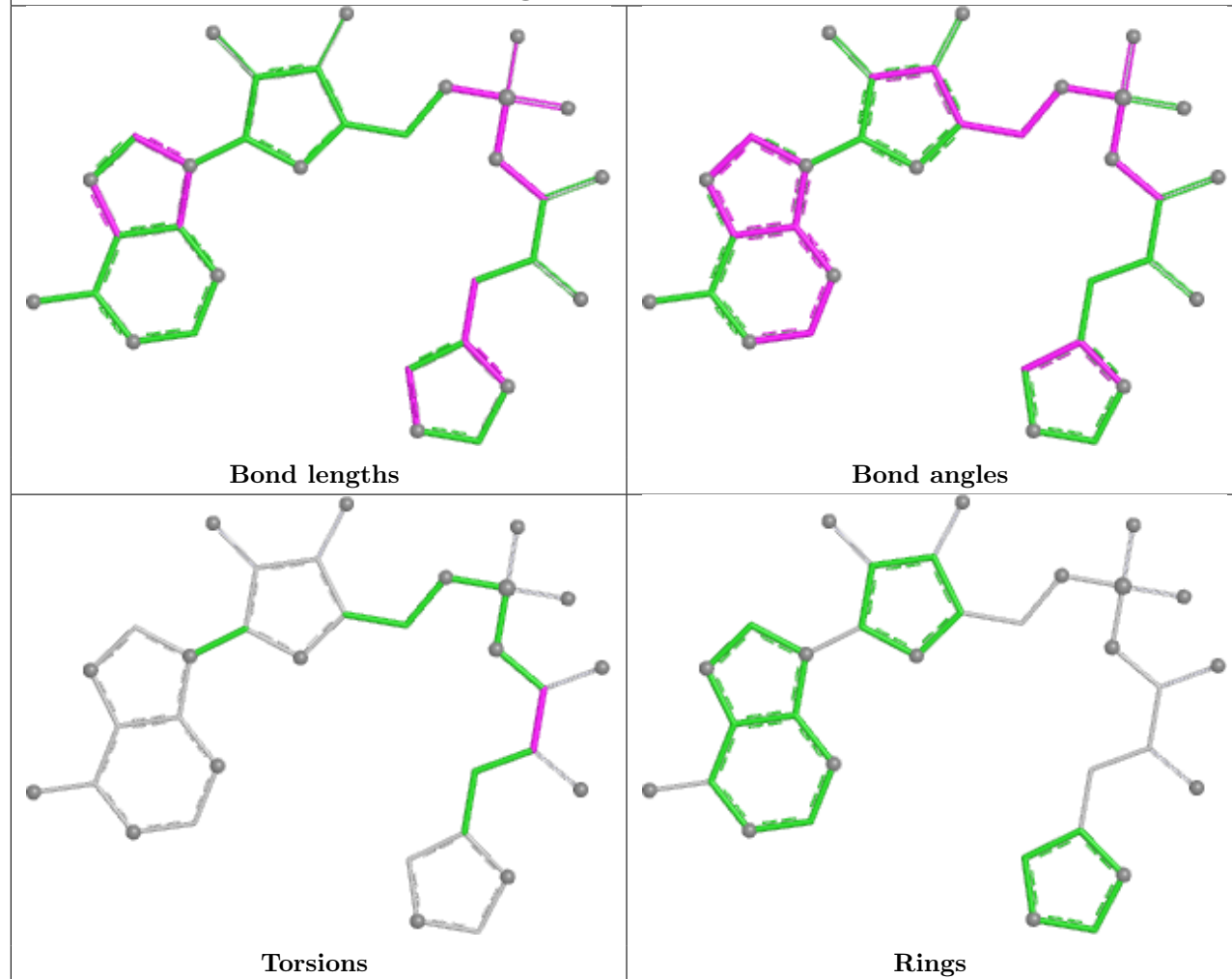
## Ligand HSS D 810

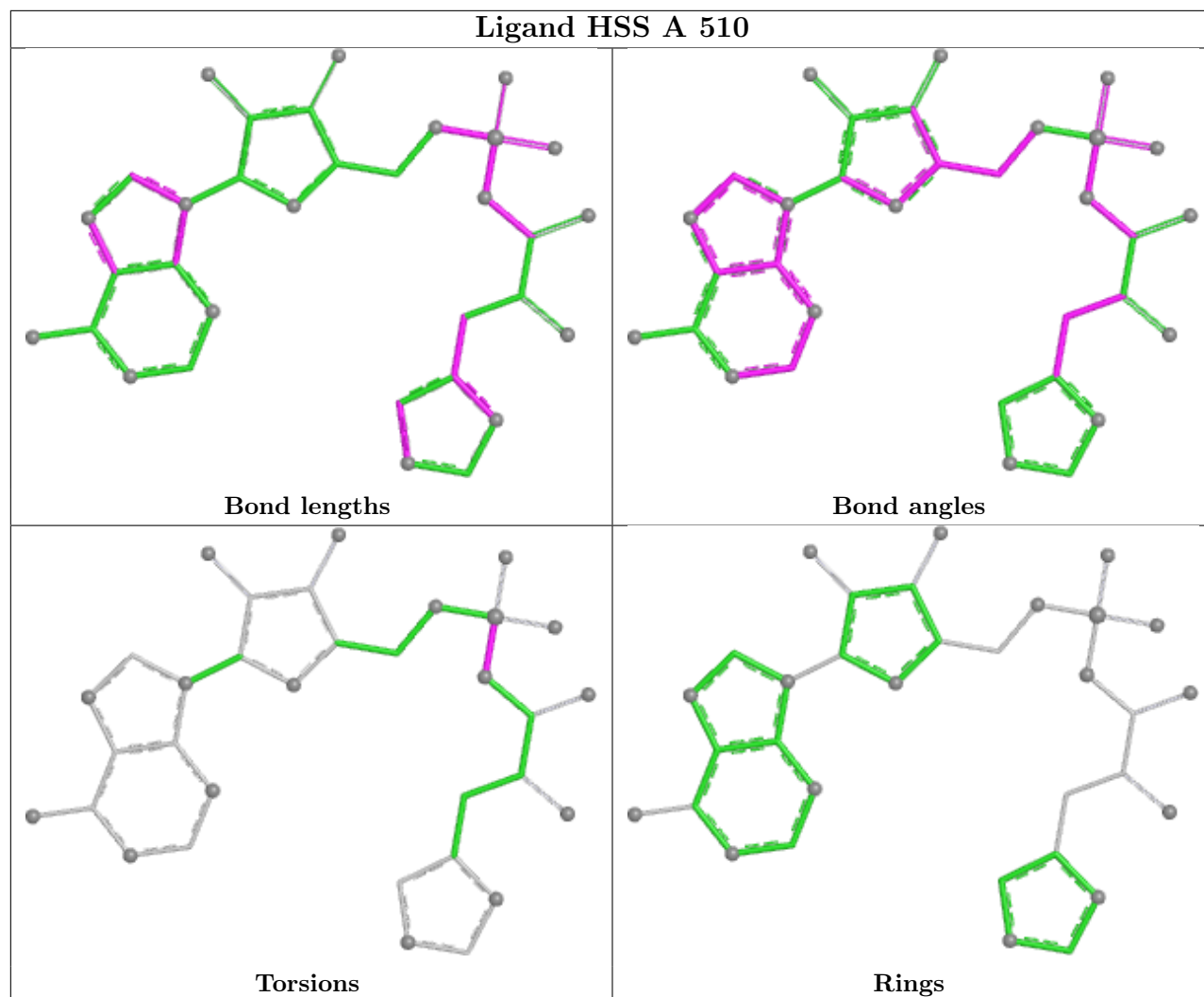


## Ligand HSS C 710



## Ligand HSS B 610





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 372/431 (86%)   | 0.35   | 19 (5%)   | 33 29 | 27, 57, 113, 140      | 0       |
| 1   | B     | 376/431 (87%)   | -0.00  | 14 (3%)   | 45 41 | 21, 50, 90, 109       | 0       |
| 1   | C     | 372/431 (86%)   | 0.33   | 21 (5%)   | 30 26 | 27, 56, 111, 128      | 0       |
| 1   | D     | 385/431 (89%)   | 0.12   | 19 (4%)   | 35 31 | 19, 51, 97, 136       | 0       |
| All | All   | 1505/1724 (87%) | 0.20   | 73 (4%)   | 35 31 | 19, 54, 104, 140      | 0       |

All (73) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 226 | GLY  | 4.7  |
| 1   | A     | 226 | GLY  | 4.5  |
| 1   | C     | 257 | LEU  | 4.5  |
| 1   | A     | 225 | LEU  | 4.2  |
| 1   | A     | 257 | LEU  | 3.7  |
| 1   | C     | 337 | GLY  | 3.6  |
| 1   | C     | 167 | SER  | 3.6  |
| 1   | D     | 276 | LEU  | 3.6  |
| 1   | D     | 185 | LEU  | 3.5  |
| 1   | A     | 180 | ALA  | 3.3  |
| 1   | A     | 174 | ARG  | 3.2  |
| 1   | B     | 257 | LEU  | 3.2  |
| 1   | A     | 338 | ALA  | 3.2  |
| 1   | B     | 328 | VAL  | 3.1  |
| 1   | D     | 184 | PHE  | 3.1  |
| 1   | C     | 137 | GLY  | 3.1  |
| 1   | B     | 178 | ARG  | 3.0  |
| 1   | C     | 258 | VAL  | 3.0  |
| 1   | D     | 59  | VAL  | 2.9  |
| 1   | A     | 167 | SER  | 2.9  |
| 1   | D     | 224 | ALA  | 2.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | B            | 137        | GLY         | 2.8         |
| 1          | B            | 256        | ARG         | 2.8         |
| 1          | C            | 274        | ASN         | 2.8         |
| 1          | D            | 356        | PRO         | 2.7         |
| 1          | A            | 255        | GLN         | 2.7         |
| 1          | B            | 277        | GLY         | 2.7         |
| 1          | D            | 182        | VAL         | 2.7         |
| 1          | A            | 228        | TYR         | 2.6         |
| 1          | B            | 323        | PHE         | 2.6         |
| 1          | C            | 165        | LEU         | 2.6         |
| 1          | B            | 75         | GLY         | 2.6         |
| 1          | C            | 171        | LEU         | 2.5         |
| 1          | A            | 323        | PHE         | 2.5         |
| 1          | A            | 274        | ASN         | 2.5         |
| 1          | A            | 258        | VAL         | 2.5         |
| 1          | D            | 328        | VAL         | 2.4         |
| 1          | C            | 336        | SER         | 2.4         |
| 1          | A            | 171        | LEU         | 2.4         |
| 1          | B            | 276        | LEU         | 2.4         |
| 1          | C            | 229        | LEU         | 2.4         |
| 1          | B            | 258        | VAL         | 2.3         |
| 1          | A            | 173        | ALA         | 2.3         |
| 1          | D            | 369        | PHE         | 2.3         |
| 1          | B            | 325        | ALA         | 2.3         |
| 1          | B            | 278        | SER         | 2.3         |
| 1          | C            | 168        | ILE         | 2.3         |
| 1          | D            | 183        | ALA         | 2.3         |
| 1          | B            | 370        | LYS         | 2.3         |
| 1          | A            | 229        | LEU         | 2.3         |
| 1          | A            | 175        | ALA         | 2.2         |
| 1          | C            | 180        | ALA         | 2.2         |
| 1          | D            | 175        | ALA         | 2.2         |
| 1          | D            | 370        | LYS         | 2.2         |
| 1          | C            | 120        | GLY         | 2.2         |
| 1          | D            | 323        | PHE         | 2.2         |
| 1          | C            | 117        | PRO         | 2.1         |
| 1          | A            | 3          | LYS         | 2.1         |
| 1          | C            | 255        | GLN         | 2.1         |
| 1          | D            | 277        | GLY         | 2.1         |
| 1          | C            | 256        | ARG         | 2.1         |
| 1          | D            | 187        | GLN         | 2.1         |
| 1          | C            | 272        | VAL         | 2.1         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 178 | ARG  | 2.1  |
| 1   | C     | 166 | ASN  | 2.1  |
| 1   | C     | 263 | TYR  | 2.1  |
| 1   | D     | 225 | LEU  | 2.1  |
| 1   | A     | 120 | GLY  | 2.1  |
| 1   | D     | 357 | GLY  | 2.1  |
| 1   | B     | 341 | GLN  | 2.0  |
| 1   | A     | 100 | ASN  | 2.0  |
| 1   | D     | 136 | GLN  | 2.0  |
| 1   | C     | 280 | GLY  | 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

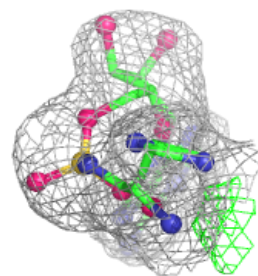
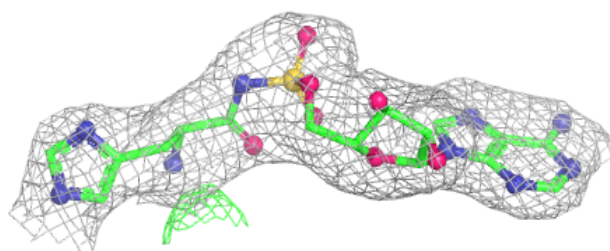
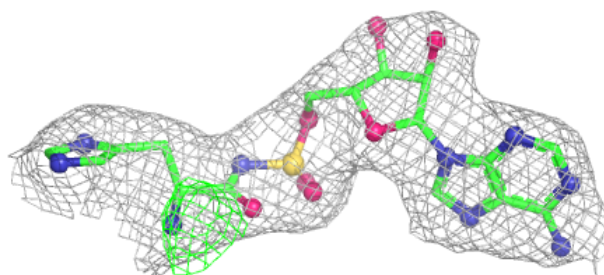
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | HSS  | A     | 510 | 33/33 | 0.95 | 0.08 | 23,48,71,77                 | 0     |
| 2   | HSS  | C     | 710 | 33/33 | 0.95 | 0.09 | 39,49,66,71                 | 0     |
| 2   | HSS  | D     | 810 | 33/33 | 0.97 | 0.06 | 15,30,37,44                 | 0     |
| 2   | HSS  | B     | 610 | 33/33 | 0.98 | 0.06 | 17,31,38,49                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

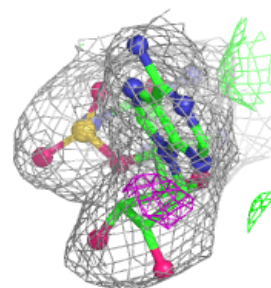
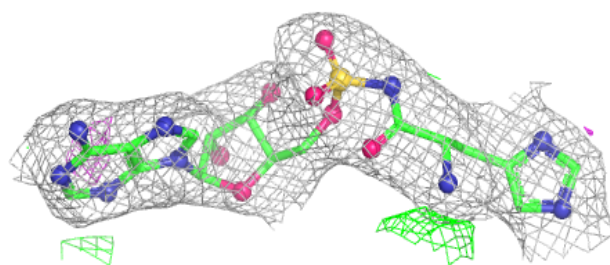
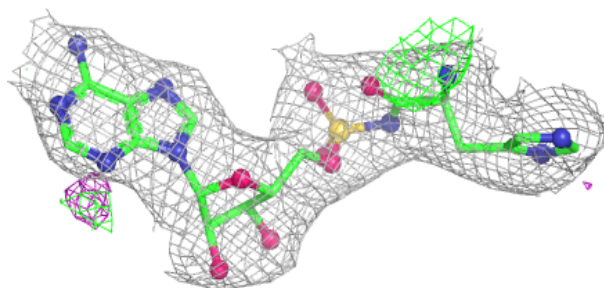


**Electron density around HSS A 510:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

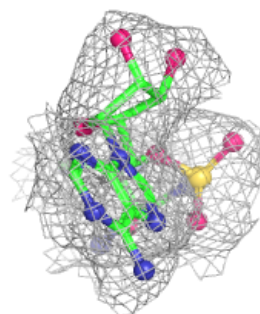
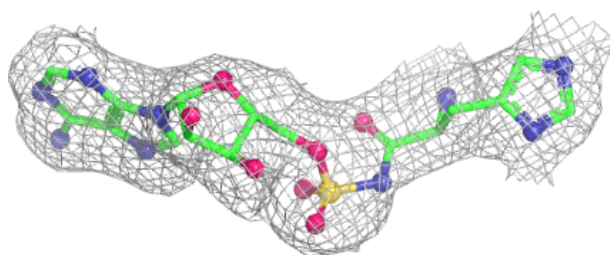
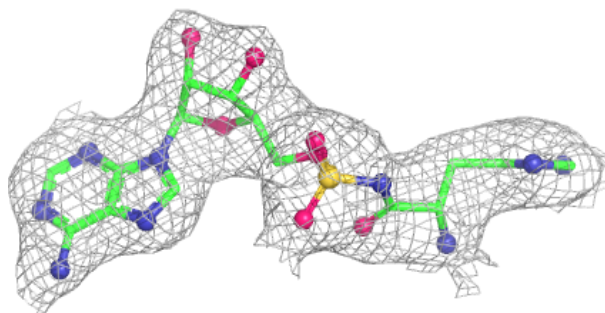
**Electron density around HSS C 710:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

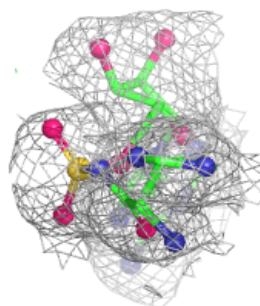
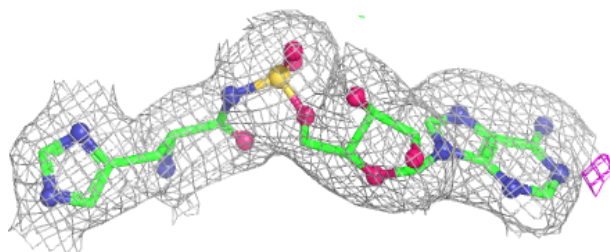
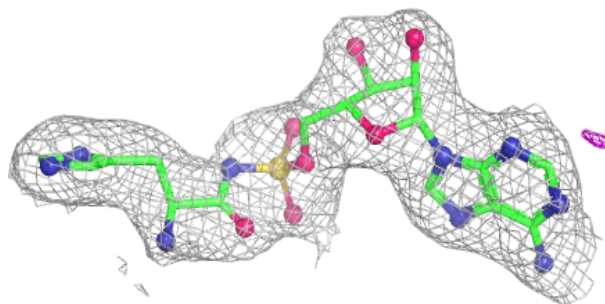


**Electron density around HSS D 810:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HSS B 610:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.