



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 1ZLA / pdb\_00001zla  
Title : X-ray Structure of a Kaposi's sarcoma herpesvirus LANA peptide bound to the nucleosomal core  
Authors : Chodaparambil, J.V.; Barbera, A.J.; Kaye, K.M.; Luger, K.  
Deposited on : 2005-05-05  
Resolution : 2.90 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                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| 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                                                             |

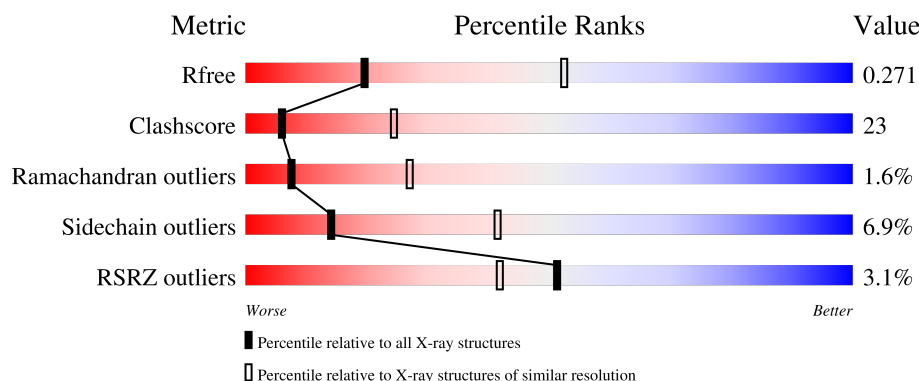
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

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   | I     | 146    | <div> <div>5%</div> <div>43%</div> <div>56%</div> <div>.</div> </div>                |
| 1   | J     | 146    | <div> <div>5%</div> <div>40%</div> <div>59%</div> <div>.</div> </div>                |
| 2   | A     | 135    | <div> <div>4%</div> <div>41%</div> <div>27%</div> <div>.</div> <div>27%</div> </div> |
| 2   | E     | 135    | <div> <div>3%</div> <div>47%</div> <div>21%</div> <div>.</div> <div>27%</div> </div> |
| 3   | B     | 102    | <div> <div>46%</div> <div>30%</div> <div>.</div> <div>23%</div> </div>               |

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| Mol | Chain | Length | Quality of chain                                            |
|-----|-------|--------|-------------------------------------------------------------|
| 3   | F     | 102    | <div><div></div><div>53%26%18%</div><div></div></div>       |
| 4   | C     | 129    | <div><div></div><div>%48%29%6%17%</div><div></div></div>    |
| 4   | G     | 129    | <div><div></div><div>2%42%32%6%18%</div><div></div></div>   |
| 5   | D     | 125    | <div><div></div><div>2%42%32%26%</div><div></div></div>     |
| 5   | H     | 125    | <div><div></div><div>2%41%30%26%</div><div></div></div>     |
| 6   | K     | 22     | <div><div></div><div>5%23%5%27%9%36%</div><div></div></div> |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12168 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 DNA chain called Palindromic 146bp Human alpha-Satellite DNA fragment.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 1   | I     | 146      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2990  | 1430 | 541 | 874 | 145 |         |         |       |
| 1   | J     | 146      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2990  | 1430 | 541 | 874 | 145 |         |         |       |

- Molecule 2 is a protein called histone H3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | A     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 811   | 511 | 158 | 139 | 3 |         |         |       |
| 2   | E     | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 811   | 511 | 158 | 139 | 3 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference |
|-------|---------|----------|--------|---------------------|-----------|
| A     | 511     | ALA      | GLY    | engineered mutation | GB 288992 |
| A     | 518     | HIS      | THR    | engineered mutation | GB 288992 |
| E     | 711     | ALA      | GLY    | engineered mutation | GB 288992 |
| E     | 718     | HIS      | THR    | engineered mutation | GB 288992 |

- Molecule 3 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | B     | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 627   | 395 | 121 | 110 | 1 |         |         |       |
| 3   | F     | 84       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 673   | 424 | 133 | 115 | 1 |         |         |       |

- Molecule 4 is a protein called Xenopus laevis-like histone H2A.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 4   | C     | 107      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 825   | 520 | 161 | 144 |         |         |       |
| 4   | G     | 106      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 818   | 516 | 160 | 142 |         |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment             | Reference   |
|-------|---------|----------|--------|---------------------|-------------|
| C     | 869     | TRP      | ALA    | engineered mutation | GB 30268540 |
| C     | 870     | GLU      | ALA    | engineered mutation | GB 30268540 |
| C     | 926     | THR      | ALA    | engineered mutation | GB 30268540 |
| G     | 1069    | TRP      | ALA    | engineered mutation | GB 30268540 |
| G     | 1070    | GLU      | ALA    | engineered mutation | GB 30268540 |
| G     | 1126    | THR      | ALA    | engineered mutation | GB 30268540 |

- Molecule 5 is a protein called histone H2B.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | D     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 459 | 131 | 137 | 2 |         |         |       |
| 5   | H     | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 729   | 459 | 131 | 137 | 2 |         |         |       |

- Molecule 6 is a protein called latent nuclear antigen.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 6   | K     | 14       | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 99    | 58 | 23 | 17 | 1 |         |         |       |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 7   | I     | 16       | Total | O  | 0       | 0       |
|     |       |          | 16    | 16 |         |         |
| 7   | J     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 7   | A     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 7   | B     | 1        | Total | O  | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 7   | C     | 6        | Total | O  | 0       | 0       |
|     |       |          | 6     | 6  |         |         |

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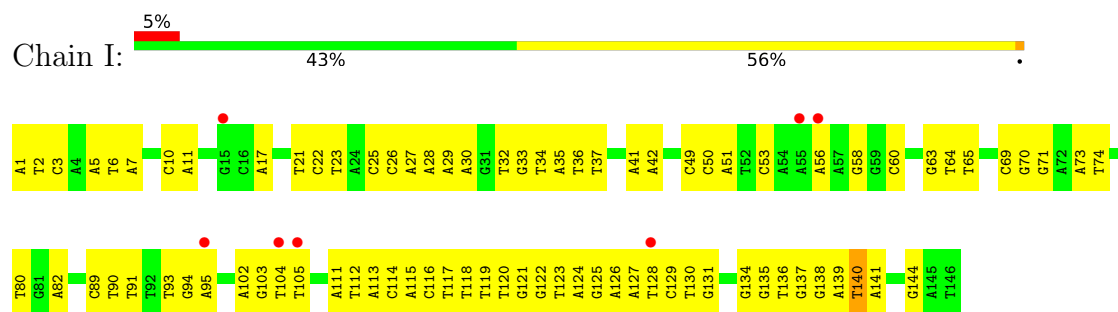
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| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 7   | D     | 8        | Total<br>8 | O<br>8 | 0       | 0       |
| 7   | E     | 4        | Total<br>4 | O<br>4 | 0       | 0       |
| 7   | F     | 6        | Total<br>6 | O<br>6 | 0       | 0       |
| 7   | G     | 7        | Total<br>7 | O<br>7 | 0       | 0       |
| 7   | H     | 5        | Total<br>5 | O<br>5 | 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.

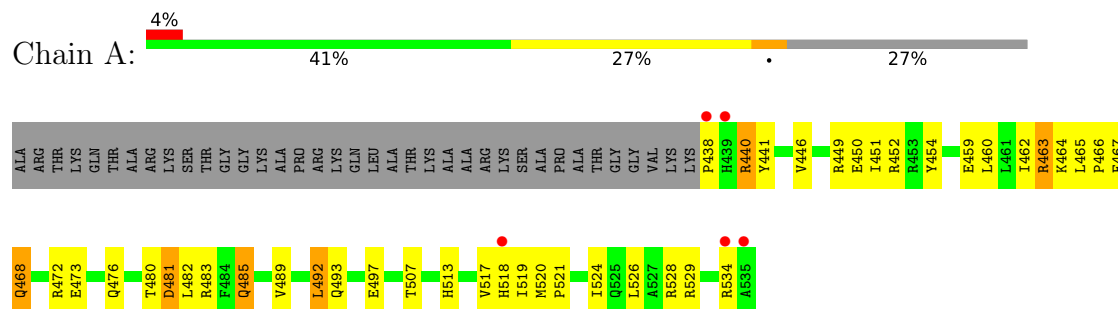
- Molecule 1: Palindromic 146bp Human alpha-Satellite DNA fragment



- Molecule 1: Palindromic 146bp Human alpha-Satellite DNA fragment



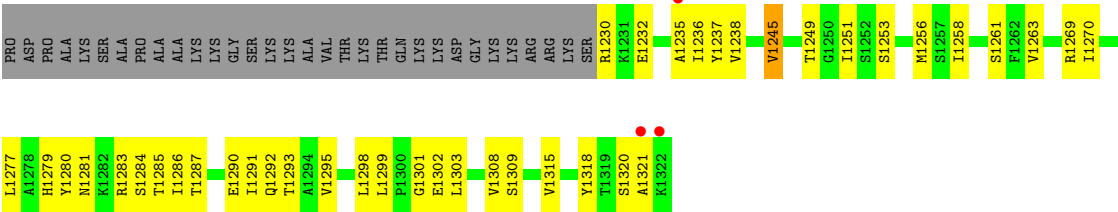
- Molecule 2: histone H3



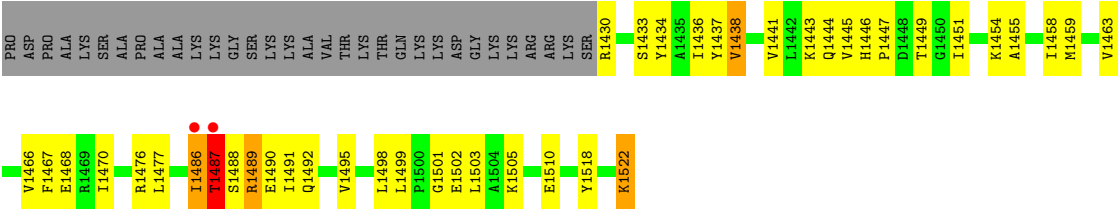
- Molecule 2: histone H3



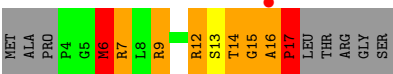
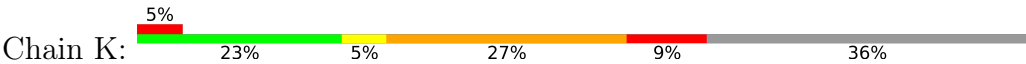




• Molecule 5: histone H2B



• Molecule 6: latent nuclear antigen



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 21 21 21                                                  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 106.16Å 109.60Å 182.24Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 50.00 – 2.90<br>50.00 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.8 (50.00-2.90)<br>90.8 (50.00-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.04                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.18 (at 2.90Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.222 , 0.277<br>0.212 , 0.271                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2208 reflections (4.94%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 52.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.264                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 55.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | 0.023 for k,h,-l                                            | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 12168                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 64.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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   | I     | 0.30         | 0/3354         | 0.65        | 0/5175          |
| 1   | J     | 0.32         | 1/3354 (0.0%)  | 0.67        | 0/5175          |
| 2   | A     | 0.59         | 0/824          | 1.09        | 3/1104 (0.3%)   |
| 2   | E     | 0.80         | 1/824 (0.1%)   | 1.02        | 3/1104 (0.3%)   |
| 3   | B     | 0.50         | 0/634          | 1.08        | 4/848 (0.5%)    |
| 3   | F     | 0.77         | 2/680 (0.3%)   | 1.30        | 9/908 (1.0%)    |
| 4   | C     | 0.63         | 1/835 (0.1%)   | 1.14        | 5/1127 (0.4%)   |
| 4   | G     | 0.56         | 0/828          | 1.19        | 11/1117 (1.0%)  |
| 5   | D     | 0.57         | 0/740          | 1.04        | 3/994 (0.3%)    |
| 5   | H     | 0.74         | 1/740 (0.1%)   | 1.03        | 3/994 (0.3%)    |
| 6   | K     | 0.68         | 0/100          | 1.97        | 2/131 (1.5%)    |
| All | All   | 0.50         | 6/12913 (0.0%) | 0.90        | 43/18677 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | I     | 0                   | 1                   |
| 1   | J     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

All (6) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | E     | 735  | ALA  | C-OXT | 15.67 | 1.54        | 1.23     |
| 5   | H     | 1522 | LYS  | C-OXT | 13.41 | 1.50        | 1.23     |
| 3   | F     | 224  | ASP  | C-N   | 7.50  | 1.44        | 1.33     |
| 1   | J     | 199  | DC   | P-OP1 | -7.33 | 1.33        | 1.48     |
| 3   | F     | 220  | LYS  | CA-C  | -6.11 | 1.44        | 1.52     |
| 4   | C     | 917  | PRO  | CA-C  | 6.08  | 1.60        | 1.52     |

All (43) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 4   | C     | 917  | PRO  | CA-N-CD    | -16.18 | 89.36       | 112.00   |
| 2   | A     | 438  | PRO  | CA-N-CD    | -13.63 | 92.92       | 112.00   |
| 6   | K     | 17   | PRO  | CA-N-CD    | -13.51 | 93.09       | 112.00   |
| 3   | F     | 219  | ARG  | O-C-N      | 11.18  | 140.89      | 123.00   |
| 3   | F     | 219  | ARG  | CA-C-N     | 9.86   | 140.38      | 121.54   |
| 3   | F     | 219  | ARG  | C-N-CA     | 9.86   | 140.38      | 121.54   |
| 4   | G     | 1112 | GLN  | OE1-CD-NE2 | -9.42  | 113.18      | 122.60   |
| 3   | F     | 219  | ARG  | CA-C-O     | 9.13   | 136.32      | 120.80   |
| 3   | B     | 30   | THR  | N-CA-C     | 7.81   | 120.66      | 110.43   |
| 4   | G     | 1117 | PRO  | CA-N-CD    | -7.79  | 101.09      | 112.00   |
| 3   | B     | 93   | GLN  | N-CA-C     | -7.28  | 104.38      | 113.18   |
| 4   | G     | 1112 | GLN  | CG-CD-NE2  | 6.80   | 126.60      | 116.40   |
| 5   | D     | 1238 | VAL  | N-CA-C     | -6.76  | 103.89      | 110.72   |
| 3   | B     | 46   | ILE  | N-CA-C     | 6.64   | 117.85      | 107.28   |
| 2   | A     | 464  | LYS  | N-CA-C     | 6.60   | 119.03      | 111.11   |
| 4   | C     | 917  | PRO  | CB-CA-C    | -6.54  | 102.39      | 110.95   |
| 5   | H     | 1489 | ARG  | N-CA-C     | -6.06  | 104.01      | 111.40   |
| 6   | K     | 6    | MET  | N-CA-C     | 5.95   | 119.75      | 110.17   |
| 2   | E     | 733  | GLU  | N-CA-C     | -5.89  | 106.09      | 113.28   |
| 3   | F     | 228  | GLY  | N-CA-C     | -5.82  | 107.69      | 115.32   |
| 4   | G     | 1118 | LYS  | CA-C-N     | -5.79  | 111.28      | 121.70   |
| 4   | G     | 1118 | LYS  | C-N-CA     | -5.79  | 111.28      | 121.70   |
| 4   | G     | 1116 | LEU  | CA-C-N     | 5.78   | 127.06      | 119.84   |
| 4   | G     | 1116 | LEU  | C-N-CA     | 5.78   | 127.06      | 119.84   |
| 3   | F     | 219  | ARG  | CB-CA-C    | 5.75   | 121.03      | 110.10   |
| 4   | G     | 1115 | LEU  | CB-CA-C    | -5.74  | 101.72      | 111.02   |
| 2   | A     | 485  | GLN  | N-CA-C     | -5.47  | 102.91      | 110.35   |
| 4   | G     | 1025 | PHE  | N-CA-C     | 5.32   | 117.23      | 109.84   |
| 3   | B     | 72   | TYR  | N-CA-C     | -5.29  | 105.18      | 111.69   |
| 4   | C     | 887  | VAL  | N-CA-C     | 5.26   | 115.48      | 110.53   |
| 5   | D     | 1235 | ALA  | N-CA-C     | 5.25   | 120.04      | 111.37   |
| 2   | E     | 685  | GLN  | N-CA-C     | -5.24  | 101.92      | 110.20   |
| 3   | F     | 224  | ASP  | CA-C-N     | -5.21  | 112.01      | 120.72   |
| 3   | F     | 224  | ASP  | C-N-CA     | -5.21  | 112.01      | 120.72   |
| 5   | H     | 1438 | VAL  | N-CA-C     | -5.20  | 105.43      | 110.42   |
| 4   | G     | 1117 | PRO  | CA-C-N     | -5.15  | 113.19      | 122.46   |
| 4   | G     | 1117 | PRO  | C-N-CA     | -5.15  | 113.19      | 122.46   |
| 4   | C     | 917  | PRO  | CA-CB-CG   | -5.09  | 94.84       | 104.50   |
| 5   | D     | 1245 | VAL  | N-CA-C     | 5.08   | 115.86      | 110.72   |
| 3   | F     | 246  | ILE  | N-CA-C     | 5.07   | 115.21      | 108.11   |
| 2   | E     | 664  | LYS  | N-CA-C     | 5.05   | 116.48      | 110.97   |
| 4   | C     | 917  | PRO  | N-CA-C     | 5.05   | 118.98      | 111.41   |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed( <sup>o</sup> ) | Ideal( <sup>o</sup> ) |
|-----|-------|------|------|--------|------|--------------------------|-----------------------|
| 5   | H     | 1499 | LEU  | N-CA-C | 5.01 | 116.38                   | 110.07                |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | I     | 140 | DT   | Sidechain |
| 1   | J     | 147 | DA   | Sidechain |

## 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   | I     | 2990  | 0        | 1651     | 100     | 0            |
| 1   | J     | 2990  | 0        | 1651     | 108     | 0            |
| 2   | A     | 811   | 0        | 846      | 63      | 0            |
| 2   | E     | 811   | 0        | 846      | 53      | 0            |
| 3   | B     | 627   | 0        | 663      | 41      | 0            |
| 3   | F     | 673   | 0        | 722      | 39      | 1            |
| 4   | C     | 825   | 0        | 878      | 45      | 0            |
| 4   | G     | 818   | 0        | 871      | 65      | 0            |
| 5   | D     | 729   | 0        | 753      | 40      | 1            |
| 5   | H     | 729   | 0        | 753      | 43      | 0            |
| 6   | K     | 99    | 0        | 104      | 31      | 0            |
| 7   | A     | 2     | 0        | 0        | 5       | 0            |
| 7   | B     | 1     | 0        | 0        | 0       | 0            |
| 7   | C     | 6     | 0        | 0        | 1       | 0            |
| 7   | D     | 8     | 0        | 0        | 2       | 0            |
| 7   | E     | 4     | 0        | 0        | 1       | 0            |
| 7   | F     | 6     | 0        | 0        | 2       | 0            |
| 7   | G     | 7     | 0        | 0        | 0       | 0            |
| 7   | H     | 5     | 0        | 0        | 0       | 0            |
| 7   | I     | 16    | 0        | 0        | 2       | 0            |
| 7   | J     | 11    | 0        | 0        | 1       | 0            |
| All | All   | 12168 | 0        | 9738     | 497     | 1            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 23.

All (497) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:1116:LEU:HB3  | 4:G:1117:PRO:HD2  | 1.26                     | 1.15              |
| 1:J:261:DA:H2''   | 1:J:262:DC:H5''   | 1.34                     | 1.08              |
| 1:J:174:DA:H2''   | 1:J:175:DA:H5''   | 1.34                     | 1.06              |
| 6:K:9:ARG:HG3     | 6:K:9:ARG:HH11    | 1.22                     | 1.04              |
| 5:H:1487:THR:O    | 5:H:1489:ARG:N    | 1.90                     | 1.03              |
| 5:H:1444:GLN:HB3  | 6:K:14:THR:HG22   | 1.35                     | 1.03              |
| 1:I:3:DC:H5       | 1:J:290:DG:H1     | 1.06                     | 0.98              |
| 2:E:734:ARG:O     | 2:E:735:ALA:HB3   | 1.63                     | 0.96              |
| 5:H:1470:ILE:HD13 | 5:H:1498:LEU:HD12 | 1.47                     | 0.96              |
| 1:J:216:DG:H4'    | 2:E:718:HIS:NE2   | 1.82                     | 0.94              |
| 2:A:520:MET:HA    | 3:B:50:ILE:HD11   | 1.52                     | 0.91              |
| 1:I:28:DA:H2''    | 1:I:29:DA:H5''    | 1.52                     | 0.90              |
| 2:A:451:ILE:HD13  | 3:B:39:ARG:O      | 1.71                     | 0.89              |
| 4:G:1017:ARG:HH12 | 4:G:1031:HIS:HD2  | 1.22                     | 0.88              |
| 1:J:197:DA:H2''   | 1:J:198:DT:H5'    | 1.56                     | 0.87              |
| 4:G:1035:ARG:HB3  | 4:G:1035:ARG:NH1  | 1.92                     | 0.85              |
| 2:A:507:THR:OG1   | 2:A:524:ILE:HD13  | 1.77                     | 0.84              |
| 1:I:22:DC:H42     | 1:J:271:DG:H1     | 1.26                     | 0.84              |
| 1:I:89:DC:H2''    | 1:I:90:DT:H71     | 1.59                     | 0.83              |
| 4:G:1116:LEU:CB   | 4:G:1117:PRO:HD2  | 2.04                     | 0.83              |
| 5:H:1487:THR:HG23 | 5:H:1490:GLU:OE1  | 1.79                     | 0.82              |
| 2:A:463:ARG:O     | 2:A:466:PRO:HD2   | 1.80                     | 0.82              |
| 1:J:246:DG:H2''   | 1:J:247:DC:C5     | 2.14                     | 0.81              |
| 4:G:1116:LEU:HB3  | 4:G:1117:PRO:CD   | 2.07                     | 0.81              |
| 1:I:127:DA:H1'    | 1:I:128:DT:H5'    | 1.63                     | 0.81              |
| 1:I:3:DC:H5       | 1:J:290:DG:N1     | 1.78                     | 0.81              |
| 2:A:518:HIS:NE2   | 3:B:45:ARG:NE     | 2.29                     | 0.80              |
| 3:B:34:ILE:HD12   | 3:B:54:THR:HG21   | 1.63                     | 0.79              |
| 5:H:1444:GLN:CB   | 6:K:14:THR:HG22   | 2.12                     | 0.79              |
| 2:A:476:GLN:NE2   | 2:A:480:THR:HA    | 1.97                     | 0.79              |
| 2:E:718:HIS:CE1   | 3:F:245:ARG:NH1   | 2.51                     | 0.79              |
| 1:I:123:DT:H2''   | 1:I:124:DA:H5'    | 1.63                     | 0.79              |
| 4:C:817:ARG:HH22  | 4:C:831:HIS:CD2   | 2.01                     | 0.78              |
| 2:E:734:ARG:O     | 2:E:735:ALA:CB    | 2.28                     | 0.78              |
| 2:A:452:ARG:HG3   | 2:A:452:ARG:HH11  | 1.48                     | 0.78              |
| 5:D:1287:THR:O    | 5:D:1291:ILE:CD1  | 2.32                     | 0.78              |
| 2:E:718:HIS:HB3   | 7:F:346:HOH:O     | 1.83                     | 0.78              |
| 2:A:520:MET:HG3   | 7:A:332:HOH:O     | 1.83                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:1017:ARG:HH12 | 4:G:1031:HIS:CD2  | 2.01                     | 0.78              |
| 1:J:151:DA:H2''   | 1:J:152:DT:C5'    | 2.14                     | 0.78              |
| 6:K:14:THR:O      | 6:K:15:GLY:O      | 2.01                     | 0.77              |
| 1:I:3:DC:H2'      | 1:I:3:DC:O2       | 1.84                     | 0.77              |
| 6:K:16:ALA:O      | 6:K:17:PRO:O      | 2.03                     | 0.77              |
| 1:J:261:DA:C2'    | 1:J:262:DC:H5''   | 2.13                     | 0.76              |
| 2:E:651:ILE:HD13  | 3:F:239:ARG:HA    | 1.67                     | 0.75              |
| 4:G:1035:ARG:CB   | 4:G:1035:ARG:HH11 | 2.00                     | 0.75              |
| 1:J:174:DA:C2'    | 1:J:175:DA:H5''   | 2.14                     | 0.74              |
| 1:J:248:DA:H2''   | 1:J:249:DG:C8     | 2.22                     | 0.74              |
| 5:H:1444:GLN:OE1  | 6:K:14:THR:HG21   | 1.86                     | 0.74              |
| 1:I:80:DT:H4'     | 3:F:245:ARG:NH1   | 2.01                     | 0.74              |
| 2:E:664:LYS:NZ    | 2:E:690:MET:HE1   | 2.02                     | 0.73              |
| 1:J:151:DA:H2''   | 1:J:152:DT:H5''   | 1.71                     | 0.73              |
| 1:J:226:DT:H2''   | 1:J:227:DG:C8     | 2.23                     | 0.73              |
| 2:A:518:HIS:HB3   | 7:A:332:HOH:O     | 1.88                     | 0.73              |
| 2:E:661:LEU:HD12  | 3:F:237:LEU:HD23  | 1.71                     | 0.73              |
| 1:J:286:DT:H2''   | 1:J:287:DA:O5'    | 1.89                     | 0.72              |
| 1:I:89:DC:H2''    | 1:I:90:DT:C7      | 2.19                     | 0.72              |
| 1:I:22:DC:N4      | 1:J:271:DG:H1     | 1.86                     | 0.72              |
| 1:I:138:DG:H2''   | 1:I:139:DA:OP2    | 1.90                     | 0.71              |
| 1:I:134:DG:H2''   | 1:I:135:DG:H5'    | 1.72                     | 0.71              |
| 1:J:227:DG:H5'    | 3:B:47:SER:HA     | 1.71                     | 0.71              |
| 3:F:287:VAL:HG11  | 3:F:302:GLY:HA3   | 1.74                     | 0.70              |
| 6:K:7:ARG:HG2     | 6:K:7:ARG:HH11    | 1.55                     | 0.70              |
| 5:D:1287:THR:O    | 5:D:1291:ILE:HD12 | 1.91                     | 0.69              |
| 5:H:1444:GLN:CD   | 6:K:14:THR:CG2    | 2.65                     | 0.69              |
| 4:C:841:GLU:HB2   | 5:D:1284:SER:HB2  | 1.74                     | 0.69              |
| 1:I:28:DA:C2'     | 1:I:29:DA:H5''    | 2.23                     | 0.69              |
| 4:C:842:ARG:HD3   | 5:D:1285:THR:OG1  | 1.93                     | 0.69              |
| 1:J:246:DG:H2''   | 1:J:247:DC:C6     | 2.28                     | 0.69              |
| 4:G:1078:ILE:HB   | 5:H:1451:ILE:HD12 | 1.76                     | 0.68              |
| 4:G:1116:LEU:CB   | 4:G:1117:PRO:CD   | 2.62                     | 0.68              |
| 1:J:197:DA:C2'    | 1:J:198:DT:H5'    | 2.23                     | 0.68              |
| 4:C:849:VAL:HG11  | 5:D:1315:VAL:HA   | 1.76                     | 0.68              |
| 5:D:1292:GLN:NE2  | 5:D:1308:VAL:HG13 | 2.08                     | 0.68              |
| 3:B:31:LYS:HB3    | 3:B:32:PRO:HD3    | 1.76                     | 0.67              |
| 4:G:1061:GLU:CD   | 6:K:9:ARG:NH1     | 2.53                     | 0.67              |
| 1:I:122:DG:H5'    | 5:H:1430:ARG:HH21 | 1.57                     | 0.67              |
| 5:D:1291:ILE:HD12 | 5:D:1291:ILE:H    | 1.58                     | 0.67              |
| 1:I:119:DT:H4'    | 1:I:120:DT:OP1    | 1.93                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:902:ILE:HG23  | 5:D:1258:ILE:HD13 | 1.77                     | 0.67              |
| 6:K:9:ARG:HH11    | 6:K:9:ARG:CG      | 2.04                     | 0.67              |
| 1:J:151:DA:C2'    | 1:J:152:DT:H5''   | 2.25                     | 0.67              |
| 4:G:1050:TYR:OH   | 5:H:1492:GLN:HG3  | 1.95                     | 0.67              |
| 1:I:82:DA:H3'     | 2:E:646:VAL:HG21  | 1.77                     | 0.66              |
| 2:E:651:ILE:HD13  | 3:F:239:ARG:O     | 1.95                     | 0.66              |
| 5:H:1502:GLU:OE1  | 5:H:1505:LYS:HD3  | 1.96                     | 0.66              |
| 5:H:1510:GLU:OE1  | 6:K:6:MET:HE2     | 1.96                     | 0.66              |
| 5:D:1298:LEU:HD23 | 5:D:1299:LEU:HD23 | 1.77                     | 0.66              |
| 5:H:1510:GLU:CD   | 6:K:6:MET:HB3     | 2.21                     | 0.65              |
| 4:C:832:ARG:HH22  | 5:D:1232:GLU:CD   | 2.05                     | 0.65              |
| 1:I:122:DG:N7     | 7:I:360:HOH:O     | 2.29                     | 0.65              |
| 3:F:226:ILE:HG12  | 3:F:255:ARG:HB3   | 1.79                     | 0.65              |
| 2:E:651:ILE:HD12  | 3:F:242:GLY:HA2   | 1.79                     | 0.64              |
| 4:G:1026:PRO:HD3  | 5:H:1437:TYR:CD2  | 2.32                     | 0.64              |
| 2:E:665:LEU:HB3   | 2:E:666:PRO:HD3   | 1.79                     | 0.64              |
| 2:E:708:ASN:O     | 2:E:712:ILE:HD13  | 1.98                     | 0.64              |
| 4:G:1035:ARG:NH1  | 4:G:1035:ARG:CB   | 2.61                     | 0.64              |
| 1:I:36:DT:H2''    | 1:I:37:DT:OP2     | 1.98                     | 0.64              |
| 2:E:718:HIS:CD2   | 3:F:245:ARG:HD2   | 2.33                     | 0.64              |
| 2:E:729:ARG:HA    | 2:E:734:ARG:HB3   | 1.80                     | 0.63              |
| 3:F:259:LYS:O     | 3:F:263:GLU:HG3   | 1.98                     | 0.63              |
| 1:J:184:DT:H2''   | 1:J:185:DG:N7     | 2.13                     | 0.63              |
| 6:K:7:ARG:HG2     | 6:K:7:ARG:NH1     | 2.13                     | 0.63              |
| 5:H:1522:LYS:O    | 5:H:1522:LYS:HG3  | 1.98                     | 0.62              |
| 1:J:217:DG:H5'    | 2:E:718:HIS:CE1   | 2.34                     | 0.62              |
| 4:G:1058:LEU:O    | 4:G:1062:ILE:HD13 | 2.00                     | 0.62              |
| 1:I:69:DC:H4'     | 2:A:518:HIS:HE1   | 1.65                     | 0.62              |
| 4:C:855:LEU:O     | 4:C:859:THR:HG23  | 1.98                     | 0.62              |
| 1:I:137:DG:H2''   | 1:I:138:DG:C8     | 2.35                     | 0.62              |
| 3:F:231:LYS:HB3   | 3:F:232:PRO:HD3   | 1.82                     | 0.62              |
| 2:E:651:ILE:HD13  | 3:F:239:ARG:CA    | 2.30                     | 0.62              |
| 2:E:664:LYS:HZ1   | 2:E:690:MET:HE1   | 1.63                     | 0.62              |
| 2:A:440:ARG:HG2   | 2:A:440:ARG:HH11  | 1.65                     | 0.61              |
| 1:I:114:DC:H4'    | 1:I:114:DC:OP1    | 1.99                     | 0.61              |
| 2:E:651:ILE:HD12  | 3:F:242:GLY:CA    | 2.31                     | 0.61              |
| 1:J:262:DC:H2'    | 1:J:263:DT:H71    | 1.83                     | 0.61              |
| 3:B:47:SER:HB3    | 3:B:50:ILE:HD13   | 1.82                     | 0.61              |
| 3:B:47:SER:HB3    | 3:B:50:ILE:CD1    | 2.30                     | 0.61              |
| 4:C:832:ARG:NH2   | 5:D:1232:GLU:OE1  | 2.34                     | 0.61              |
| 4:C:906:GLY:HA3   | 2:E:658:THR:HG22  | 1.83                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:258:DT:H2'    | 1:J:259:DA:C8     | 2.37                     | 0.60              |
| 1:I:21:DT:H2''    | 1:I:22:DC:O5'     | 2.01                     | 0.60              |
| 1:J:151:DA:H2''   | 1:J:152:DT:H5'    | 1.83                     | 0.60              |
| 1:J:235:DC:H2''   | 1:J:236:DT:OP2    | 2.00                     | 0.60              |
| 3:B:59:LYS:HE2    | 3:B:63:GLU:OE2    | 2.02                     | 0.60              |
| 4:C:831:HIS:CD2   | 4:C:848:PRO:HG3   | 2.37                     | 0.60              |
| 1:I:25:DC:H2''    | 1:I:26:DC:H5'     | 1.83                     | 0.60              |
| 1:I:94:DG:H2''    | 1:I:95:DA:C8      | 2.37                     | 0.59              |
| 2:A:521:PRO:HD2   | 7:A:304:HOH:O     | 2.02                     | 0.59              |
| 2:E:718:HIS:CE1   | 3:F:245:ARG:CZ    | 2.86                     | 0.59              |
| 5:D:1287:THR:O    | 5:D:1291:ILE:HD13 | 2.02                     | 0.59              |
| 5:H:1444:GLN:CD   | 6:K:14:THR:HG21   | 2.27                     | 0.59              |
| 5:H:1470:ILE:HD13 | 5:H:1498:LEU:CD1  | 2.28                     | 0.59              |
| 1:I:63:DG:H2''    | 1:I:64:DT:OP2     | 2.02                     | 0.59              |
| 2:A:476:GLN:HE22  | 2:A:480:THR:HA    | 1.68                     | 0.59              |
| 5:H:1434:TYR:O    | 5:H:1438:VAL:HG23 | 2.03                     | 0.59              |
| 5:H:1491:ILE:HD12 | 5:H:1491:ILE:H    | 1.68                     | 0.59              |
| 1:I:22:DC:H4'     | 1:I:22:DC:OP1     | 2.03                     | 0.58              |
| 1:I:125:DG:H1     | 1:J:168:DC:H42    | 1.51                     | 0.58              |
| 6:K:14:THR:C      | 6:K:15:GLY:O      | 2.44                     | 0.58              |
| 1:J:239:DT:H2''   | 1:J:240:DG:H8     | 1.68                     | 0.58              |
| 6:K:14:THR:O      | 6:K:15:GLY:C      | 2.46                     | 0.58              |
| 1:I:10:DC:H2''    | 1:I:11:DA:C8      | 2.39                     | 0.58              |
| 2:A:517:VAL:O     | 3:B:45:ARG:HB2    | 2.03                     | 0.58              |
| 4:C:884:GLN:OE1   | 4:C:888:ARG:HD2   | 2.04                     | 0.58              |
| 4:G:1015:LYS:HE2  | 4:G:1019:SER:HB3  | 1.84                     | 0.58              |
| 4:G:1113:SER:C    | 4:G:1115:LEU:H    | 2.13                     | 0.57              |
| 5:H:1444:GLN:CD   | 6:K:14:THR:HG22   | 2.29                     | 0.57              |
| 4:G:1031:HIS:HE1  | 4:G:1035:ARG:NH2  | 2.01                     | 0.57              |
| 1:I:94:DG:H2''    | 1:I:95:DA:H8      | 1.69                     | 0.57              |
| 1:I:131:DG:H3'    | 4:G:1076:THR:OG1  | 2.05                     | 0.57              |
| 3:F:230:THR:HB    | 3:F:232:PRO:HD2   | 1.85                     | 0.57              |
| 2:E:651:ILE:CD1   | 3:F:239:ARG:HA    | 2.34                     | 0.57              |
| 4:C:831:HIS:HE1   | 4:C:835:ARG:NH2   | 2.03                     | 0.57              |
| 3:F:236:ARG:O     | 3:F:239:ARG:HB2   | 2.05                     | 0.57              |
| 1:I:117:DT:H2''   | 1:I:118:DT:H71    | 1.87                     | 0.57              |
| 2:A:528:ARG:HD3   | 2:A:534:ARG:HH12  | 1.69                     | 0.57              |
| 1:I:117:DT:C2'    | 1:I:118:DT:H71    | 2.35                     | 0.57              |
| 6:K:15:GLY:O      | 6:K:16:ALA:HB3    | 2.05                     | 0.57              |
| 1:J:247:DC:H2''   | 1:J:248:DA:OP2    | 2.05                     | 0.57              |
| 4:C:826:PRO:HD3   | 5:D:1237:TYR:CD2  | 2.40                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:1017:ARG:NH1  | 4:G:1031:HIS:HD2  | 1.99                     | 0.56              |
| 3:F:238:ALA:HB1   | 3:F:243:VAL:HB    | 1.86                     | 0.56              |
| 3:B:47:SER:CB     | 3:B:50:ILE:HD13   | 2.35                     | 0.56              |
| 5:D:1287:THR:H    | 5:D:1290:GLU:HG2  | 1.69                     | 0.56              |
| 1:J:252:DT:H2''   | 1:J:253:DC:C6     | 2.41                     | 0.56              |
| 2:A:440:ARG:HH11  | 2:A:440:ARG:CG    | 2.19                     | 0.56              |
| 1:I:124:DA:H2''   | 1:I:125:DG:C8     | 2.41                     | 0.56              |
| 4:G:1017:ARG:HG2  | 5:H:1518:TYR:HE1  | 1.71                     | 0.55              |
| 1:I:93:DT:H2''    | 1:I:94:DG:H5'     | 1.87                     | 0.55              |
| 2:A:519:ILE:C     | 7:A:332:HOH:O     | 2.48                     | 0.55              |
| 2:E:663:ARG:HE    | 2:E:663:ARG:HA    | 1.70                     | 0.55              |
| 5:H:1436:ILE:HG13 | 5:H:1437:TYR:N    | 2.21                     | 0.55              |
| 1:J:162:DC:H1'    | 1:J:163:DA:C5     | 2.40                     | 0.55              |
| 5:D:1286:ILE:HG22 | 5:D:1291:ILE:HD11 | 1.88                     | 0.55              |
| 1:J:281:DG:H2''   | 1:J:282:DT:O5'    | 2.06                     | 0.55              |
| 4:G:1031:HIS:CD2  | 4:G:1048:PRO:HG3  | 2.42                     | 0.55              |
| 2:A:518:HIS:NE2   | 3:B:45:ARG:CZ     | 2.69                     | 0.55              |
| 3:B:59:LYS:O      | 3:B:63:GLU:HG3    | 2.07                     | 0.55              |
| 1:I:53:DC:H42     | 1:J:240:DG:H1     | 1.54                     | 0.55              |
| 4:C:862:ILE:HD11  | 4:C:887:VAL:CG2   | 2.37                     | 0.55              |
| 1:J:155:DC:H2''   | 1:J:156:DC:C6     | 2.41                     | 0.55              |
| 2:E:718:HIS:CB    | 7:F:346:HOH:O     | 2.46                     | 0.55              |
| 5:H:1451:ILE:HD11 | 5:H:1455:ALA:HB1  | 1.88                     | 0.55              |
| 1:J:214:DG:H2''   | 1:J:215:DC:C6     | 2.42                     | 0.54              |
| 1:I:49:DC:H1'     | 1:I:50:DC:C6      | 2.42                     | 0.54              |
| 1:J:227:DG:C5'    | 3:B:47:SER:HA     | 2.37                     | 0.54              |
| 1:J:263:DT:H2''   | 1:J:264:DT:OP2    | 2.07                     | 0.54              |
| 2:A:460:LEU:HD13  | 2:A:493:GLN:NE2   | 2.23                     | 0.54              |
| 3:B:24:ASP:CG     | 3:B:25:ASN:H      | 2.15                     | 0.54              |
| 3:B:78:ARG:NH1    | 3:B:82:THR:HG23   | 2.22                     | 0.54              |
| 4:C:831:HIS:HE1   | 4:C:835:ARG:CZ    | 2.20                     | 0.54              |
| 1:I:73:DA:H1'     | 1:I:74:DT:H5'     | 1.90                     | 0.54              |
| 3:F:226:ILE:O     | 3:F:255:ARG:HD3   | 2.08                     | 0.54              |
| 1:J:233:DG:H1'    | 1:J:234:DC:H5'    | 1.90                     | 0.54              |
| 2:E:680:THR:HB    | 2:E:681:ASP:OD1   | 2.08                     | 0.54              |
| 4:C:829:ARG:NH1   | 5:D:1232:GLU:HB3  | 2.23                     | 0.53              |
| 1:I:1:DA:H2''     | 1:I:2:DT:OP2      | 2.07                     | 0.53              |
| 2:A:451:ILE:CD1   | 3:B:39:ARG:O      | 2.50                     | 0.53              |
| 2:A:518:HIS:C     | 7:A:332:HOH:O     | 2.51                     | 0.53              |
| 2:E:712:ILE:CD1   | 2:E:712:ILE:N     | 2.71                     | 0.53              |
| 4:C:817:ARG:HH22  | 4:C:831:HIS:CG    | 2.27                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:G:1031:HIS:CE1  | 4:G:1035:ARG:NH2  | 2.77                     | 0.53              |
| 4:C:851:LEU:HD13  | 5:D:1270:ILE:HG21 | 1.91                     | 0.53              |
| 2:A:529:ARG:HA    | 2:A:534:ARG:HB2   | 1.90                     | 0.53              |
| 6:K:16:ALA:O      | 6:K:17:PRO:C      | 2.49                     | 0.53              |
| 1:J:264:DT:C2'    | 1:J:265:DT:H71    | 2.38                     | 0.53              |
| 5:H:1443:LYS:O    | 5:H:1447:PRO:HG3  | 2.09                     | 0.53              |
| 1:J:176:DA:H2''   | 1:J:177:DG:OP2    | 2.09                     | 0.52              |
| 5:D:1281:ASN:O    | 5:D:1283:ARG:HG2  | 2.09                     | 0.52              |
| 3:F:230:THR:CB    | 3:F:232:PRO:HD2   | 2.39                     | 0.52              |
| 4:G:1061:GLU:CG   | 6:K:9:ARG:NH1     | 2.72                     | 0.52              |
| 6:K:12:ARG:HG3    | 6:K:13:SER:N      | 2.24                     | 0.52              |
| 4:G:1110:ASN:C    | 4:G:1111:ILE:HD12 | 2.35                     | 0.52              |
| 1:I:5:DA:H2''     | 1:I:6:DT:C5'      | 2.40                     | 0.52              |
| 2:A:463:ARG:C     | 2:A:466:PRO:HD2   | 2.34                     | 0.52              |
| 1:J:175:DA:H2''   | 1:J:176:DA:C8     | 2.44                     | 0.52              |
| 1:J:274:DT:H2''   | 1:J:275:DC:OP2    | 2.09                     | 0.52              |
| 1:I:130:DT:H2''   | 1:I:131:DG:N7     | 2.25                     | 0.52              |
| 2:E:664:LYS:HZ2   | 2:E:690:MET:HE1   | 1.73                     | 0.52              |
| 1:I:112:DT:H5'    | 4:G:1042:ARG:HG2  | 1.91                     | 0.52              |
| 1:I:58:DG:H1      | 1:J:235:DC:H42    | 1.58                     | 0.52              |
| 2:A:452:ARG:HG3   | 2:A:452:ARG:NH1   | 2.21                     | 0.52              |
| 4:G:1066:ALA:HB2  | 4:G:1083:LEU:HD23 | 1.90                     | 0.52              |
| 1:I:136:DT:H1'    | 1:I:137:DG:H5'    | 1.92                     | 0.52              |
| 4:C:911:ILE:N     | 4:C:911:ILE:HD12  | 2.24                     | 0.52              |
| 5:H:1436:ILE:HD11 | 5:H:1437:TYR:CZ   | 2.45                     | 0.52              |
| 1:I:30:DA:OP2     | 4:C:832:ARG:HD3   | 2.10                     | 0.52              |
| 2:A:519:ILE:HG13  | 2:A:519:ILE:O     | 2.09                     | 0.51              |
| 4:G:1062:ILE:HD11 | 4:G:1093:LEU:HD21 | 1.91                     | 0.51              |
| 6:K:9:ARG:HG3     | 6:K:9:ARG:NH1     | 2.04                     | 0.51              |
| 1:J:253:DC:H4'    | 1:J:254:DC:OP1    | 2.10                     | 0.51              |
| 2:E:720:MET:HE2   | 2:E:722:LYS:HE3   | 1.92                     | 0.51              |
| 1:J:172:DC:H2''   | 1:J:173:DA:N7     | 2.25                     | 0.51              |
| 1:J:216:DG:O3'    | 2:E:718:HIS:CE1   | 2.63                     | 0.51              |
| 4:G:1061:GLU:CD   | 6:K:9:ARG:HH11    | 2.18                     | 0.51              |
| 1:I:34:DT:H2''    | 1:I:35:DA:O5'     | 2.09                     | 0.51              |
| 1:I:121:DG:N7     | 7:I:335:HOH:O     | 2.35                     | 0.51              |
| 2:E:729:ARG:HG3   | 2:E:735:ALA:HA    | 1.93                     | 0.51              |
| 1:J:217:DG:H5'    | 2:E:718:HIS:ND1   | 2.25                     | 0.51              |
| 2:A:513:HIS:HB2   | 2:E:726:LEU:HD22  | 1.93                     | 0.51              |
| 1:I:126:DA:H2''   | 1:I:127:DA:OP2    | 2.10                     | 0.51              |
| 1:J:152:DT:H2''   | 1:J:153:DA:C8     | 2.46                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:207:DA:H5''   | 7:J:358:HOH:O     | 2.10                     | 0.51              |
| 1:J:287:DA:H2'    | 1:J:288:DT:C6     | 2.45                     | 0.51              |
| 1:I:26:DC:H1'     | 1:I:27:DA:C5      | 2.46                     | 0.51              |
| 1:I:111:DA:H4'    | 4:G:1042:ARG:NH1  | 2.25                     | 0.51              |
| 2:A:460:LEU:HB3   | 2:A:497:GLU:OE2   | 2.11                     | 0.51              |
| 4:G:1118:LYS:HG2  | 4:G:1119:LYS:N    | 2.24                     | 0.51              |
| 1:J:165:DA:H4'    | 4:G:1077:ARG:NH2  | 2.25                     | 0.50              |
| 1:J:272:DA:H1'    | 1:J:273:DA:H5'    | 1.94                     | 0.50              |
| 4:G:1058:LEU:O    | 4:G:1062:ILE:CD1  | 2.58                     | 0.50              |
| 1:J:151:DA:H1'    | 1:J:152:DT:H5''   | 1.93                     | 0.50              |
| 1:J:216:DG:H4'    | 2:E:718:HIS:CE1   | 2.46                     | 0.50              |
| 4:C:831:HIS:CE1   | 4:C:835:ARG:NH2   | 2.79                     | 0.50              |
| 1:J:195:DC:H4'    | 1:J:196:DC:OP1    | 2.11                     | 0.50              |
| 2:A:451:ILE:HD12  | 3:B:42:GLY:HA2    | 1.94                     | 0.50              |
| 1:I:125:DG:H1'    | 1:I:126:DA:H5'    | 1.94                     | 0.50              |
| 3:B:34:ILE:HD12   | 3:B:54:THR:CG2    | 2.38                     | 0.50              |
| 1:J:181:DA:H2''   | 1:J:182:DT:OP2    | 2.12                     | 0.50              |
| 1:I:113:DA:H2''   | 1:I:114:DC:O5'    | 2.11                     | 0.50              |
| 1:J:197:DA:H1'    | 1:J:198:DT:C5'    | 2.43                     | 0.49              |
| 2:A:460:LEU:HB3   | 2:A:493:GLN:NE2   | 2.27                     | 0.49              |
| 4:C:888:ARG:NH1   | 7:C:353:HOH:O     | 2.44                     | 0.49              |
| 2:A:446:VAL:O     | 2:A:450:GLU:HG3   | 2.12                     | 0.49              |
| 1:J:268:DG:H2''   | 1:J:269:DT:O5'    | 2.12                     | 0.49              |
| 1:J:274:DT:H1'    | 1:J:275:DC:H5'    | 1.94                     | 0.49              |
| 2:A:483:ARG:O     | 3:B:80:THR:HA     | 2.13                     | 0.49              |
| 4:C:837:GLY:HA3   | 4:C:839:TYR:CE1   | 2.47                     | 0.49              |
| 1:I:56:DA:H2      | 1:J:238:DT:O2     | 1.95                     | 0.49              |
| 4:G:1037:GLY:HA3  | 4:G:1039:TYR:CE1  | 2.48                     | 0.49              |
| 1:I:29:DA:H2''    | 1:I:30:DA:O5'     | 2.13                     | 0.49              |
| 4:C:835:ARG:HG2   | 4:C:835:ARG:HH11  | 1.77                     | 0.49              |
| 5:D:1298:LEU:HD23 | 5:D:1299:LEU:CD2  | 2.43                     | 0.49              |
| 4:G:1035:ARG:HH11 | 4:G:1035:ARG:HB2  | 1.76                     | 0.49              |
| 6:K:7:ARG:NH1     | 6:K:13:SER:HB3    | 2.28                     | 0.49              |
| 1:J:195:DC:H1'    | 1:J:196:DC:C6     | 2.48                     | 0.49              |
| 4:G:1062:ILE:HD11 | 4:G:1093:LEU:CD2  | 2.42                     | 0.49              |
| 1:I:49:DC:H1'     | 1:I:50:DC:C5      | 2.47                     | 0.48              |
| 2:A:473:GLU:OE1   | 3:B:25:ASN:ND2    | 2.41                     | 0.48              |
| 4:G:1102:ILE:HG23 | 5:H:1458:ILE:HD13 | 1.95                     | 0.48              |
| 1:I:6:DT:H2''     | 1:I:7:DA:C8       | 2.48                     | 0.48              |
| 2:A:451:ILE:HD13  | 3:B:39:ARG:C      | 2.36                     | 0.48              |
| 4:C:918:LYS:CG    | 4:C:919:LYS:H     | 2.25                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:D:1292:GLN:HE21 | 5:D:1308:VAL:HG13 | 1.76                     | 0.48              |
| 2:E:663:ARG:HA    | 2:E:663:ARG:NE    | 2.27                     | 0.48              |
| 4:G:1111:ILE:HD12 | 4:G:1111:ILE:N    | 2.29                     | 0.48              |
| 1:J:203:DA:H2''   | 1:J:204:DG:C8     | 2.49                     | 0.48              |
| 4:G:1026:PRO:HB2  | 4:G:1029:ARG:HB3  | 1.95                     | 0.48              |
| 3:F:231:LYS:N     | 3:F:232:PRO:CD    | 2.76                     | 0.48              |
| 1:J:197:DA:H1'    | 1:J:198:DT:H5'    | 1.94                     | 0.48              |
| 4:C:825:PHE:HZ    | 4:C:859:THR:HG21  | 1.78                     | 0.48              |
| 5:D:1261:SER:HB3  | 3:F:302:GLY:OXT   | 2.14                     | 0.48              |
| 1:J:239:DT:H2''   | 1:J:240:DG:C8     | 2.48                     | 0.48              |
| 1:I:3:DC:O2       | 1:I:3:DC:C2'      | 2.58                     | 0.48              |
| 3:B:101:GLY:O     | 3:B:102:GLY:C     | 2.57                     | 0.48              |
| 4:G:1119:LYS:HE2  | 4:G:1119:LYS:HB3  | 1.36                     | 0.48              |
| 1:I:2:DT:H1'      | 1:I:3:DC:H5'      | 1.95                     | 0.47              |
| 1:I:36:DT:H1'     | 1:I:37:DT:H5'     | 1.96                     | 0.47              |
| 1:I:125:DG:H2''   | 1:I:126:DA:OP2    | 2.14                     | 0.47              |
| 1:J:248:DA:H2''   | 1:J:249:DG:N7     | 2.28                     | 0.47              |
| 1:I:26:DC:H1'     | 1:I:27:DA:C4      | 2.48                     | 0.47              |
| 2:A:528:ARG:HB2   | 2:A:534:ARG:HH11  | 1.78                     | 0.47              |
| 1:I:64:DT:H1'     | 1:I:65:DT:H5'     | 1.96                     | 0.47              |
| 3:F:287:VAL:HG11  | 3:F:302:GLY:CA    | 2.44                     | 0.47              |
| 1:I:117:DT:H2''   | 1:I:118:DT:OP2    | 2.15                     | 0.47              |
| 1:I:115:DA:H61    | 1:J:178:DT:H3     | 1.62                     | 0.47              |
| 1:J:281:DG:H1'    | 1:J:282:DT:H5'    | 1.96                     | 0.47              |
| 3:F:226:ILE:HD11  | 3:F:255:ARG:O     | 2.15                     | 0.47              |
| 4:C:850:TYR:OH    | 5:D:1292:GLN:HG3  | 2.14                     | 0.47              |
| 5:D:1279:HIS:O    | 5:D:1280:TYR:C    | 2.57                     | 0.47              |
| 2:E:651:ILE:HD13  | 3:F:239:ARG:C     | 2.40                     | 0.47              |
| 4:G:1061:GLU:CG   | 6:K:9:ARG:HH12    | 2.28                     | 0.47              |
| 1:I:2:DT:H2''     | 1:I:3:DC:O5'      | 2.14                     | 0.47              |
| 5:D:1318:TYR:O    | 5:D:1321:ALA:HB3  | 2.15                     | 0.47              |
| 4:G:1047:ALA:N    | 4:G:1048:PRO:HD2  | 2.30                     | 0.47              |
| 5:H:1503:LEU:HD13 | 6:K:9:ARG:CZ      | 2.44                     | 0.47              |
| 1:I:60:DC:H5'     | 2:A:463:ARG:CZ    | 2.44                     | 0.47              |
| 1:J:162:DC:H1'    | 1:J:163:DA:C4     | 2.50                     | 0.47              |
| 4:G:1080:PRO:HG3  | 5:H:1458:ILE:HD12 | 1.96                     | 0.47              |
| 4:G:1081:ARG:HD3  | 4:G:1081:ARG:C    | 2.40                     | 0.47              |
| 4:G:1081:ARG:NH2  | 4:G:1107:VAL:O    | 2.48                     | 0.47              |
| 1:J:195:DC:H1'    | 1:J:196:DC:C5     | 2.50                     | 0.47              |
| 2:E:724:ILE:HD11  | 3:F:250:ILE:HD12  | 1.96                     | 0.47              |
| 1:I:5:DA:H2''     | 1:I:6:DT:H5''     | 1.95                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:238:DT:H72    | 2:A:465:LEU:HD22  | 1.98                     | 0.46              |
| 2:E:712:ILE:HD13  | 2:E:712:ILE:H     | 1.80                     | 0.46              |
| 1:J:164:DG:H2''   | 1:J:165:DA:OP2    | 2.15                     | 0.46              |
| 1:J:176:DA:OP2    | 4:G:1032:ARG:HD3  | 2.14                     | 0.46              |
| 1:J:217:DG:C5'    | 2:E:718:HIS:ND1   | 2.78                     | 0.46              |
| 4:G:1015:LYS:HE2  | 4:G:1019:SER:CB   | 2.44                     | 0.46              |
| 2:A:462:ILE:HD11  | 3:B:37:LEU:HD11   | 1.97                     | 0.46              |
| 5:H:1459:MET:O    | 5:H:1463:VAL:HG23 | 2.16                     | 0.46              |
| 1:I:3:DC:H5       | 1:J:290:DG:C2     | 2.33                     | 0.46              |
| 5:D:1236:ILE:HG13 | 5:D:1237:TYR:N    | 2.30                     | 0.46              |
| 2:E:663:ARG:HB2   | 2:E:666:PRO:HG2   | 1.98                     | 0.46              |
| 4:G:1040:ALA:CB   | 5:H:1486:ILE:HG13 | 2.45                     | 0.46              |
| 2:A:460:LEU:HD13  | 2:A:493:GLN:CD    | 2.41                     | 0.46              |
| 3:F:225:ASN:C     | 3:F:227:GLN:N     | 2.72                     | 0.46              |
| 3:F:233:ALA:HA    | 3:F:236:ARG:NH2   | 2.31                     | 0.46              |
| 1:I:7:DA:C2       | 1:J:287:DA:C2     | 3.03                     | 0.46              |
| 1:J:150:DA:H4'    | 1:J:151:DA:OP1    | 2.16                     | 0.46              |
| 4:C:826:PRO:O     | 4:C:830:VAL:HG23  | 2.15                     | 0.46              |
| 5:H:1466:VAL:O    | 5:H:1467:PHE:C    | 2.58                     | 0.46              |
| 2:A:451:ILE:HD12  | 3:B:42:GLY:CA     | 2.46                     | 0.46              |
| 1:I:69:DC:H4'     | 2:A:518:HIS:CE1   | 2.49                     | 0.45              |
| 2:A:518:HIS:NE2   | 3:B:45:ARG:NH2    | 2.64                     | 0.45              |
| 5:H:1451:ILE:HG23 | 5:H:1451:ILE:O    | 2.16                     | 0.45              |
| 1:I:5:DA:C2'      | 1:I:6:DT:H5''     | 2.46                     | 0.45              |
| 3:F:226:ILE:CG1   | 3:F:255:ARG:HB3   | 2.46                     | 0.45              |
| 1:I:28:DA:H2''    | 1:I:29:DA:C5'     | 2.37                     | 0.45              |
| 1:J:149:DC:H2'    | 1:J:150:DA:C8     | 2.51                     | 0.45              |
| 2:E:724:ILE:O     | 2:E:728:ARG:HG3   | 2.16                     | 0.45              |
| 4:G:1113:SER:C    | 4:G:1115:LEU:N    | 2.74                     | 0.45              |
| 1:J:175:DA:C2'    | 1:J:176:DA:C8     | 2.99                     | 0.45              |
| 1:I:25:DC:N4      | 1:I:26:DC:H42     | 2.15                     | 0.45              |
| 1:I:144:DG:H1     | 1:J:149:DC:H42    | 1.63                     | 0.45              |
| 4:G:1061:GLU:OE2  | 6:K:9:ARG:NH1     | 2.49                     | 0.45              |
| 1:I:104:DT:H2''   | 1:I:105:DT:H71    | 1.99                     | 0.45              |
| 4:G:1031:HIS:CE1  | 4:G:1035:ARG:HH21 | 2.34                     | 0.45              |
| 1:I:32:DT:H2''    | 1:I:33:DG:O5'     | 2.16                     | 0.45              |
| 5:H:1491:ILE:O    | 5:H:1495:VAL:HG23 | 2.17                     | 0.45              |
| 6:K:12:ARG:CG     | 6:K:13:SER:N      | 2.79                     | 0.45              |
| 2:A:521:PRO:HD3   | 3:B:50:ILE:CD1    | 2.47                     | 0.45              |
| 1:J:148:DT:H2''   | 1:J:149:DC:O5'    | 2.17                     | 0.45              |
| 1:J:181:DA:H1'    | 1:J:182:DT:H5'    | 1.98                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:473:GLU:OE1  | 3:B:25:ASN:HB2    | 2.17                     | 0.45              |
| 4:C:840:ALA:HA   | 4:G:1038:ASN:OD1  | 2.17                     | 0.44              |
| 3:F:226:ILE:HD12 | 3:F:259:LYS:HB2   | 1.98                     | 0.44              |
| 1:I:114:DC:H2''  | 1:I:115:DA:O5'    | 2.17                     | 0.44              |
| 2:A:526:LEU:HD22 | 2:E:713:HIS:CG    | 2.51                     | 0.44              |
| 4:G:1047:ALA:HB1 | 5:H:1491:ILE:HD11 | 1.99                     | 0.44              |
| 1:I:121:DG:H5''  | 5:H:1437:TYR:OH   | 2.18                     | 0.44              |
| 1:J:153:DA:H5'   | 2:A:441:TYR:OH    | 2.17                     | 0.44              |
| 1:I:129:DC:C2'   | 1:I:130:DT:H72    | 2.48                     | 0.44              |
| 1:J:237:DT:H4'   | 2:A:463:ARG:NH1   | 2.32                     | 0.44              |
| 1:J:257:DA:H2''  | 1:J:258:DT:O5'    | 2.18                     | 0.44              |
| 2:A:528:ARG:HB2  | 2:A:534:ARG:NH1   | 2.33                     | 0.44              |
| 3:F:235:ARG:O    | 3:F:236:ARG:C     | 2.60                     | 0.44              |
| 1:I:124:DA:H2''  | 1:I:125:DG:N7     | 2.32                     | 0.44              |
| 1:J:149:DC:H2''  | 1:J:150:DA:O5'    | 2.18                     | 0.44              |
| 1:J:182:DT:H1'   | 1:J:183:DT:H5'    | 2.00                     | 0.44              |
| 1:J:268:DG:H1'   | 1:J:269:DT:H5'    | 1.99                     | 0.44              |
| 2:E:685:GLN:O    | 2:E:686:SER:C     | 2.61                     | 0.44              |
| 4:G:1025:PHE:CD1 | 4:G:1056:GLU:HG3  | 2.52                     | 0.44              |
| 4:C:854:VAL:HG21 | 5:D:1295:VAL:HG21 | 1.99                     | 0.44              |
| 1:I:27:DA:H2''   | 1:I:28:DA:OP2     | 2.18                     | 0.44              |
| 2:A:485:GLN:HG3  | 3:B:82:THR:HA     | 2.00                     | 0.44              |
| 5:D:1230:ARG:N   | 7:D:315:HOH:O     | 2.50                     | 0.44              |
| 1:I:141:DA:C2    | 1:J:153:DA:C2     | 3.06                     | 0.43              |
| 1:J:287:DA:H2'   | 1:J:288:DT:C7     | 2.48                     | 0.43              |
| 3:B:68:ASP:OD2   | 3:B:92:ARG:NH1    | 2.50                     | 0.43              |
| 2:E:718:HIS:NE2  | 3:F:245:ARG:HD2   | 2.33                     | 0.43              |
| 5:H:1476:ARG:O   | 5:H:1477:LEU:C    | 2.60                     | 0.43              |
| 1:J:197:DA:C1'   | 1:J:198:DT:H5'    | 2.48                     | 0.43              |
| 6:K:12:ARG:HG3   | 6:K:13:SER:H      | 1.82                     | 0.43              |
| 1:I:70:DG:H2''   | 1:I:71:DG:C8      | 2.54                     | 0.43              |
| 2:A:454:TYR:CZ   | 3:B:36:ARG:HG2    | 2.53                     | 0.43              |
| 2:A:481:ASP:OD2  | 3:B:79:LYS:NZ     | 2.39                     | 0.43              |
| 4:C:855:LEU:HD22 | 5:D:1263:VAL:HG13 | 2.00                     | 0.43              |
| 4:C:919:LYS:O    | 4:C:920:THR:C     | 2.61                     | 0.43              |
| 2:A:467:PHE:CZ   | 2:A:493:GLN:HA    | 2.54                     | 0.43              |
| 3:F:262:LEU:HD23 | 3:F:262:LEU:HA    | 1.84                     | 0.43              |
| 1:I:17:DA:H8     | 1:I:17:DA:OP2     | 2.01                     | 0.43              |
| 1:I:123:DT:C2'   | 1:I:124:DA:H5'    | 2.42                     | 0.43              |
| 4:C:906:GLY:CA   | 2:E:658:THR:HG22  | 2.47                     | 0.43              |
| 2:E:639:HIS:ND1  | 2:E:640:ARG:N     | 2.66                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:674:ILE:O     | 2:E:678:PHE:HD1   | 2.01                     | 0.43              |
| 2:E:667:PHE:HB3   | 7:E:343:HOH:O     | 2.19                     | 0.43              |
| 1:I:128:DT:H1'    | 1:I:129:DC:H5'    | 2.00                     | 0.43              |
| 1:J:147:DA:H2''   | 1:J:148:DT:OP2    | 2.18                     | 0.43              |
| 1:J:272:DA:H2''   | 1:J:273:DA:O5'    | 2.18                     | 0.43              |
| 5:D:1286:ILE:HG22 | 5:D:1291:ILE:CD1  | 2.49                     | 0.43              |
| 1:I:140:DT:H1'    | 1:I:141:DA:C8     | 2.54                     | 0.43              |
| 2:A:451:ILE:HD11  | 3:B:43:VAL:O      | 2.19                     | 0.43              |
| 1:I:116:DC:H2''   | 1:I:117:DT:OP2    | 2.18                     | 0.42              |
| 3:F:233:ALA:HA    | 3:F:236:ARG:CZ    | 2.49                     | 0.42              |
| 4:G:1031:HIS:HA   | 4:G:1048:PRO:HB3  | 2.00                     | 0.42              |
| 4:G:1064:GLU:HA   | 5:H:1445:VAL:HG11 | 2.00                     | 0.42              |
| 1:I:41:DA:C6      | 1:I:42:DA:C6      | 3.08                     | 0.42              |
| 4:C:825:PHE:CZ    | 4:C:859:THR:HG21  | 2.54                     | 0.42              |
| 1:I:5:DA:H1'      | 1:I:6:DT:H5''     | 2.00                     | 0.42              |
| 1:J:149:DC:C2'    | 1:J:150:DA:C8     | 3.02                     | 0.42              |
| 1:J:172:DC:H1'    | 1:J:173:DA:C5     | 2.54                     | 0.42              |
| 2:A:482:LEU:HD23  | 3:B:79:LYS:O      | 2.19                     | 0.42              |
| 5:H:1454:LYS:HE3  | 5:H:1454:LYS:HB2  | 1.94                     | 0.42              |
| 1:I:22:DC:H2''    | 1:I:23:DT:O5'     | 2.19                     | 0.42              |
| 4:G:1020:ARG:HH11 | 4:G:1020:ARG:HG2  | 1.84                     | 0.42              |
| 1:J:284:DG:H2''   | 1:J:285:DA:C8     | 2.55                     | 0.42              |
| 2:A:452:ARG:NH1   | 2:A:452:ARG:CG    | 2.80                     | 0.42              |
| 1:I:112:DT:C5'    | 4:G:1042:ARG:HG2  | 2.49                     | 0.42              |
| 1:J:211:DT:H2''   | 1:J:212:DC:C6     | 2.55                     | 0.42              |
| 2:A:492:LEU:HD12  | 2:A:492:LEU:HA    | 1.90                     | 0.42              |
| 5:H:1446:HIS:HB3  | 5:H:1449:THR:OG1  | 2.19                     | 0.42              |
| 1:J:278:DC:H2''   | 1:J:279:DA:N7     | 2.34                     | 0.42              |
| 3:B:26:ILE:HG23   | 3:B:27:GLN:N      | 2.34                     | 0.42              |
| 4:C:880:PRO:HB3   | 5:D:1258:ILE:CD1  | 2.50                     | 0.42              |
| 1:I:102:DA:H2''   | 1:I:103:DG:OP2    | 2.19                     | 0.42              |
| 1:I:113:DA:C2     | 1:J:181:DA:C2     | 3.08                     | 0.42              |
| 1:J:215:DC:H1'    | 1:J:216:DG:C8     | 2.54                     | 0.42              |
| 2:A:529:ARG:HH11  | 2:A:529:ARG:HG3   | 1.85                     | 0.42              |
| 4:C:829:ARG:HH11  | 5:D:1232:GLU:HB3  | 1.84                     | 0.42              |
| 4:C:881:ARG:NH2   | 4:C:907:VAL:O     | 2.40                     | 0.42              |
| 5:D:1251:ILE:HG21 | 5:D:1256:MET:HE2  | 2.02                     | 0.42              |
| 1:I:64:DT:H2''    | 1:I:65:DT:O5'     | 2.20                     | 0.42              |
| 2:E:651:ILE:HD11  | 3:F:243:VAL:O     | 2.20                     | 0.42              |
| 4:G:1040:ALA:HB2  | 5:H:1486:ILE:HG13 | 2.01                     | 0.42              |
| 1:I:80:DT:C4'     | 3:F:245:ARG:NH1   | 2.79                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:C:850:TYR:OH    | 5:D:1308:VAL:HA   | 2.20                     | 0.42              |
| 3:F:252:GLU:OE2   | 3:F:255:ARG:NH1   | 2.53                     | 0.42              |
| 5:H:1487:THR:C    | 5:H:1489:ARG:H    | 2.07                     | 0.42              |
| 1:J:150:DA:H1'    | 1:J:151:DA:C8     | 2.54                     | 0.41              |
| 2:A:468:GLN:HG2   | 2:A:489:VAL:HG11  | 2.01                     | 0.41              |
| 5:D:1291:ILE:O    | 5:D:1295:VAL:HG23 | 2.20                     | 0.41              |
| 4:G:1079:ILE:HG12 | 4:G:1082:HIS:CE1  | 2.55                     | 0.41              |
| 1:J:165:DA:H4'    | 4:G:1077:ARG:CZ   | 2.50                     | 0.41              |
| 4:G:1050:TYR:O    | 4:G:1054:VAL:HG23 | 2.20                     | 0.41              |
| 1:I:90:DT:OP2     | 2:E:669:ARG:NH2   | 2.43                     | 0.41              |
| 2:A:451:ILE:HD13  | 3:B:39:ARG:HA     | 2.02                     | 0.41              |
| 4:C:876:THR:O     | 5:D:1249:THR:HG23 | 2.19                     | 0.41              |
| 5:D:1269:ARG:HB3  | 5:D:1298:LEU:HD11 | 2.03                     | 0.41              |
| 1:J:151:DA:C1'    | 1:J:152:DT:H5''   | 2.49                     | 0.41              |
| 4:C:824:GLN:N     | 4:C:856:GLU:OE1   | 2.52                     | 0.41              |
| 2:E:712:ILE:HD12  | 2:E:716:ARG:O     | 2.20                     | 0.41              |
| 3:F:249:LEU:HD23  | 3:F:249:LEU:HA    | 1.73                     | 0.41              |
| 4:G:1114:VAL:O    | 4:G:1114:VAL:HG22 | 2.20                     | 0.41              |
| 1:J:165:DA:C2     | 1:J:166:DT:C2     | 3.08                     | 0.41              |
| 2:A:521:PRO:HD3   | 3:B:50:ILE:HD12   | 2.01                     | 0.41              |
| 4:C:884:GLN:CD    | 4:C:888:ARG:HG3   | 2.45                     | 0.41              |
| 2:E:717:VAL:HG23  | 2:E:718:HIS:HD2   | 1.85                     | 0.41              |
| 6:K:6:MET:HE2     | 6:K:6:MET:HB3     | 2.00                     | 0.41              |
| 1:I:91:DT:OP1     | 2:E:664:LYS:N     | 2.50                     | 0.41              |
| 5:D:1245:VAL:O    | 7:D:300:HOH:O     | 2.22                     | 0.41              |
| 5:D:1277:LEU:CD2  | 5:D:1293:THR:HB   | 2.50                     | 0.41              |
| 4:G:1085:LEU:O    | 4:G:1089:ASN:HB2  | 2.21                     | 0.41              |
| 2:A:446:VAL:O     | 2:A:449:ARG:HB3   | 2.20                     | 0.41              |
| 4:C:913:SER:C     | 4:C:915:LEU:N     | 2.79                     | 0.41              |
| 1:I:136:DT:H2''   | 1:I:137:DG:O5'    | 2.21                     | 0.41              |
| 1:J:223:DC:H2''   | 1:J:224:DG:N7     | 2.36                     | 0.41              |
| 1:J:198:DT:H6     | 1:J:198:DT:H2'    | 1.78                     | 0.41              |
| 2:E:661:LEU:HD13  | 3:F:236:ARG:HB3   | 2.02                     | 0.41              |
| 5:H:1437:TYR:O    | 5:H:1441:VAL:HG23 | 2.21                     | 0.41              |
| 1:J:258:DT:H2''   | 1:J:259:DA:H5'    | 2.02                     | 0.41              |
| 3:B:61:PHE:O      | 3:B:65:VAL:HG23   | 2.21                     | 0.41              |
| 4:C:887:VAL:HG11  | 4:C:897:LEU:HD12  | 2.01                     | 0.41              |
| 5:H:1491:ILE:HD12 | 5:H:1491:ILE:N    | 2.32                     | 0.40              |
| 1:J:267:DG:H5''   | 5:D:1237:TYR:OH   | 2.21                     | 0.40              |
| 3:B:47:SER:HB3    | 3:B:50:ILE:HD11   | 2.02                     | 0.40              |
| 4:G:1074:LYS:HA   | 4:G:1074:LYS:HD3  | 1.86                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:A:451:ILE:HD13 | 3:B:39:ARG:CA     | 2.51                     | 0.40              |
| 2:A:518:HIS:CD2  | 3:B:45:ARG:HB3    | 2.56                     | 0.40              |
| 4:C:890:ASP:O    | 4:C:891:GLU:C     | 2.63                     | 0.40              |
| 5:D:1303:LEU:HA  | 5:D:1303:LEU:HD23 | 1.82                     | 0.40              |
| 1:I:51:DA:P      | 2:A:472:ARG:HH22  | 2.45                     | 0.40              |
| 1:J:156:DC:H2"   | 1:J:157:DA:C8     | 2.56                     | 0.40              |
| 4:C:847:ALA:HB3  | 4:C:848:PRO:CD    | 2.51                     | 0.40              |
| 4:G:1061:GLU:HG3 | 6:K:9:ARG:HH12    | 1.87                     | 0.40              |

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

| Atom-1           | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------------|--------------------------|-------------------|
| 5:D:1302:GLU:OE2 | 3:F:219:ARG:NH2[3_544] | 1.70                     | 0.50              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 2   | A     | 96/135 (71%)   | 90 (94%)  | 5 (5%)   | 1 (1%)   | 12          | 39  |
| 2   | E     | 96/135 (71%)   | 91 (95%)  | 5 (5%)   | 0        | 100         | 100 |
| 3   | B     | 77/102 (76%)   | 74 (96%)  | 3 (4%)   | 0        | 100         | 100 |
| 3   | F     | 82/102 (80%)   | 78 (95%)  | 3 (4%)   | 1 (1%)   | 10          | 34  |
| 4   | C     | 105/129 (81%)  | 95 (90%)  | 10 (10%) | 0        | 100         | 100 |
| 4   | G     | 104/129 (81%)  | 95 (91%)  | 6 (6%)   | 3 (3%)   | 3           | 15  |
| 5   | D     | 91/125 (73%)   | 82 (90%)  | 8 (9%)   | 1 (1%)   | 11          | 36  |
| 5   | H     | 91/125 (73%)   | 81 (89%)  | 6 (7%)   | 4 (4%)   | 2           | 8   |
| 6   | K     | 12/22 (54%)    | 9 (75%)   | 1 (8%)   | 2 (17%)  | 0           | 0   |
| All | All   | 754/1004 (75%) | 695 (92%) | 47 (6%)  | 12 (2%)  | 7           | 27  |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | F     | 220  | LYS  |
| 4   | G     | 1117 | PRO  |
| 5   | H     | 1488 | SER  |
| 5   | H     | 1501 | GLY  |
| 5   | D     | 1301 | GLY  |
| 5   | H     | 1486 | ILE  |
| 6   | K     | 15   | GLY  |
| 5   | H     | 1487 | THR  |
| 2   | A     | 481  | ASP  |
| 6   | K     | 16   | ALA  |
| 4   | G     | 1116 | LEU  |
| 4   | G     | 1114 | VAL  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 2   | A     | 85/110 (77%)  | 80 (94%)  | 5 (6%)   | 18          | 48 |
| 2   | E     | 85/110 (77%)  | 82 (96%)  | 3 (4%)   | 32          | 66 |
| 3   | B     | 64/78 (82%)   | 63 (98%)  | 1 (2%)   | 55          | 83 |
| 3   | F     | 69/78 (88%)   | 66 (96%)  | 3 (4%)   | 26          | 60 |
| 4   | C     | 85/104 (82%)  | 76 (89%)  | 9 (11%)  | 6           | 22 |
| 4   | G     | 84/104 (81%)  | 73 (87%)  | 11 (13%) | 4           | 13 |
| 5   | D     | 79/104 (76%)  | 76 (96%)  | 3 (4%)   | 29          | 64 |
| 5   | H     | 79/104 (76%)  | 76 (96%)  | 3 (4%)   | 29          | 64 |
| 6   | K     | 10/16 (62%)   | 4 (40%)   | 6 (60%)  | 0           | 0  |
| All | All   | 640/808 (79%) | 596 (93%) | 44 (7%)  | 14          | 41 |

All (44) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 440 | ARG  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | A     | 459  | GLU  |
| 2   | A     | 463  | ARG  |
| 2   | A     | 468  | GLN  |
| 2   | A     | 492  | LEU  |
| 3   | B     | 50   | ILE  |
| 4   | C     | 829  | ARG  |
| 4   | C     | 876  | THR  |
| 4   | C     | 881  | ARG  |
| 4   | C     | 888  | ARG  |
| 4   | C     | 909  | PRO  |
| 4   | C     | 914  | VAL  |
| 4   | C     | 917  | PRO  |
| 4   | C     | 918  | LYS  |
| 4   | C     | 919  | LYS  |
| 5   | D     | 1253 | SER  |
| 5   | D     | 1309 | SER  |
| 5   | D     | 1320 | SER  |
| 2   | E     | 680  | THR  |
| 2   | E     | 712  | ILE  |
| 2   | E     | 734  | ARG  |
| 3   | F     | 220  | LYS  |
| 3   | F     | 245  | ARG  |
| 3   | F     | 293  | GLN  |
| 4   | G     | 1035 | ARG  |
| 4   | G     | 1042 | ARG  |
| 4   | G     | 1064 | GLU  |
| 4   | G     | 1081 | ARG  |
| 4   | G     | 1088 | ARG  |
| 4   | G     | 1091 | GLU  |
| 4   | G     | 1100 | VAL  |
| 4   | G     | 1116 | LEU  |
| 4   | G     | 1117 | PRO  |
| 4   | G     | 1118 | LYS  |
| 4   | G     | 1119 | LYS  |
| 5   | H     | 1433 | SER  |
| 5   | H     | 1468 | GLU  |
| 5   | H     | 1487 | THR  |
| 6   | K     | 6    | MET  |
| 6   | K     | 7    | ARG  |
| 6   | K     | 9    | ARG  |
| 6   | K     | 12   | ARG  |
| 6   | K     | 14   | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | K     | 17  | PRO  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | A     | 439  | HIS  |
| 2   | A     | 476  | GLN  |
| 2   | A     | 493  | GLN  |
| 3   | B     | 93   | GLN  |
| 4   | C     | 831  | HIS  |
| 4   | C     | 838  | ASN  |
| 5   | D     | 1244 | GLN  |
| 5   | D     | 1292 | GLN  |
| 2   | E     | 676  | GLN  |
| 3   | F     | 264  | ASN  |
| 4   | G     | 1031 | HIS  |
| 4   | G     | 1038 | ASN  |
| 4   | G     | 1112 | GLN  |
| 5   | H     | 1444 | GLN  |
| 5   | H     | 1446 | HIS  |

### 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](#)

There are no ligands in this entry.

## 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   | I     | 146/146 (100%)  | 0.49   | 7 (4%)    | 35  | 28  | 43, 83, 142, 166      | 0       |
| 1   | J     | 146/146 (100%)  | 0.58   | 7 (4%)    | 35  | 28  | 43, 86, 141, 181      | 0       |
| 2   | A     | 98/135 (72%)    | -0.18  | 5 (5%)    | 33  | 26  | 18, 35, 72, 113       | 0       |
| 2   | E     | 98/135 (72%)    | -0.34  | 4 (4%)    | 41  | 33  | 11, 30, 90, 161       | 0       |
| 3   | B     | 79/102 (77%)    | -0.43  | 0         | 100 | 100 | 12, 33, 60, 106       | 0       |
| 3   | F     | 84/102 (82%)    | -0.61  | 0         | 100 | 100 | 11, 28, 49, 121       | 0       |
| 4   | C     | 107/129 (82%)   | -0.42  | 1 (0%)    | 81  | 75  | 14, 31, 68, 194       | 0       |
| 4   | G     | 106/129 (82%)   | -0.24  | 3 (2%)    | 55  | 46  | 9, 38, 91, 178        | 0       |
| 5   | D     | 93/125 (74%)    | -0.30  | 3 (3%)    | 50  | 41  | 16, 34, 60, 127       | 0       |
| 5   | H     | 93/125 (74%)    | -0.18  | 2 (2%)    | 62  | 53  | 17, 40, 80, 137       | 0       |
| 6   | K     | 14/22 (63%)     | 0.25   | 1 (7%)    | 22  | 17  | 29, 58, 158, 177      | 0       |
| All | All   | 1064/1296 (82%) | -0.09  | 33 (3%)   | 51  | 42  | 9, 41, 118, 194       | 0       |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | A     | 438  | PRO  | 5.1  |
| 2   | A     | 518  | HIS  | 4.5  |
| 2   | E     | 638  | PRO  | 4.2  |
| 4   | G     | 1117 | PRO  | 4.2  |
| 2   | E     | 735  | ALA  | 3.8  |
| 5   | H     | 1486 | ILE  | 3.4  |
| 2   | E     | 718  | HIS  | 3.1  |
| 1   | I     | 15   | DG   | 3.1  |
| 2   | A     | 439  | HIS  | 3.1  |
| 1   | I     | 104  | DT   | 3.0  |
| 1   | J     | 233  | DG   | 2.9  |
| 4   | C     | 920  | THR  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | A     | 535  | ALA  | 2.9  |
| 4   | G     | 1118 | LYS  | 2.6  |
| 1   | I     | 95   | DA   | 2.6  |
| 2   | E     | 734  | ARG  | 2.5  |
| 1   | J     | 234  | DC   | 2.5  |
| 1   | I     | 105  | DT   | 2.4  |
| 5   | D     | 1321 | ALA  | 2.4  |
| 1   | J     | 223  | DC   | 2.4  |
| 1   | I     | 55   | DA   | 2.3  |
| 6   | K     | 16   | ALA  | 2.2  |
| 5   | D     | 1322 | LYS  | 2.2  |
| 2   | A     | 534  | ARG  | 2.2  |
| 5   | D     | 1235 | ALA  | 2.1  |
| 1   | J     | 275  | DC   | 2.1  |
| 5   | H     | 1487 | THR  | 2.1  |
| 1   | I     | 128  | DT   | 2.1  |
| 1   | J     | 242  | DT   | 2.1  |
| 1   | J     | 273  | DA   | 2.1  |
| 1   | I     | 56   | DA   | 2.0  |
| 4   | G     | 1014 | ALA  | 2.0  |
| 1   | J     | 274  | DT   | 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.