



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:58 AM UTC

PDB ID : 1FLO / pdb\_00001flo  
Title : FLP Recombinase-Holliday Junction Complex I  
Authors : Chen, Y.; Narendra, U.; Iype, L.E.; Cox, M.M.; Rice, P.A.  
Deposited on : 2000-08-14  
Resolution : 2.65 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>.

---

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  
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

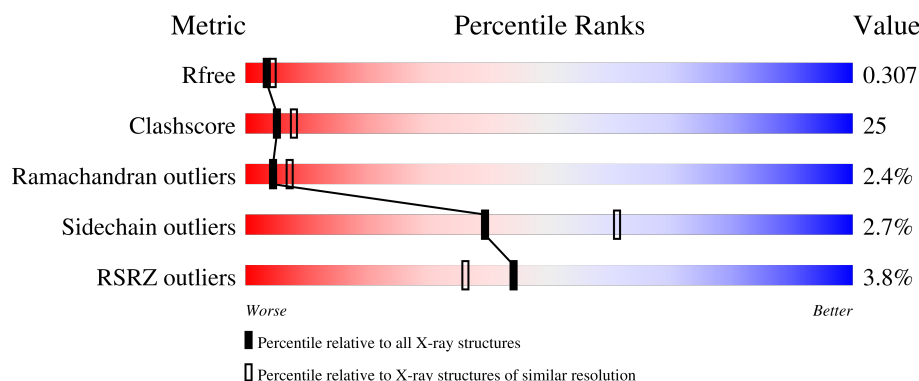
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

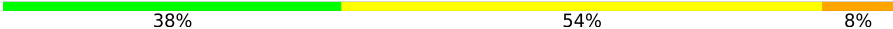
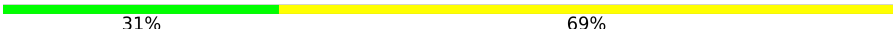
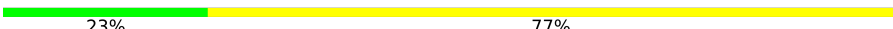
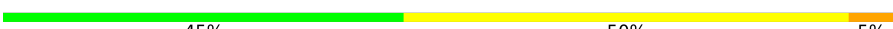
The reported resolution of this entry is 2.65 Å.

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                      | 1110 (2.66-2.66)                                      |
| Clashscore            | 190562                      | 1141 (2.66-2.66)                                      |
| Ramachandran outliers | 187476                      | 1126 (2.66-2.66)                                      |
| Sidechain outliers    | 187428                      | 1126 (2.66-2.66)                                      |
| RSRZ outliers         | 180081                      | 1110 (2.66-2.66)                                      |

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   | E     | 13     |  |
| 1   | G     | 13     |  |
| 1   | I     | 13     |  |
| 1   | K     | 13     |  |
| 2   | F     | 20     |  |

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain                                                                         |
|-----|-------|--------|------------------------------------------------------------------------------------------|
| 2   | H     | 20     | <div><div></div><div>55%</div><div>40%</div><div>5%</div></div>                          |
| 2   | J     | 20     | <div><div></div><div>20%</div><div>75%</div><div>5%</div></div>                          |
| 2   | L     | 20     | <div><div></div><div>5%</div><div>20%</div><div>75%</div><div>5%</div></div>             |
| 3   | A     | 422    | <div><div></div><div>2%</div><div>61%</div><div>32%</div><div>•</div><div>•</div></div>  |
| 3   | B     | 422    | <div><div></div><div>4%</div><div>63%</div><div>30%</div><div>•</div><div>•</div></div>  |
| 3   | C     | 422    | <div><div></div><div>3%</div><div>49%</div><div>42%</div><div>5%</div><div>•</div></div> |
| 3   | D     | 422    | <div><div></div><div>7%</div><div>45%</div><div>46%</div><div>•</div><div>•</div></div>  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16064 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 SYMMETRIZED FRT DNA SITES.

| Mol | Chain | Residues | Atoms |     |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| 1   | E     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 259   | 127 | 41 | 79 | 12 |         |         |       |
| 1   | G     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 259   | 127 | 41 | 79 | 12 |         |         |       |
| 1   | I     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 259   | 127 | 41 | 79 | 12 |         |         |       |
| 1   | K     | 13       | Total | C   | N  | O  | P  | 0       | 0       | 0     |
|     |       |          | 259   | 127 | 41 | 79 | 12 |         |         |       |

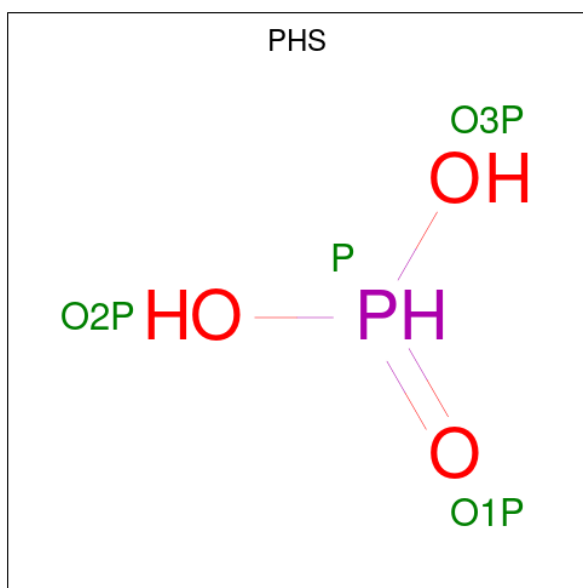
- Molecule 2 is a DNA chain called SYMMETRIZED FRT DNA SITES.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | F     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 410   | 198 | 78 | 115 | 19 |         |         |       |
| 2   | H     | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 395   | 189 | 75 | 112 | 19 |         |         |       |
| 2   | J     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 391   | 189 | 75 | 109 | 18 |         |         |       |
| 2   | L     | 19       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 391   | 189 | 75 | 109 | 18 |         |         |       |

- Molecule 3 is a protein called FLP RECOMBINASE.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 3   | A     | 405      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3297  | 2128 | 553 | 605 | 11 |         |         |       |
| 3   | B     | 408      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3323  | 2141 | 564 | 607 | 11 |         |         |       |
| 3   | C     | 404      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3304  | 2133 | 560 | 600 | 11 |         |         |       |
| 3   | D     | 405      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3308  | 2135 | 560 | 602 | 11 |         |         |       |

- Molecule 4 is PHOSPHONIC ACID (CCD ID: PHS) (formula:  $\text{H}_3\text{O}_3\text{P}$ ).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | E     | 1        | Total O P<br>4 3 1 | 0       | 0       |
| 4   | G     | 1        | Total O P<br>4 3 1 | 0       | 0       |
| 4   | I     | 1        | Total O P<br>4 3 1 | 0       | 0       |
| 4   | K     | 1        | Total O P<br>4 3 1 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | E     | 10       | Total O<br>10 10   | 0       | 0       |
| 5   | F     | 10       | Total O<br>10 10   | 0       | 0       |
| 5   | G     | 3        | Total O<br>3 3     | 0       | 0       |
| 5   | H     | 6        | Total O<br>6 6     | 0       | 0       |
| 5   | L     | 1        | Total O<br>1 1     | 0       | 0       |
| 5   | A     | 103      | Total O<br>103 103 | 0       | 0       |
| 5   | B     | 38       | Total O<br>38 38   | 0       | 0       |

*Continued on next page...*

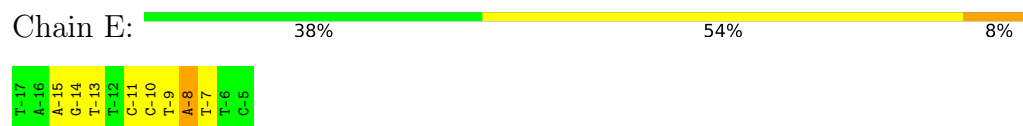
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5   | C     | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 5   | D     | 6        | Total<br>6  | O<br>6  | 0       | 0       |

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

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: SYMMETRIZED FRT DNA SITES



- Molecule 1: SYMMETRIZED FRT DNA SITES



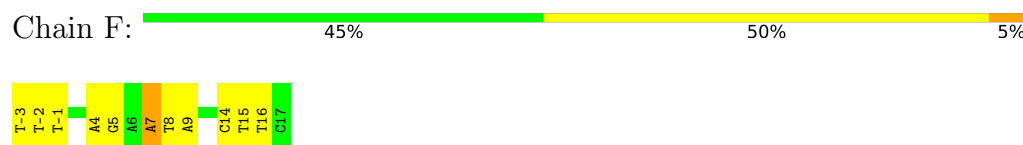
- Molecule 1: SYMMETRIZED FRT DNA SITES



- Molecule 1: SYMMETRIZED FRT DNA SITES



- Molecule 2: SYMMETRIZED FRT DNA SITES

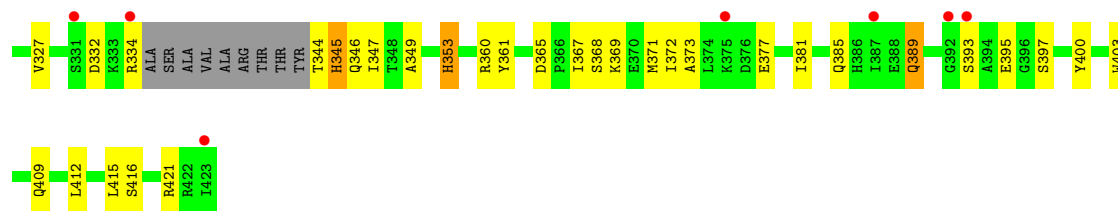


- Molecule 2: SYMMETRIZED FRT DNA SITES

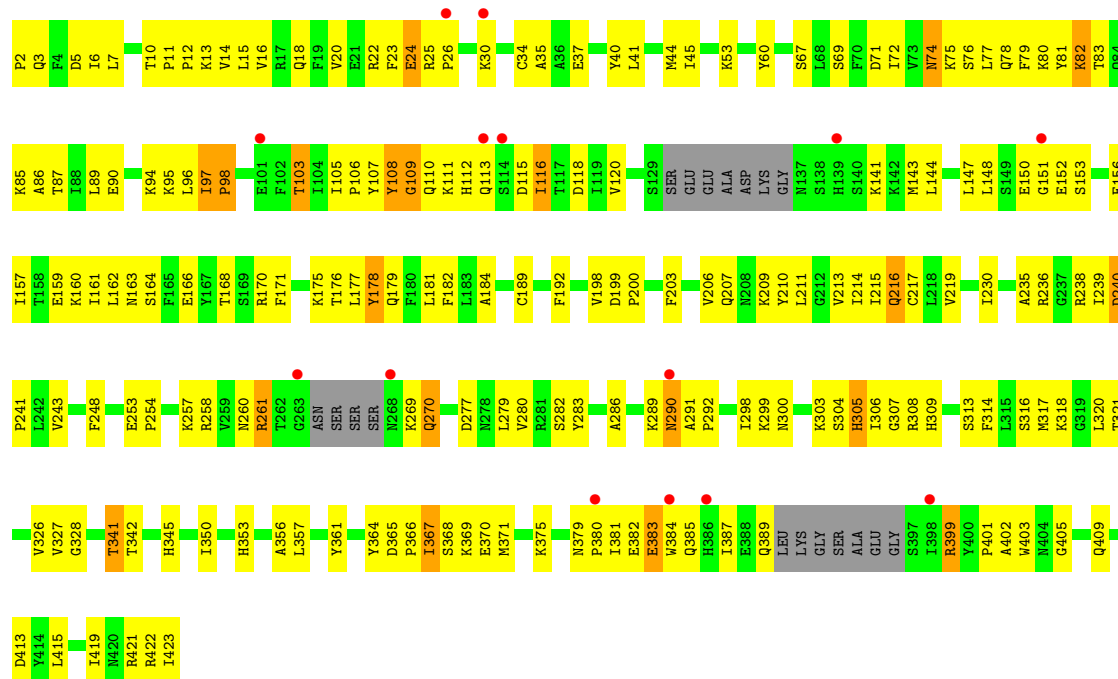




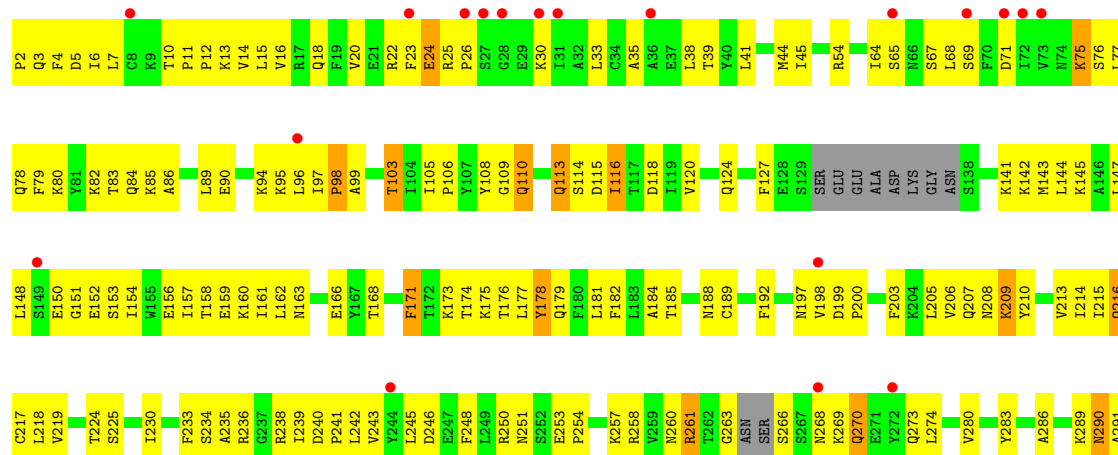


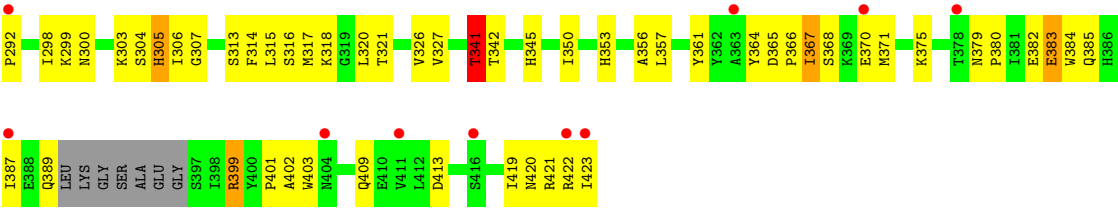


• Molecule 3: FLP RECOMBINASE



• Molecule 3: FLP RECOMBINASE





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 81.48Å 180.18Å 98.60Å<br>90.00° 97.02° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 15.00 – 2.65<br>15.00 – 2.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.5 (15.00-2.65)<br>88.0 (15.00-2.65)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.05                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.79 (at 2.60Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.0                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.249 , 0.297<br>0.264 , 0.307                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7133 reflections (9.15%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.101                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 70.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 16064                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 70.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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   | E     | 0.37         | 0/288          | 1.03        | 2/442 (0.5%)    |
| 1   | G     | 0.33         | 0/288          | 0.97        | 1/442 (0.2%)    |
| 1   | I     | 0.31         | 0/288          | 0.90        | 0/442           |
| 1   | K     | 0.30         | 0/288          | 0.82        | 0/442           |
| 2   | F     | 0.43         | 0/461          | 0.92        | 2/710 (0.3%)    |
| 2   | H     | 0.38         | 0/444          | 0.89        | 2/685 (0.3%)    |
| 2   | J     | 0.31         | 0/440          | 0.79        | 0/678           |
| 2   | L     | 0.30         | 0/440          | 0.77        | 1/678 (0.1%)    |
| 3   | A     | 0.59         | 1/3370 (0.0%)  | 1.03        | 19/4551 (0.4%)  |
| 3   | B     | 0.45         | 0/3397         | 1.02        | 14/4585 (0.3%)  |
| 3   | C     | 0.42         | 0/3378         | 0.93        | 14/4563 (0.3%)  |
| 3   | D     | 0.40         | 0/3382         | 0.91        | 9/4568 (0.2%)   |
| All | All   | 0.45         | 1/16464 (0.0%) | 0.95        | 64/22786 (0.3%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | H     | 0                   | 1                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | A     | 198 | VAL  | CA-CB | 5.48 | 1.60        | 1.54     |

All (64) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 3   | B     | 110 | GLN  | N-CA-C      | -15.33 | 95.58       | 113.21   |
| 3   | A     | 97  | ILE  | CA-C-N      | 11.20  | 132.08      | 119.32   |
| 3   | A     | 97  | ILE  | C-N-CA      | 11.20  | 132.08      | 119.32   |
| 3   | B     | 97  | ILE  | CA-C-N      | 10.22  | 130.97      | 119.32   |
| 3   | B     | 97  | ILE  | C-N-CA      | 10.22  | 130.97      | 119.32   |
| 3   | D     | 216 | GLN  | OE1-CD-NE2  | -9.82  | 112.78      | 122.60   |
| 3   | B     | 216 | GLN  | OE1-CD-NE2  | -9.81  | 112.79      | 122.60   |
| 3   | A     | 216 | GLN  | OE1-CD-NE2  | -9.79  | 112.81      | 122.60   |
| 3   | C     | 216 | GLN  | OE1-CD-NE2  | -9.77  | 112.83      | 122.60   |
| 3   | D     | 269 | LYS  | N-CA-C      | 7.49   | 119.81      | 109.18   |
| 3   | C     | 269 | LYS  | N-CA-C      | 7.49   | 119.81      | 109.18   |
| 2   | F     | 7   | DA   | N9-C1'-C2'  | -7.33  | 102.50      | 113.50   |
| 3   | B     | 25  | ARG  | CA-C-N      | 7.25   | 128.91      | 119.84   |
| 3   | B     | 25  | ARG  | C-N-CA      | 7.25   | 128.91      | 119.84   |
| 3   | A     | 324 | THR  | N-CA-C      | 7.12   | 119.71      | 111.02   |
| 3   | C     | 399 | ARG  | N-CA-C      | -7.08  | 104.11      | 112.89   |
| 3   | C     | 383 | GLU  | N-CA-C      | -7.03  | 104.58      | 113.01   |
| 3   | B     | 112 | HIS  | N-CA-C      | -7.01  | 101.13      | 110.24   |
| 3   | A     | 152 | GLU  | N-CA-C      | 6.97   | 120.11      | 110.35   |
| 3   | B     | 166 | GLU  | N-CA-C      | 6.75   | 119.49      | 111.33   |
| 3   | D     | 399 | ARG  | N-CA-C      | -6.71  | 104.57      | 112.89   |
| 3   | D     | 216 | GLN  | CG-CD-NE2   | 6.70   | 126.45      | 116.40   |
| 3   | C     | 216 | GLN  | CG-CD-NE2   | 6.69   | 126.43      | 116.40   |
| 3   | B     | 216 | GLN  | CG-CD-NE2   | 6.68   | 126.42      | 116.40   |
| 3   | A     | 216 | GLN  | CG-CD-NE2   | 6.68   | 126.41      | 116.40   |
| 2   | F     | 7   | DA   | C4'-C3'-O3' | 6.58   | 119.88      | 110.00   |
| 3   | B     | 152 | GLU  | N-CA-C      | 6.52   | 119.48      | 110.35   |
| 3   | D     | 383 | GLU  | N-CA-C      | -6.22  | 104.95      | 112.54   |
| 3   | B     | 199 | ASP  | CA-C-N      | 6.15   | 126.04      | 119.28   |
| 3   | B     | 199 | ASP  | C-N-CA      | 6.15   | 126.04      | 119.28   |
| 3   | C     | 97  | ILE  | CA-C-N      | 6.05   | 127.40      | 119.84   |
| 3   | C     | 97  | ILE  | C-N-CA      | 6.05   | 127.40      | 119.84   |
| 2   | H     | 7   | DA   | C4'-C3'-O3' | 6.03   | 119.05      | 110.00   |
| 3   | C     | 166 | GLU  | N-CA-C      | 5.99   | 118.30      | 111.11   |
| 3   | A     | 22  | ARG  | N-CA-C      | 5.91   | 118.50      | 111.71   |
| 3   | A     | 166 | GLU  | N-CA-C      | 5.88   | 119.28      | 111.75   |
| 3   | A     | 290 | ASN  | N-CA-C      | 5.88   | 122.03      | 114.56   |
| 3   | D     | 24  | GLU  | N-CA-C      | -5.84  | 105.65      | 112.89   |
| 3   | A     | 199 | ASP  | CA-C-N      | 5.82   | 125.51      | 119.05   |
| 3   | A     | 199 | ASP  | C-N-CA      | 5.82   | 125.51      | 119.05   |
| 3   | C     | 405 | GLY  | N-CA-C      | -5.69  | 108.31      | 115.08   |
| 3   | C     | 24  | GLU  | N-CA-C      | -5.67  | 106.19      | 113.23   |
| 2   | H     | 7   | DA   | N9-C1'-C2'  | -5.66  | 105.01      | 113.50   |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 3   | A     | 350 | ILE  | CA-C-N     | 5.53  | 125.45      | 119.76   |
| 3   | A     | 350 | ILE  | C-N-CA     | 5.53  | 125.45      | 119.76   |
| 3   | A     | 35  | ALA  | N-CA-C     | 5.52  | 116.97      | 111.07   |
| 3   | A     | 231 | TYR  | N-CA-C     | 5.52  | 118.25      | 109.81   |
| 3   | D     | 341 | THR  | N-CA-C     | 5.48  | 118.17      | 111.82   |
| 2   | L     | 5   | DG   | N9-C1'-C2' | 5.46  | 121.69      | 113.50   |
| 3   | B     | 231 | TYR  | N-CA-C     | 5.44  | 118.14      | 109.81   |
| 1   | G     | -11 | DC   | N1-C1'-C2' | 5.39  | 121.59      | 113.50   |
| 3   | D     | 218 | LEU  | N-CA-C     | 5.35  | 118.18      | 109.24   |
| 1   | E     | -11 | DC   | N1-C1'-C2' | 5.35  | 121.52      | 113.50   |
| 3   | A     | 379 | ASN  | CA-C-N     | 5.32  | 124.95      | 119.05   |
| 3   | A     | 379 | ASN  | C-N-CA     | 5.32  | 124.95      | 119.05   |
| 3   | D     | 197 | ASN  | N-CA-C     | 5.31  | 119.24      | 112.87   |
| 1   | E     | -8  | DA   | N9-C1'-C2' | 5.27  | 121.41      | 113.50   |
| 3   | B     | 266 | SER  | N-CA-C     | -5.24 | 106.66      | 113.16   |
| 3   | A     | 70  | PHE  | N-CA-C     | 5.18  | 116.67      | 108.96   |
| 3   | A     | 29  | GLU  | N-CA-C     | 5.13  | 117.27      | 111.11   |
| 3   | C     | 240 | ASP  | CA-C-N     | 5.10  | 124.55      | 119.24   |
| 3   | C     | 240 | ASP  | C-N-CA     | 5.10  | 124.55      | 119.24   |
| 3   | C     | 74  | ASN  | N-CA-C     | -5.05 | 107.12      | 113.28   |
| 3   | C     | 108 | TYR  | N-CA-C     | -5.01 | 105.89      | 112.41   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 2   | H     | 7   | 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   | E     | 259   | 0        | 150      | 12      | 0            |
| 1   | G     | 259   | 0        | 150      | 13      | 0            |
| 1   | I     | 259   | 0        | 150      | 9       | 0            |
| 1   | K     | 259   | 0        | 150      | 13      | 0            |
| 2   | F     | 410   | 0        | 228      | 14      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | H     | 395   | 0        | 216      | 13      | 0            |
| 2   | J     | 391   | 0        | 217      | 25      | 0            |
| 2   | L     | 391   | 0        | 217      | 25      | 0            |
| 3   | A     | 3297  | 0        | 3339     | 129     | 0            |
| 3   | B     | 3323  | 0        | 3369     | 137     | 0            |
| 3   | C     | 3304  | 0        | 3350     | 207     | 0            |
| 3   | D     | 3308  | 0        | 3354     | 213     | 0            |
| 4   | E     | 4     | 0        | 0        | 1       | 0            |
| 4   | G     | 4     | 0        | 0        | 0       | 0            |
| 4   | I     | 4     | 0        | 0        | 0       | 0            |
| 4   | K     | 4     | 0        | 0        | 0       | 0            |
| 5   | A     | 103   | 0        | 0        | 7       | 0            |
| 5   | B     | 38    | 0        | 0        | 1       | 0            |
| 5   | C     | 16    | 0        | 0        | 7       | 0            |
| 5   | D     | 6     | 0        | 0        | 0       | 0            |
| 5   | E     | 10    | 0        | 0        | 1       | 0            |
| 5   | F     | 10    | 0        | 0        | 1       | 0            |
| 5   | G     | 3     | 0        | 0        | 0       | 0            |
| 5   | H     | 6     | 0        | 0        | 0       | 0            |
| 5   | L     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 16064 | 0        | 14890    | 757     | 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 25.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:399:ARG:HH22 | 3:D:419:ILE:HG21 | 1.15                     | 1.09              |
| 2:J:15:DT:H2''   | 2:J:16:DT:H5''   | 1.36                     | 1.07              |
| 3:C:83:THR:HG22  | 3:C:85:LYS:H     | 1.20                     | 1.07              |
| 3:A:148:LEU:HD12 | 3:D:345:HIS:HB2  | 1.41                     | 1.03              |
| 3:D:83:THR:HG22  | 3:D:85:LYS:H     | 1.23                     | 1.02              |
| 3:D:86:ALA:O     | 3:D:90:GLU:HG2   | 1.62                     | 1.00              |
| 3:C:367:ILE:HG23 | 3:C:368:SER:H    | 1.29                     | 0.97              |
| 3:B:109:GLY:C    | 3:B:111:LYS:H    | 1.61                     | 0.96              |
| 3:C:399:ARG:HH22 | 3:C:419:ILE:HG21 | 1.27                     | 0.96              |
| 3:D:10:THR:HG21  | 3:D:15:LEU:HD13  | 1.43                     | 0.96              |
| 1:G:-10:DC:H2'   | 1:G:-9:DT:H72    | 1.48                     | 0.95              |
| 1:E:-10:DC:H2'   | 1:E:-9:DT:H72    | 1.48                     | 0.94              |
| 3:B:72:ILE:HD12  | 3:B:72:ILE:H     | 1.31                     | 0.93              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:258:ARG:HE   | 3:A:260:ASN:HD21 | 1.17                     | 0.93              |
| 3:C:86:ALA:O     | 3:C:90:GLU:HG2   | 1.66                     | 0.92              |
| 3:B:309:HIS:HD2  | 3:C:345:HIS:HE2  | 1.09                     | 0.92              |
| 3:B:25:ARG:H     | 3:B:26:PRO:HD3   | 1.34                     | 0.91              |
| 3:C:71:ASP:HB2   | 3:C:76:SER:OG    | 1.70                     | 0.91              |
| 3:A:188:ASN:HD21 | 3:A:231:TYR:H    | 0.97                     | 0.91              |
| 3:D:367:ILE:HG23 | 3:D:368:SER:H    | 1.34                     | 0.91              |
| 3:B:188:ASN:HD21 | 3:B:231:TYR:H    | 1.08                     | 0.91              |
| 3:A:214:ILE:HD12 | 3:A:233:PHE:HB3  | 1.55                     | 0.89              |
| 3:D:25:ARG:HG2   | 3:D:30:LYS:HZ1   | 1.37                     | 0.89              |
| 3:A:352:ASP:HB2  | 5:A:475:HOH:O    | 1.72                     | 0.88              |
| 3:D:341:THR:HG22 | 3:D:342:THR:HG23 | 1.53                     | 0.88              |
| 2:L:9:DA:H2''    | 2:L:10:DG:H5'    | 1.56                     | 0.86              |
| 3:C:10:THR:HG21  | 3:C:15:LEU:HD13  | 1.57                     | 0.86              |
| 3:B:309:HIS:CD2  | 3:C:345:HIS:HE2  | 1.93                     | 0.86              |
| 3:C:341:THR:HG22 | 3:C:342:THR:HG23 | 1.57                     | 0.86              |
| 3:D:116:ILE:HD12 | 3:D:116:ILE:H    | 1.41                     | 0.86              |
| 3:A:92:SER:HB3   | 3:C:116:ILE:HD11 | 1.59                     | 0.85              |
| 2:J:9:DA:H2''    | 2:J:10:DG:H5'    | 1.58                     | 0.85              |
| 3:A:188:ASN:ND2  | 3:A:231:TYR:H    | 1.74                     | 0.85              |
| 3:C:25:ARG:HG2   | 3:C:30:LYS:HZ1   | 1.39                     | 0.85              |
| 3:B:123:LEU:HD13 | 3:C:44:MET:HE3   | 1.59                     | 0.84              |
| 3:C:24:GLU:C     | 3:C:26:PRO:HD3   | 2.04                     | 0.83              |
| 2:F:15:DT:H2''   | 2:F:16:DT:H5'    | 1.60                     | 0.83              |
| 3:B:258:ARG:HE   | 3:B:260:ASN:HD21 | 1.25                     | 0.82              |
| 3:C:143:MET:HG3  | 3:C:298:ILE:HD11 | 1.61                     | 0.82              |
| 3:B:349:ALA:HA   | 5:B:441:HOH:O    | 1.81                     | 0.81              |
| 3:D:2:PRO:HB2    | 3:D:5:ASP:OD2    | 1.80                     | 0.81              |
| 2:F:7:DA:H2'     | 2:F:8:DT:H72     | 1.63                     | 0.81              |
| 3:A:345:HIS:HE1  | 3:A:347:ILE:HG23 | 1.46                     | 0.81              |
| 3:A:38:LEU:HD21  | 3:A:79:PHE:CE2   | 2.16                     | 0.80              |
| 2:L:7:DA:H2'     | 2:L:8:DT:H72     | 1.64                     | 0.80              |
| 3:B:148:LEU:HD12 | 3:C:345:HIS:HB2  | 1.64                     | 0.80              |
| 3:D:77:LEU:HD23  | 3:D:78:GLN:N     | 1.97                     | 0.79              |
| 3:C:3:GLN:O      | 3:C:7:LEU:HD13   | 1.83                     | 0.79              |
| 3:D:399:ARG:NH2  | 3:D:419:ILE:HG21 | 1.97                     | 0.79              |
| 3:C:116:ILE:HD12 | 3:C:116:ILE:H    | 1.45                     | 0.79              |
| 3:D:143:MET:HG3  | 3:D:298:ILE:HD11 | 1.62                     | 0.79              |
| 3:B:108:TYR:CE1  | 3:B:110:GLN:HB2  | 2.18                     | 0.79              |
| 3:B:367:ILE:HD11 | 3:C:364:TYR:CE1  | 2.18                     | 0.78              |
| 3:B:112:HIS:C    | 3:B:114:SER:H    | 1.92                     | 0.78              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:345:HIS:HE1  | 3:B:347:ILE:HG23 | 1.49                     | 0.78              |
| 3:B:214:ILE:HD12 | 3:B:233:PHE:HB3  | 1.65                     | 0.78              |
| 3:B:135:LYS:HB2  | 3:B:138:SER:HB2  | 1.65                     | 0.77              |
| 3:D:24:GLU:C     | 3:D:26:PRO:HD3   | 2.08                     | 0.77              |
| 3:C:143:MET:O    | 3:C:147:LEU:HD13 | 1.85                     | 0.77              |
| 2:L:13:DA:H2''   | 2:L:14:DC:H5''   | 1.67                     | 0.76              |
| 3:A:116:ILE:O    | 3:A:120:VAL:HG23 | 1.86                     | 0.76              |
| 2:J:15:DT:C2'    | 2:J:16:DT:H5''   | 2.16                     | 0.76              |
| 3:C:379:ASN:HD22 | 3:C:382:GLU:HG3  | 1.49                     | 0.76              |
| 3:A:211:LEU:HD12 | 3:A:214:ILE:HD11 | 1.66                     | 0.76              |
| 3:D:423:ILE:H    | 3:D:423:ILE:HD12 | 1.50                     | 0.75              |
| 2:J:14:DC:H2''   | 2:J:15:DT:H5''   | 1.69                     | 0.75              |
| 2:L:12:DA:H5''   | 5:L:73:HOH:O     | 1.86                     | 0.75              |
| 3:A:148:LEU:CD1  | 3:D:345:HIS:HB2  | 2.16                     | 0.74              |
| 3:B:92:SER:HB3   | 3:D:116:ILE:HD11 | 1.67                     | 0.74              |
| 3:B:188:ASN:ND2  | 3:B:231:TYR:H    | 1.85                     | 0.74              |
| 3:C:176:THR:CG2  | 3:C:248:PHE:HA   | 2.17                     | 0.74              |
| 3:D:379:ASN:HD22 | 3:D:382:GLU:HG3  | 1.53                     | 0.74              |
| 2:L:14:DC:H2''   | 2:L:15:DT:H5''   | 1.68                     | 0.74              |
| 3:B:116:ILE:O    | 3:B:120:VAL:HG23 | 1.87                     | 0.74              |
| 3:B:260:ASN:H    | 3:B:261:ARG:NH1  | 1.86                     | 0.74              |
| 3:D:22:ARG:HG2   | 3:D:30:LYS:HG2   | 1.69                     | 0.74              |
| 3:C:22:ARG:HG2   | 3:C:30:LYS:HG2   | 1.69                     | 0.74              |
| 3:D:22:ARG:HA    | 3:D:30:LYS:HD2   | 1.70                     | 0.73              |
| 3:D:178:TYR:HD1  | 3:D:178:TYR:H    | 1.36                     | 0.73              |
| 3:C:71:ASP:HB3   | 3:C:76:SER:H     | 1.53                     | 0.73              |
| 1:G:-10:DC:C2'   | 1:G:-9:DT:H72    | 2.19                     | 0.73              |
| 3:B:211:LEU:HD12 | 3:B:214:ILE:HD11 | 1.69                     | 0.73              |
| 3:D:116:ILE:HD12 | 3:D:116:ILE:N    | 2.03                     | 0.73              |
| 3:D:176:THR:CG2  | 3:D:248:PHE:HA   | 2.19                     | 0.73              |
| 3:C:214:ILE:HG22 | 3:C:215:ILE:N    | 2.04                     | 0.72              |
| 3:C:71:ASP:CG    | 3:C:74:ASN:HB3   | 2.15                     | 0.72              |
| 3:C:209:LYS:HE3  | 3:C:210:TYR:CZ   | 2.23                     | 0.72              |
| 1:E:-10:DC:C2'   | 1:E:-9:DT:H72    | 2.18                     | 0.72              |
| 3:B:287:LEU:HD12 | 3:B:291:ALA:HB2  | 1.70                     | 0.72              |
| 3:D:399:ARG:HH12 | 3:D:419:ILE:HB   | 1.53                     | 0.72              |
| 3:A:92:SER:CB    | 3:C:116:ILE:HD11 | 2.20                     | 0.72              |
| 3:A:260:ASN:C    | 3:A:261:ARG:HD3  | 2.15                     | 0.72              |
| 3:C:22:ARG:HA    | 3:C:30:LYS:HD2   | 1.69                     | 0.72              |
| 3:D:78:GLN:HG2   | 3:D:103:THR:OG1  | 1.89                     | 0.72              |
| 3:D:217:CYS:SG   | 3:D:230:ILE:HB   | 2.29                     | 0.72              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:178:TYR:HD1  | 3:C:178:TYR:H    | 1.38                     | 0.71              |
| 3:D:77:LEU:HD23  | 3:D:78:GLN:H     | 1.54                     | 0.71              |
| 2:J:14:DC:H2''   | 2:J:15:DT:C5'    | 2.21                     | 0.71              |
| 3:A:260:ASN:H    | 3:A:261:ARG:NH1  | 1.87                     | 0.71              |
| 3:B:367:ILE:HD11 | 3:C:364:TYR:HE1  | 1.51                     | 0.71              |
| 3:C:423:ILE:HD12 | 3:C:423:ILE:H    | 1.55                     | 0.71              |
| 3:A:54:ARG:HD2   | 3:A:260:ASN:HD22 | 1.55                     | 0.71              |
| 3:A:123:LEU:HD13 | 3:D:44:MET:HE3   | 1.72                     | 0.71              |
| 3:B:109:GLY:C    | 3:B:111:LYS:N    | 2.35                     | 0.70              |
| 2:J:13:DA:H2''   | 2:J:14:DC:H5''   | 1.73                     | 0.70              |
| 3:C:2:PRO:HB2    | 3:C:5:ASP:OD2    | 1.91                     | 0.70              |
| 3:C:116:ILE:O    | 3:C:120:VAL:HG23 | 1.91                     | 0.70              |
| 3:B:332:ASP:O    | 3:B:334:ARG:HD3  | 1.92                     | 0.70              |
| 3:A:258:ARG:NE   | 3:A:260:ASN:HD21 | 1.88                     | 0.70              |
| 3:D:116:ILE:H    | 3:D:116:ILE:CD1  | 2.03                     | 0.70              |
| 3:A:214:ILE:CD1  | 3:A:233:PHE:HB3  | 2.21                     | 0.70              |
| 2:H:7:DA:H2'     | 2:H:8:DT:H72     | 1.72                     | 0.70              |
| 3:B:25:ARG:N     | 3:B:26:PRO:HD3   | 1.99                     | 0.70              |
| 3:C:96:LEU:C     | 3:C:98:PRO:HD3   | 2.16                     | 0.69              |
| 3:C:116:ILE:H    | 3:C:116:ILE:CD1  | 2.05                     | 0.69              |
| 2:J:7:DA:H2'     | 2:J:8:DT:H72     | 1.75                     | 0.69              |
| 3:C:153:SER:O    | 3:C:157:ILE:HG13 | 1.92                     | 0.69              |
| 3:D:3:GLN:O      | 3:D:7:LEU:HD13   | 1.93                     | 0.69              |
| 3:D:116:ILE:O    | 3:D:120:VAL:HG23 | 1.92                     | 0.69              |
| 3:D:110:GLN:O    | 3:D:110:GLN:HG2  | 1.93                     | 0.69              |
| 3:C:364:TYR:O    | 3:C:366:PRO:HD3  | 1.92                     | 0.69              |
| 3:C:116:ILE:HD12 | 3:C:116:ILE:N    | 2.07                     | 0.68              |
| 3:D:316:SER:HA   | 3:D:321:THR:HG22 | 1.75                     | 0.68              |
| 3:B:260:ASN:C    | 3:B:261:ARG:HD3  | 2.18                     | 0.68              |
| 3:B:11:PRO:HD2   | 3:B:14:VAL:HG21  | 1.75                     | 0.68              |
| 3:D:143:MET:O    | 3:D:147:LEU:HD13 | 1.92                     | 0.68              |
| 3:C:399:ARG:NH2  | 3:C:419:ILE:HG21 | 2.05                     | 0.68              |
| 2:L:14:DC:H2''   | 2:L:15:DT:C5'    | 2.24                     | 0.68              |
| 3:A:160:LYS:HG3  | 5:A:509:HOH:O    | 1.93                     | 0.67              |
| 3:B:112:HIS:O    | 3:B:114:SER:N    | 2.22                     | 0.67              |
| 3:D:364:TYR:O    | 3:D:366:PRO:HD3  | 1.94                     | 0.67              |
| 3:B:92:SER:CB    | 3:D:116:ILE:HD11 | 2.23                     | 0.67              |
| 3:C:316:SER:HA   | 3:C:321:THR:HG22 | 1.77                     | 0.67              |
| 3:B:54:ARG:HD2   | 3:B:260:ASN:HD22 | 1.59                     | 0.67              |
| 3:A:143:MET:HG3  | 3:A:298:ILE:HD11 | 1.76                     | 0.67              |
| 3:A:287:LEU:HD12 | 3:A:291:ALA:HB2  | 1.76                     | 0.67              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:240:ASP:OD2  | 3:C:243:VAL:HG23 | 1.95                     | 0.67              |
| 3:B:43:TRP:CD2   | 3:B:52:ILE:HD13  | 2.30                     | 0.67              |
| 3:C:170:ARG:HG2  | 3:C:171:PHE:CE2  | 2.30                     | 0.67              |
| 1:K:-13:DT:H2''  | 1:K:-12:DT:H5'   | 1.76                     | 0.66              |
| 3:A:353:HIS:HD2  | 5:A:523:HOH:O    | 1.78                     | 0.66              |
| 3:D:240:ASP:OD2  | 3:D:243:VAL:HG23 | 1.95                     | 0.66              |
| 4:E:-4:PHS:O2P   | 2:J:-3:DT:H5''   | 1.95                     | 0.66              |
| 2:F:-2:DT:H2''   | 2:F:-1:DT:H5'    | 1.76                     | 0.66              |
| 3:A:353:HIS:HB2  | 3:A:371:MET:HE3  | 1.77                     | 0.66              |
| 3:C:399:ARG:HH12 | 3:C:419:ILE:HB   | 1.60                     | 0.66              |
| 3:D:200:PRO:O    | 3:D:203:PHE:HD1  | 1.79                     | 0.66              |
| 3:A:198:VAL:HA   | 3:A:219:VAL:HG22 | 1.77                     | 0.65              |
| 3:C:178:TYR:HE2  | 3:C:286:ALA:HB2  | 1.62                     | 0.65              |
| 3:D:365:ASP:HB3  | 3:D:370:GLU:H    | 1.60                     | 0.65              |
| 2:J:15:DT:H2''   | 2:J:16:DT:C5'    | 2.22                     | 0.65              |
| 3:C:200:PRO:O    | 3:C:203:PHE:HD1  | 1.80                     | 0.65              |
| 3:D:80:LYS:HA    | 3:D:105:ILE:O    | 1.96                     | 0.65              |
| 2:H:-2:DT:H2''   | 2:H:-1:DT:H5'    | 1.78                     | 0.64              |
| 2:J:-3:DT:H5'    | 2:J:-3:DT:H6     | 1.62                     | 0.64              |
| 2:L:-3:DT:H6     | 2:L:-3:DT:H5'    | 1.62                     | 0.64              |
| 3:D:313:SER:O    | 3:D:317:MET:HG3  | 1.97                     | 0.64              |
| 3:B:176:THR:CG2  | 3:B:248:PHE:HA   | 2.28                     | 0.64              |
| 3:C:77:LEU:HD23  | 3:C:78:GLN:N     | 2.11                     | 0.64              |
| 3:D:69:SER:OG    | 3:D:78:GLN:HB2   | 1.96                     | 0.64              |
| 3:D:83:THR:HG22  | 3:D:85:LYS:N     | 2.07                     | 0.64              |
| 3:D:96:LEU:HB3   | 3:D:97:ILE:HD12  | 1.79                     | 0.64              |
| 3:D:290:ASN:O    | 3:D:292:PRO:HD3  | 1.98                     | 0.64              |
| 1:I:-17:DT:H2''  | 1:I:-16:DA:H5'   | 1.79                     | 0.64              |
| 3:B:258:ARG:NE   | 3:B:260:ASN:HD21 | 1.95                     | 0.64              |
| 3:B:198:VAL:HA   | 3:B:219:VAL:HG22 | 1.79                     | 0.64              |
| 3:C:83:THR:HG22  | 3:C:85:LYS:N     | 2.03                     | 0.64              |
| 3:A:24:GLU:C     | 3:A:26:PRO:HD3   | 2.23                     | 0.63              |
| 3:B:353:HIS:HB2  | 3:B:371:MET:HE3  | 1.81                     | 0.63              |
| 3:C:45:ILE:HG21  | 3:C:89:LEU:HD12  | 1.80                     | 0.63              |
| 3:C:309:HIS:HE1  | 5:C:427:HOH:O    | 1.80                     | 0.63              |
| 2:F:7:DA:H2'     | 2:F:8:DT:C7      | 2.28                     | 0.63              |
| 1:I:-13:DT:H2''  | 1:I:-12:DT:H5'   | 1.79                     | 0.63              |
| 3:C:217:CYS:SG   | 3:C:230:ILE:HB   | 2.37                     | 0.63              |
| 3:A:345:HIS:CE1  | 3:A:347:ILE:HG23 | 2.32                     | 0.63              |
| 3:A:367:ILE:HD11 | 3:D:364:TYR:CE1  | 2.33                     | 0.63              |
| 3:C:67:SER:O     | 3:C:79:PHE:HA    | 1.98                     | 0.63              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:67:SER:O     | 3:D:79:PHE:HA    | 1.97                     | 0.63              |
| 3:B:246:ASP:O    | 3:B:250:ARG:HG3  | 1.99                     | 0.63              |
| 3:C:421:ARG:HD3  | 3:C:421:ARG:C    | 2.24                     | 0.63              |
| 3:D:162:LEU:CD1  | 3:D:179:GLN:HG3  | 2.29                     | 0.63              |
| 2:F:14:DC:H2''   | 2:F:15:DT:H5'    | 1.80                     | 0.63              |
| 3:D:210:TYR:CD1  | 3:D:356:ALA:HB2  | 2.33                     | 0.63              |
| 3:C:109:GLY:HA2  | 3:C:112:HIS:CE1  | 2.34                     | 0.63              |
| 3:C:81:TYR:HD2   | 3:C:83:THR:HG1   | 1.46                     | 0.62              |
| 3:C:96:LEU:C     | 3:C:97:ILE:HD12  | 2.24                     | 0.62              |
| 3:D:367:ILE:HG23 | 3:D:368:SER:N    | 2.12                     | 0.62              |
| 3:C:69:SER:OG    | 3:C:78:GLN:HG3   | 1.99                     | 0.62              |
| 2:H:14:DC:H2''   | 2:H:15:DT:C5'    | 2.29                     | 0.62              |
| 3:B:323:LEU:O    | 3:B:327:VAL:HG23 | 1.99                     | 0.62              |
| 3:D:236:ARG:HB2  | 3:D:361:TYR:CZ   | 2.34                     | 0.62              |
| 3:D:10:THR:CG2   | 3:D:15:LEU:HD13  | 2.24                     | 0.62              |
| 3:A:43:TRP:CD2   | 3:A:52:ILE:HD13  | 2.35                     | 0.62              |
| 3:A:343:TYR:HA   | 3:C:141:LYS:HE2  | 1.82                     | 0.62              |
| 3:C:78:GLN:HB3   | 3:C:103:THR:OG1  | 1.98                     | 0.62              |
| 3:C:365:ASP:HB3  | 3:C:370:GLU:H    | 1.65                     | 0.62              |
| 3:B:80:LYS:HA    | 3:B:105:ILE:O    | 2.00                     | 0.62              |
| 3:C:10:THR:CG2   | 3:C:15:LEU:HD13  | 2.28                     | 0.62              |
| 3:A:52:ILE:HG22  | 3:A:262:THR:OG1  | 2.00                     | 0.61              |
| 2:L:2:DA:H1'     | 2:L:3:DA:H5''    | 1.82                     | 0.61              |
| 3:D:199:ASP:HB2  | 3:D:270:GLN:HE21 | 1.66                     | 0.61              |
| 3:D:379:ASN:O    | 3:D:383:GLU:HG3  | 2.00                     | 0.61              |
| 2:J:2:DA:H1'     | 2:J:3:DA:H5''    | 1.81                     | 0.61              |
| 3:C:25:ARG:HG2   | 3:C:30:LYS:NZ    | 2.15                     | 0.61              |
| 3:D:153:SER:O    | 3:D:157:ILE:HG13 | 2.00                     | 0.61              |
| 3:D:178:TYR:HE2  | 3:D:286:ALA:HB2  | 1.66                     | 0.61              |
| 3:B:38:LEU:HD21  | 3:B:79:PHE:CE2   | 2.34                     | 0.61              |
| 3:C:361:TYR:OH   | 3:C:422:ARG:NH1  | 2.34                     | 0.61              |
| 3:A:353:HIS:CD2  | 5:A:523:HOH:O    | 2.54                     | 0.61              |
| 3:B:2:PRO:HB2    | 3:B:5:ASP:OD2    | 2.01                     | 0.60              |
| 3:D:68:LEU:HD12  | 3:D:77:LEU:HD21  | 1.83                     | 0.60              |
| 1:E:-15:DA:H1'   | 1:E:-14:DG:H5''  | 1.83                     | 0.60              |
| 3:A:194:ASP:O    | 3:A:219:VAL:HG21 | 2.01                     | 0.60              |
| 3:C:236:ARG:HB2  | 3:C:361:TYR:CZ   | 2.35                     | 0.60              |
| 3:D:214:ILE:HG22 | 3:D:215:ILE:N    | 2.16                     | 0.60              |
| 3:D:254:PRO:HG3  | 3:D:403:TRP:CZ3  | 2.37                     | 0.60              |
| 2:F:14:DC:H2''   | 2:F:15:DT:C5'    | 2.32                     | 0.60              |
| 3:A:196:LYS:CE   | 3:A:197:ASN:ND2  | 2.64                     | 0.60              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:148:LEU:CD1  | 3:C:345:HIS:HB2  | 2.30                     | 0.60              |
| 3:B:421:ARG:HG2  | 3:B:421:ARG:O    | 2.02                     | 0.60              |
| 3:D:181:LEU:O    | 3:D:184:ALA:HB3  | 2.02                     | 0.60              |
| 3:A:148:LEU:HD12 | 3:D:345:HIS:CB   | 2.26                     | 0.60              |
| 3:D:41:LEU:O     | 3:D:45:ILE:HG13  | 2.02                     | 0.60              |
| 3:D:198:VAL:HG22 | 3:D:219:VAL:HG22 | 1.84                     | 0.60              |
| 2:H:14:DC:H2''   | 2:H:15:DT:H5'    | 1.84                     | 0.59              |
| 3:B:309:HIS:HD2  | 3:C:345:HIS:NE2  | 1.92                     | 0.59              |
| 3:D:260:ASN:O    | 3:D:261:ARG:HB3  | 2.02                     | 0.59              |
| 3:A:120:VAL:HG11 | 3:D:16:VAL:HG11  | 1.84                     | 0.59              |
| 3:A:236:ARG:HB2  | 3:A:361:TYR:CE2  | 2.38                     | 0.59              |
| 3:A:421:ARG:O    | 3:A:421:ARG:HG2  | 2.03                     | 0.59              |
| 3:C:326:VAL:HG12 | 3:C:350:ILE:HD13 | 1.85                     | 0.59              |
| 2:L:12:DA:H2''   | 2:L:13:DA:OP2    | 2.02                     | 0.59              |
| 3:C:277:ASP:N    | 5:C:430:HOH:O    | 2.35                     | 0.59              |
| 3:D:210:TYR:HE1  | 3:D:353:HIS:HA   | 1.67                     | 0.59              |
| 3:A:162:LEU:HD23 | 3:A:239:ILE:HD12 | 1.85                     | 0.59              |
| 3:C:170:ARG:HG2  | 3:C:171:PHE:CD2  | 2.38                     | 0.59              |
| 3:C:401:PRO:O    | 3:C:402:ALA:HB3  | 2.02                     | 0.59              |
| 3:B:365:ASP:OD2  | 3:B:367:ILE:HG22 | 2.03                     | 0.59              |
| 3:C:214:ILE:CG2  | 3:C:215:ILE:N    | 2.65                     | 0.59              |
| 3:B:88:ILE:HG21  | 3:D:113:GLN:HG3  | 1.84                     | 0.58              |
| 3:D:383:GLU:O    | 3:D:387:ILE:HG12 | 2.03                     | 0.58              |
| 3:A:80:LYS:HA    | 3:A:105:ILE:O    | 2.02                     | 0.58              |
| 3:B:162:LEU:HD23 | 3:B:239:ILE:HD12 | 1.83                     | 0.58              |
| 3:B:344:THR:HG21 | 3:D:144:LEU:HG   | 1.84                     | 0.58              |
| 3:C:16:VAL:O     | 3:C:20:VAL:HG23  | 2.04                     | 0.58              |
| 3:C:361:TYR:CE2  | 3:C:380:PRO:HD3  | 2.38                     | 0.58              |
| 3:A:367:ILE:HD13 | 3:D:353:HIS:CD2  | 2.38                     | 0.58              |
| 3:D:421:ARG:HD3  | 3:D:421:ARG:C    | 2.29                     | 0.58              |
| 3:C:96:LEU:HB3   | 3:C:97:ILE:HD12  | 1.85                     | 0.58              |
| 3:D:25:ARG:HG2   | 3:D:30:LYS:NZ    | 2.14                     | 0.58              |
| 3:A:365:ASP:OD2  | 3:A:367:ILE:HG22 | 2.04                     | 0.58              |
| 3:B:345:HIS:CE1  | 3:B:347:ILE:HG23 | 2.35                     | 0.58              |
| 3:C:327:VAL:HG22 | 3:C:350:ILE:HD12 | 1.84                     | 0.58              |
| 2:J:12:DA:H2''   | 2:J:13:DA:OP2    | 2.03                     | 0.58              |
| 1:K:-10:DC:H2'   | 1:K:-9:DT:H72    | 1.85                     | 0.58              |
| 3:B:127:PHE:HE2  | 3:C:11:PRO:HG3   | 1.68                     | 0.58              |
| 2:L:15:DT:H2'    | 2:L:16:DT:H72    | 1.85                     | 0.58              |
| 3:A:246:ASP:O    | 3:A:250:ARG:HG3  | 2.04                     | 0.58              |
| 3:D:290:ASN:O    | 3:D:290:ASN:CG   | 2.47                     | 0.57              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:119:ILE:O    | 3:A:123:LEU:HG   | 2.04                     | 0.57              |
| 3:B:194:ASP:O    | 3:B:219:VAL:HG21 | 2.03                     | 0.57              |
| 3:C:203:PHE:HA   | 3:C:216:GLN:O    | 2.04                     | 0.57              |
| 1:G:-15:DA:H1'   | 1:G:-14:DG:H5''  | 1.86                     | 0.57              |
| 3:B:113:GLN:O    | 3:B:115:ASP:N    | 2.37                     | 0.57              |
| 3:B:23:PHE:O     | 3:B:26:PRO:HG3   | 2.04                     | 0.57              |
| 1:K:-14:DG:H2''  | 1:K:-13:DT:C5'   | 2.34                     | 0.57              |
| 3:A:176:THR:CG2  | 3:A:248:PHE:HA   | 2.35                     | 0.57              |
| 3:C:109:GLY:HA2  | 3:C:112:HIS:HE1  | 1.68                     | 0.57              |
| 3:C:379:ASN:ND2  | 3:C:382:GLU:HG3  | 2.19                     | 0.57              |
| 3:D:68:LEU:CD1   | 3:D:77:LEU:HD21  | 2.34                     | 0.57              |
| 2:H:14:DC:C6     | 2:H:15:DT:H72    | 2.40                     | 0.57              |
| 3:C:383:GLU:O    | 3:C:387:ILE:HG12 | 2.04                     | 0.57              |
| 3:D:96:LEU:C     | 3:D:98:PRO:HD3   | 2.30                     | 0.57              |
| 3:B:236:ARG:HH11 | 3:B:236:ARG:HG3  | 1.69                     | 0.57              |
| 3:C:97:ILE:HD12  | 3:C:97:ILE:N     | 2.20                     | 0.57              |
| 3:C:168:THR:HG23 | 5:C:432:HOH:O    | 2.04                     | 0.57              |
| 3:C:313:SER:O    | 3:C:317:MET:HG3  | 2.05                     | 0.57              |
| 3:D:209:LYS:HE3  | 3:D:210:TYR:CZ   | 2.40                     | 0.57              |
| 3:C:192:PHE:CE2  | 3:C:280:VAL:HB   | 2.40                     | 0.57              |
| 3:B:25:ARG:N     | 3:B:26:PRO:CD    | 2.67                     | 0.56              |
| 3:B:143:MET:HG3  | 3:B:298:ILE:HD11 | 1.86                     | 0.56              |
| 3:B:196:LYS:HE3  | 3:B:197:ASN:ND2  | 2.20                     | 0.56              |
| 3:C:210:TYR:CD1  | 3:C:356:ALA:HB2  | 2.41                     | 0.56              |
| 3:C:379:ASN:O    | 3:C:383:GLU:HG3  | 2.05                     | 0.56              |
| 3:D:213:VAL:HG13 | 3:D:384:TRP:HE1  | 1.70                     | 0.56              |
| 3:A:389:GLN:OE1  | 3:A:389:GLN:HA   | 2.04                     | 0.56              |
| 3:B:353:HIS:CD2  | 3:B:353:HIS:H    | 2.23                     | 0.56              |
| 3:B:72:ILE:HD12  | 3:B:72:ILE:N     | 2.13                     | 0.56              |
| 3:C:260:ASN:O    | 3:C:261:ARG:HB3  | 2.05                     | 0.56              |
| 3:D:213:VAL:HG13 | 3:D:384:TRP:NE1  | 2.21                     | 0.56              |
| 3:A:135:LYS:HB2  | 3:A:138:SER:OG   | 2.06                     | 0.56              |
| 3:A:236:ARG:HG3  | 3:A:236:ARG:HH11 | 1.70                     | 0.56              |
| 3:D:13:LYS:O     | 3:D:16:VAL:HG22  | 2.06                     | 0.56              |
| 2:H:7:DA:H2'     | 2:H:8:DT:C7      | 2.36                     | 0.56              |
| 1:K:-8:DA:H1'    | 1:K:-7:DT:H5''   | 1.88                     | 0.56              |
| 3:B:135:LYS:HB2  | 3:B:138:SER:CB   | 2.35                     | 0.56              |
| 3:B:217:CYS:SG   | 3:B:230:ILE:HB   | 2.45                     | 0.56              |
| 3:C:383:GLU:HG2  | 3:C:421:ARG:NH1  | 2.21                     | 0.56              |
| 3:D:144:LEU:O    | 3:D:148:LEU:HG   | 2.06                     | 0.56              |
| 3:B:183:LEU:O    | 3:B:187:ILE:HG12 | 2.06                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:261:ARG:HD3  | 3:B:261:ARG:N    | 2.21                     | 0.56              |
| 3:D:162:LEU:HD11 | 3:D:179:GLN:HG3  | 1.87                     | 0.56              |
| 3:B:389:GLN:HA   | 3:B:389:GLN:OE1  | 2.05                     | 0.55              |
| 1:G:-10:DC:H2'   | 1:G:-9:DT:C7     | 2.31                     | 0.55              |
| 1:I:-14:DG:H2''  | 1:I:-13:DT:C5'   | 2.35                     | 0.55              |
| 3:D:239:ILE:N    | 3:D:239:ILE:HD12 | 2.21                     | 0.55              |
| 3:C:108:TYR:O    | 3:C:110:GLN:N    | 2.39                     | 0.55              |
| 3:B:24:GLU:O     | 3:B:25:ARG:HB2   | 2.06                     | 0.55              |
| 1:I:-15:DA:H8    | 1:I:-15:DA:OP2   | 1.90                     | 0.55              |
| 3:A:127:PHE:HE2  | 3:D:11:PRO:HG3   | 1.72                     | 0.55              |
| 3:D:203:PHE:HA   | 3:D:216:GLN:O    | 2.07                     | 0.55              |
| 1:G:-5:DC:H2''   | 2:L:-3:DT:H5''   | 1.88                     | 0.55              |
| 3:C:365:ASP:OD1  | 3:C:367:ILE:HG22 | 2.05                     | 0.55              |
| 3:C:80:LYS:HA    | 3:C:105:ILE:O    | 2.06                     | 0.55              |
| 3:C:421:ARG:HD3  | 3:C:421:ARG:O    | 2.06                     | 0.55              |
| 3:D:75:LYS:HD3   | 3:D:99:ALA:O     | 2.06                     | 0.55              |
| 3:D:210:TYR:CE1  | 3:D:353:HIS:HA   | 2.41                     | 0.55              |
| 3:A:122:SER:O    | 3:A:126:GLN:HG3  | 2.07                     | 0.55              |
| 1:E:-10:DC:C2'   | 1:E:-9:DT:C7     | 2.84                     | 0.55              |
| 1:K:-14:DG:H2''  | 1:K:-13:DT:H5'   | 1.89                     | 0.55              |
| 3:A:236:ARG:O    | 3:A:236:ARG:HD3  | 2.07                     | 0.54              |
| 3:C:254:PRO:HG3  | 3:C:403:TRP:CZ3  | 2.43                     | 0.54              |
| 3:D:401:PRO:O    | 3:D:402:ALA:HB3  | 2.06                     | 0.54              |
| 1:K:-13:DT:H2'   | 1:K:-12:DT:H71   | 1.88                     | 0.54              |
| 1:G:-15:DA:H2''  | 1:G:-14:DG:H5'   | 1.89                     | 0.54              |
| 3:B:11:PRO:HG3   | 3:D:127:PHE:CE2  | 2.42                     | 0.54              |
| 3:C:144:LEU:O    | 3:C:148:LEU:HG   | 2.08                     | 0.54              |
| 1:I:-13:DT:H2'   | 1:I:-12:DT:H72   | 1.89                     | 0.54              |
| 2:L:7:DA:H2'     | 2:L:8:DT:C7      | 2.37                     | 0.54              |
| 3:C:236:ARG:HB2  | 3:C:361:TYR:CE1  | 2.42                     | 0.54              |
| 3:B:214:ILE:CD1  | 3:B:233:PHE:HB3  | 2.35                     | 0.54              |
| 3:C:157:ILE:O    | 3:C:161:ILE:HG13 | 2.08                     | 0.54              |
| 3:C:290:ASN:O    | 3:C:292:PRO:HD3  | 2.08                     | 0.54              |
| 3:C:107:TYR:CZ   | 3:C:109:GLY:HA3  | 2.41                     | 0.54              |
| 3:A:117:THR:HG23 | 5:A:506:HOH:O    | 2.07                     | 0.54              |
| 3:C:162:LEU:CD1  | 3:C:179:GLN:HG3  | 2.37                     | 0.54              |
| 3:C:25:ARG:HB3   | 3:C:30:LYS:HZ2   | 1.73                     | 0.54              |
| 3:D:365:ASP:OD1  | 3:D:367:ILE:HG22 | 2.08                     | 0.54              |
| 2:J:7:DA:H2'     | 2:J:8:DT:C7      | 2.38                     | 0.54              |
| 3:B:96:LEU:HD11  | 3:D:116:ILE:HG21 | 1.89                     | 0.54              |
| 3:D:192:PHE:CE2  | 3:D:280:VAL:HB   | 2.43                     | 0.54              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:-15:DA:H2''  | 1:G:-14:DG:C5'   | 2.38                     | 0.54              |
| 1:I:-14:DG:H2''  | 1:I:-13:DT:H5'   | 1.88                     | 0.54              |
| 3:A:88:ILE:HG21  | 3:C:113:GLN:NE2  | 2.23                     | 0.54              |
| 3:B:10:THR:OG1   | 3:B:15:LEU:HD21  | 2.07                     | 0.54              |
| 3:D:238:ARG:C    | 3:D:239:ILE:HD12 | 2.33                     | 0.54              |
| 3:B:112:HIS:CD2  | 3:B:112:HIS:H    | 2.25                     | 0.53              |
| 3:B:196:LYS:CE   | 3:B:197:ASN:ND2  | 2.72                     | 0.53              |
| 3:C:143:MET:HG3  | 3:C:298:ILE:CD1  | 2.37                     | 0.53              |
| 3:C:178:TYR:CE2  | 3:C:286:ALA:HB2  | 2.43                     | 0.53              |
| 3:C:150:GLU:O    | 3:C:152:GLU:N    | 2.39                     | 0.53              |
| 3:D:11:PRO:HB2   | 3:D:14:VAL:CG2   | 2.39                     | 0.53              |
| 3:C:13:LYS:HA    | 3:C:16:VAL:HG22  | 1.90                     | 0.53              |
| 3:C:239:ILE:HD12 | 3:C:239:ILE:N    | 2.23                     | 0.53              |
| 3:B:123:LEU:CD1  | 3:C:44:MET:HE3   | 2.36                     | 0.53              |
| 3:A:341:THR:HG22 | 3:A:341:THR:O    | 2.08                     | 0.53              |
| 3:A:217:CYS:SG   | 3:A:230:ILE:HB   | 2.48                     | 0.53              |
| 3:A:96:LEU:HD11  | 3:C:116:ILE:HG21 | 1.91                     | 0.53              |
| 3:C:367:ILE:HG23 | 3:C:368:SER:N    | 2.08                     | 0.53              |
| 3:D:78:GLN:HB3   | 3:D:105:ILE:HD11 | 1.90                     | 0.53              |
| 2:L:13:DA:C2'    | 2:L:14:DC:H5''   | 2.38                     | 0.52              |
| 3:C:289:LYS:C    | 3:C:291:ALA:H    | 2.17                     | 0.52              |
| 3:D:399:ARG:NH1  | 3:D:419:ILE:HB   | 2.22                     | 0.52              |
| 2:L:15:DT:H2''   | 2:L:16:DT:O5'    | 2.09                     | 0.52              |
| 3:A:121:SER:O    | 3:A:125:LEU:HG   | 2.09                     | 0.52              |
| 1:E:-10:DC:H2'   | 1:E:-9:DT:C7     | 2.29                     | 0.52              |
| 2:L:9:DA:H5'     | 3:D:303:LYS:HB2  | 1.91                     | 0.52              |
| 3:D:38:LEU:HD21  | 3:D:79:PHE:CE2   | 2.44                     | 0.52              |
| 3:D:150:GLU:O    | 3:D:152:GLU:N    | 2.41                     | 0.52              |
| 3:D:67:SER:CB    | 3:D:80:LYS:H     | 2.23                     | 0.52              |
| 3:D:152:GLU:HA   | 3:D:156:GLU:OE1  | 2.09                     | 0.52              |
| 3:A:261:ARG:HD3  | 3:A:261:ARG:N    | 2.25                     | 0.52              |
| 3:A:323:LEU:O    | 3:A:327:VAL:HG23 | 2.09                     | 0.52              |
| 3:C:97:ILE:N     | 3:C:98:PRO:HD3   | 2.25                     | 0.52              |
| 3:D:236:ARG:O    | 3:D:236:ARG:HD3  | 2.10                     | 0.52              |
| 3:A:309:HIS:HD2  | 3:D:345:HIS:NE2  | 2.08                     | 0.52              |
| 3:B:236:ARG:HG3  | 3:B:236:ARG:NH1  | 2.25                     | 0.52              |
| 3:C:22:ARG:NH1   | 3:C:30:LYS:O     | 2.43                     | 0.52              |
| 3:C:41:LEU:O     | 3:C:45:ILE:HG13  | 2.10                     | 0.52              |
| 3:D:143:MET:HG3  | 3:D:298:ILE:CD1  | 2.38                     | 0.52              |
| 2:L:8:DT:H4'     | 3:D:305:HIS:CD2  | 2.45                     | 0.52              |
| 3:B:236:ARG:HB2  | 3:B:361:TYR:CE2  | 2.45                     | 0.52              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:23:PHE:CD2   | 3:C:97:ILE:HG21  | 2.44                     | 0.52              |
| 3:C:210:TYR:HE1  | 3:C:353:HIS:HA   | 1.75                     | 0.52              |
| 3:D:45:ILE:HG21  | 3:D:89:LEU:HD12  | 1.90                     | 0.52              |
| 3:C:238:ARG:C    | 3:C:239:ILE:HD12 | 2.35                     | 0.52              |
| 1:K:-16:DA:H2''  | 1:K:-15:DA:OP2   | 2.10                     | 0.51              |
| 3:C:25:ARG:N     | 3:C:26:PRO:HD3   | 2.25                     | 0.51              |
| 3:D:25:ARG:N     | 3:D:26:PRO:HD3   | 2.25                     | 0.51              |
| 3:D:318:LYS:C    | 3:D:320:LEU:H    | 2.19                     | 0.51              |
| 1:K:-8:DA:C2     | 2:L:9:DA:C2      | 2.99                     | 0.51              |
| 3:A:73:VAL:HG12  | 3:A:74:ASN:HD22  | 1.74                     | 0.51              |
| 2:L:-3:DT:H2''   | 2:L:-2:DT:C6     | 2.46                     | 0.51              |
| 3:A:269:LYS:HE2  | 3:A:269:LYS:HA   | 1.93                     | 0.51              |
| 3:D:71:ASP:HB2   | 3:D:76:SER:OG    | 2.10                     | 0.51              |
| 1:E:-15:DA:H2''  | 1:E:-14:DG:C5'   | 2.40                     | 0.51              |
| 3:D:77:LEU:HD22  | 3:D:79:PHE:HD2   | 1.76                     | 0.51              |
| 2:F:-2:DT:H1'    | 2:F:-1:DT:H5''   | 1.91                     | 0.51              |
| 3:C:156:GLU:O    | 3:C:160:LYS:HD3  | 2.11                     | 0.51              |
| 3:A:236:ARG:HG3  | 3:A:236:ARG:NH1  | 2.25                     | 0.51              |
| 1:G:-14:DG:H1'   | 1:G:-13:DT:H5''  | 1.93                     | 0.51              |
| 3:A:196:LYS:HE3  | 3:A:197:ASN:ND2  | 2.24                     | 0.51              |
| 3:D:4:PHE:HZ     | 3:D:261:ARG:HA   | 1.75                     | 0.51              |
| 1:I:-10:DC:H2'   | 1:I:-9:DT:H72    | 1.92                     | 0.51              |
| 3:A:74:ASN:HD22  | 3:A:74:ASN:N     | 2.07                     | 0.51              |
| 3:D:3:GLN:O      | 3:D:6:ILE:HB     | 2.11                     | 0.51              |
| 1:G:-8:DA:H1'    | 1:G:-7:DT:H5''   | 1.92                     | 0.50              |
| 3:A:26:PRO:HB3   | 3:A:72:ILE:HG23  | 1.93                     | 0.50              |
| 3:C:14:VAL:O     | 3:C:18:GLN:HG3   | 2.11                     | 0.50              |
| 3:D:208:ASN:OD1  | 3:D:210:TYR:HB2  | 2.11                     | 0.50              |
| 1:E:-15:DA:H2''  | 1:E:-14:DG:H5'   | 1.93                     | 0.50              |
| 3:A:381:ILE:O    | 3:A:385:GLN:HG3  | 2.11                     | 0.50              |
| 3:B:70:PHE:HE1   | 3:B:72:ILE:HD11  | 1.76                     | 0.50              |
| 3:C:94:LYS:C     | 3:C:96:LEU:H     | 2.19                     | 0.50              |
| 3:D:365:ASP:OD1  | 3:D:367:ILE:CG2  | 2.59                     | 0.50              |
| 2:F:7:DA:H2''    | 2:F:8:DT:C6      | 2.46                     | 0.50              |
| 3:A:368:SER:O    | 3:A:369:LYS:HB2  | 2.11                     | 0.50              |
| 3:D:168:THR:HG21 | 3:D:290:ASN:OD1  | 2.11                     | 0.50              |
| 3:B:112:HIS:CD2  | 3:B:112:HIS:N    | 2.79                     | 0.50              |
| 3:C:210:TYR:CE1  | 3:C:353:HIS:HA   | 2.47                     | 0.50              |
| 3:D:22:ARG:HA    | 3:D:30:LYS:CD    | 2.40                     | 0.50              |
| 3:D:156:GLU:O    | 3:D:160:LYS:HD3  | 2.11                     | 0.50              |
| 3:C:303:LYS:O    | 3:C:306:ILE:HG22 | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:16:VAL:O     | 3:D:20:VAL:HG23  | 2.12                     | 0.50              |
| 3:D:178:TYR:CE2  | 3:D:286:ALA:HB2  | 2.44                     | 0.50              |
| 2:L:9:DA:H2''    | 2:L:10:DG:C5'    | 2.35                     | 0.50              |
| 3:A:361:TYR:O    | 3:A:374:LEU:HG   | 2.12                     | 0.50              |
| 3:B:317:MET:HE2  | 3:B:318:LYS:N    | 2.27                     | 0.50              |
| 3:C:213:VAL:HG13 | 3:C:384:TRP:HE1  | 1.77                     | 0.50              |
| 3:D:78:GLN:HG2   | 3:D:103:THR:HG1  | 1.75                     | 0.50              |
| 3:D:157:ILE:O    | 3:D:161:ILE:HG13 | 2.12                     | 0.49              |
| 3:D:375:LYS:O    | 3:D:375:LYS:HG3  | 2.12                     | 0.49              |
| 2:J:13:DA:C2'    | 2:J:14:DC:H5''   | 2.42                     | 0.49              |
| 2:J:-3:DT:H2''   | 2:J:-2:DT:C6     | 2.48                     | 0.49              |
| 3:D:236:ARG:HB2  | 3:D:361:TYR:CE1  | 2.47                     | 0.49              |
| 3:B:13:LYS:HG2   | 3:D:124:GLN:OE1  | 2.12                     | 0.49              |
| 3:B:344:THR:CG2  | 3:D:144:LEU:HG   | 2.43                     | 0.49              |
| 3:C:235:ALA:HB3  | 3:C:241:PRO:HD3  | 1.94                     | 0.49              |
| 3:D:94:LYS:C     | 3:D:96:LEU:H     | 2.20                     | 0.49              |
| 3:A:199:ASP:O    | 3:A:202:SER:OG   | 2.28                     | 0.49              |
| 3:C:115:ASP:O    | 3:C:118:ASP:HB2  | 2.11                     | 0.49              |
| 3:C:290:ASN:O    | 3:C:290:ASN:CG   | 2.55                     | 0.49              |
| 2:H:4:DA:H1'     | 2:H:5:DG:H5''    | 1.95                     | 0.49              |
| 1:K:-13:DT:H2''  | 1:K:-12:DT:C5'   | 2.42                     | 0.49              |
| 3:A:124:GLN:OE1  | 3:D:13:LYS:HG2   | 2.12                     | 0.49              |
| 3:A:353:HIS:CD2  | 3:A:353:HIS:H    | 2.29                     | 0.49              |
| 3:C:71:ASP:CB    | 3:C:76:SER:H     | 2.25                     | 0.49              |
| 3:C:116:ILE:HD13 | 5:C:438:HOH:O    | 2.13                     | 0.49              |
| 3:C:327:VAL:HA   | 3:C:350:ILE:CD1  | 2.42                     | 0.49              |
| 3:D:326:VAL:HG12 | 3:D:350:ILE:HD13 | 1.93                     | 0.49              |
| 2:H:-2:DT:H1'    | 2:H:-1:DT:H5''   | 1.95                     | 0.49              |
| 3:A:73:VAL:HG12  | 3:A:74:ASN:ND2   | 2.27                     | 0.49              |
| 3:A:345:HIS:ND1  | 3:A:345:HIS:C    | 2.70                     | 0.49              |
| 1:E:-10:DC:H2''  | 1:E:-9:DT:C6     | 2.48                     | 0.49              |
| 1:G:-10:DC:OP2   | 3:B:2:PRO:HA     | 2.12                     | 0.49              |
| 3:B:393:SER:C    | 3:B:395:GLU:H    | 2.21                     | 0.49              |
| 3:C:257:LYS:HE2  | 3:C:258:ARG:O    | 2.11                     | 0.49              |
| 3:A:2:PRO:HB2    | 3:A:5:ASP:OD2    | 2.13                     | 0.49              |
| 3:D:257:LYS:HE2  | 3:D:258:ARG:O    | 2.13                     | 0.49              |
| 3:C:200:PRO:HA   | 3:C:203:PHE:CE1  | 2.48                     | 0.49              |
| 2:J:7:DA:H2''    | 2:J:8:DT:C6      | 2.48                     | 0.48              |
| 1:K:-13:DT:C2'   | 1:K:-12:DT:H71   | 2.44                     | 0.48              |
| 2:L:6:DA:H2''    | 2:L:7:DA:OP2     | 2.12                     | 0.48              |
| 3:A:74:ASN:N     | 3:A:74:ASN:ND2   | 2.61                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:D:185:THR:OG1  | 3:D:307:GLY:HA3  | 2.12                     | 0.48              |
| 3:D:379:ASN:ND2  | 3:D:382:GLU:HG3  | 2.24                     | 0.48              |
| 2:F:-2:DT:H2''   | 2:F:-1:DT:C5'    | 2.42                     | 0.48              |
| 2:J:8:DT:H4'     | 3:C:305:HIS:CD2  | 2.48                     | 0.48              |
| 3:A:317:MET:HE2  | 3:A:318:LYS:HG2  | 1.95                     | 0.48              |
| 3:C:299:LYS:O    | 3:C:300:ASN:HB2  | 2.13                     | 0.48              |
| 3:C:385:GLN:O    | 3:C:389:GLN:HG3  | 2.13                     | 0.48              |
| 3:A:198:VAL:HG22 | 3:A:219:VAL:HG23 | 1.95                     | 0.48              |
| 3:D:3:GLN:HA     | 3:D:6:ILE:HD12   | 1.95                     | 0.48              |
| 3:D:115:ASP:O    | 3:D:118:ASP:HB2  | 2.14                     | 0.48              |
| 3:D:214:ILE:CG2  | 3:D:215:ILE:N    | 2.75                     | 0.48              |
| 1:G:-10:DC:C2'   | 1:G:-9:DT:C7     | 2.88                     | 0.48              |
| 3:A:176:THR:HG21 | 3:A:248:PHE:HA   | 1.96                     | 0.48              |
| 3:D:236:ARG:HD3  | 3:D:236:ARG:C    | 2.38                     | 0.48              |
| 3:C:236:ARG:O    | 3:C:236:ARG:HD3  | 2.13                     | 0.48              |
| 3:D:13:LYS:HA    | 3:D:16:VAL:HG22  | 1.95                     | 0.48              |
| 3:D:159:GLU:HG3  | 3:D:163:ASN:HD21 | 1.78                     | 0.48              |
| 3:D:200:PRO:HA   | 3:D:203:PHE:CE1  | 2.47                     | 0.48              |
| 3:A:367:ILE:HG23 | 3:A:368:SER:N    | 2.29                     | 0.48              |
| 3:B:269:LYS:HE2  | 3:B:269:LYS:HA   | 1.96                     | 0.48              |
| 3:B:254:PRO:HG3  | 3:B:403:TRP:CZ3  | 2.49                     | 0.48              |
| 3:B:412:LEU:O    | 3:B:416:SER:HB2  | 2.14                     | 0.48              |
| 3:D:423:ILE:H    | 3:D:423:ILE:CD1  | 2.24                     | 0.48              |
| 3:A:34:CYS:C     | 5:A:428:HOH:O    | 2.56                     | 0.48              |
| 3:B:86:ALA:O     | 3:B:90:GLU:HG3   | 2.12                     | 0.48              |
| 3:A:317:MET:HE1  | 3:A:318:LYS:HE2  | 1.96                     | 0.48              |
| 3:D:4:PHE:HD2    | 3:D:54:ARG:NH1   | 2.10                     | 0.48              |
| 3:A:393:SER:C    | 3:A:395:GLU:H    | 2.21                     | 0.47              |
| 3:D:199:ASP:HB2  | 3:D:270:GLN:NE2  | 2.28                     | 0.47              |
| 2:J:14:DC:H2''   | 2:J:15:DT:H5'    | 1.96                     | 0.47              |
| 3:A:269:LYS:HE2  | 3:A:269:LYS:CA   | 2.44                     | 0.47              |
| 3:B:72:ILE:H     | 3:B:72:ILE:CD1   | 2.08                     | 0.47              |
| 3:B:112:HIS:C    | 3:B:114:SER:N    | 2.60                     | 0.47              |
| 3:D:233:PHE:CD2  | 3:D:233:PHE:N    | 2.82                     | 0.47              |
| 3:D:254:PRO:HG3  | 3:D:403:TRP:CE3  | 2.49                     | 0.47              |
| 3:C:365:ASP:OD1  | 3:C:367:ILE:CG2  | 2.62                     | 0.47              |
| 3:D:178:TYR:HD1  | 3:D:178:TYR:N    | 2.08                     | 0.47              |
| 3:D:289:LYS:C    | 3:D:291:ALA:H    | 2.22                     | 0.47              |
| 3:D:421:ARG:HD3  | 3:D:421:ARG:O    | 2.14                     | 0.47              |
| 5:E:70:HOH:O     | 3:A:309:HIS:HE1  | 1.97                     | 0.47              |
| 3:A:367:ILE:HG23 | 3:A:368:SER:H    | 1.80                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:299:LYS:O    | 3:B:300:ASN:HB2  | 2.13                     | 0.47              |
| 3:B:334:ARG:CD   | 3:B:334:ARG:H    | 2.27                     | 0.47              |
| 3:C:375:LYS:O    | 3:C:375:LYS:HG3  | 2.14                     | 0.47              |
| 3:D:176:THR:HG23 | 3:D:248:PHE:HA   | 1.96                     | 0.47              |
| 3:C:152:GLU:HA   | 3:C:156:GLU:OE1  | 2.13                     | 0.47              |
| 3:C:399:ARG:NH1  | 3:C:419:ILE:HB   | 2.26                     | 0.47              |
| 3:C:423:ILE:HD12 | 3:C:423:ILE:N    | 2.24                     | 0.47              |
| 1:E:-14:DG:H1'   | 1:E:-13:DT:H5''  | 1.96                     | 0.47              |
| 3:B:148:LEU:HD12 | 3:C:345:HIS:CB   | 2.41                     | 0.47              |
| 3:C:213:VAL:HG13 | 3:C:384:TRP:NE1  | 2.29                     | 0.47              |
| 3:D:357:LEU:HB2  | 3:D:371:MET:HE1  | 1.97                     | 0.47              |
| 2:J:14:DC:C2'    | 2:J:15:DT:H5''   | 2.43                     | 0.47              |
| 3:B:29:GLU:CD    | 3:B:29:GLU:H     | 2.23                     | 0.47              |
| 3:B:367:ILE:HG23 | 3:B:368:SER:N    | 2.30                     | 0.47              |
| 3:C:308:ARG:NH2  | 3:C:328:GLY:O    | 2.48                     | 0.47              |
| 2:H:7:DA:H2''    | 2:H:8:DT:C6      | 2.50                     | 0.47              |
| 3:B:367:ILE:HG23 | 3:B:368:SER:H    | 1.80                     | 0.47              |
| 3:C:162:LEU:HD11 | 3:C:179:GLN:HG3  | 1.96                     | 0.47              |
| 3:D:327:VAL:HA   | 3:D:350:ILE:CD1  | 2.45                     | 0.47              |
| 2:L:14:DC:C2'    | 2:L:15:DT:H5''   | 2.41                     | 0.47              |
| 3:C:365:ASP:O    | 3:C:369:LYS:HA   | 2.14                     | 0.47              |
| 3:D:153:SER:OG   | 3:D:156:GLU:HG3  | 2.15                     | 0.47              |
| 3:B:372:ILE:HG22 | 3:B:373:ALA:O    | 2.15                     | 0.46              |
| 2:F:14:DC:C6     | 2:F:15:DT:H72    | 2.50                     | 0.46              |
| 1:K:-15:DA:OP2   | 1:K:-15:DA:H8    | 1.98                     | 0.46              |
| 3:B:400:TYR:CZ   | 3:B:415:LEU:HD23 | 2.50                     | 0.46              |
| 3:D:213:VAL:CG1  | 3:D:384:TRP:HE1  | 2.28                     | 0.46              |
| 1:K:-16:DA:H1'   | 1:K:-15:DA:C8    | 2.50                     | 0.46              |
| 3:D:39:THR:OG1   | 3:D:64:ILE:HD12  | 2.14                     | 0.46              |
| 3:D:97:ILE:HG22  | 3:D:97:ILE:O     | 2.16                     | 0.46              |
| 3:D:423:ILE:HD12 | 3:D:423:ILE:N    | 2.24                     | 0.46              |
| 5:F:21:HOH:O     | 3:A:82:LYS:HE2   | 2.14                     | 0.46              |
| 3:A:7:LEU:C      | 3:A:7:LEU:HD23   | 2.40                     | 0.46              |
| 3:B:122:SER:O    | 3:B:126:GLN:HG3  | 2.15                     | 0.46              |
| 3:C:13:LYS:O     | 3:C:16:VAL:HG22  | 2.15                     | 0.46              |
| 3:C:314:PHE:O    | 3:C:318:LYS:HG2  | 2.16                     | 0.46              |
| 3:D:11:PRO:HB2   | 3:D:14:VAL:HG23  | 1.97                     | 0.46              |
| 2:H:-3:DT:H2''   | 2:H:-2:DT:H5'    | 1.98                     | 0.46              |
| 2:H:14:DC:H2''   | 2:H:15:DT:H5''   | 1.98                     | 0.46              |
| 3:A:372:ILE:HG22 | 3:A:373:ALA:O    | 2.15                     | 0.46              |
| 3:D:260:ASN:O    | 3:D:261:ARG:CB   | 2.63                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:6:DA:OP1     | 3:C:53:LYS:HE3   | 2.16                     | 0.46              |
| 3:A:5:ASP:O      | 3:A:9:LYS:HG2    | 2.16                     | 0.46              |
| 3:B:381:ILE:O    | 3:B:385:GLN:HG3  | 2.16                     | 0.46              |
| 3:C:200:PRO:HA   | 3:C:203:PHE:HE1  | 1.80                     | 0.46              |
| 3:C:415:LEU:O    | 3:C:419:ILE:HG12 | 2.16                     | 0.46              |
| 3:D:23:PHE:CD2   | 3:D:97:ILE:HG21  | 2.51                     | 0.46              |
| 3:D:142:LYS:O    | 3:D:145:LYS:HB3  | 2.16                     | 0.46              |
| 3:A:188:ASN:HB3  | 3:A:228:ARG:NH2  | 2.30                     | 0.46              |
| 3:B:52:ILE:HG22  | 3:B:262:THR:OG1  | 2.16                     | 0.46              |
| 3:B:176:THR:HG21 | 3:B:248:PHE:HA   | 1.95                     | 0.46              |
| 3:C:189:CYS:HB3  | 3:C:327:VAL:HG12 | 1.97                     | 0.46              |
| 3:C:320:LEU:HD21 | 3:C:364:TYR:CE2  | 2.51                     | 0.46              |
| 3:D:25:ARG:HB3   | 3:D:30:LYS:HZ2   | 1.80                     | 0.46              |
| 3:B:23:PHE:N     | 3:B:23:PHE:CD1   | 2.84                     | 0.46              |
| 3:B:121:SER:O    | 3:B:125:LEU:HG   | 2.15                     | 0.46              |
| 3:C:213:VAL:O    | 3:C:214:ILE:HG13 | 2.16                     | 0.46              |
| 3:B:368:SER:O    | 3:B:369:LYS:HB2  | 2.16                     | 0.46              |
| 3:C:214:ILE:CG2  | 3:C:215:ILE:H    | 2.29                     | 0.46              |
| 3:D:263:GLY:C    | 3:D:266:SER:N    | 2.74                     | 0.46              |
| 3:B:397:SER:HB2  | 3:B:409:GLN:HE22 | 1.80                     | 0.45              |
| 1:I:-8:DA:H1'    | 1:I:-7:DT:H5''   | 1.98                     | 0.45              |
| 3:D:154:ILE:O    | 3:D:158:THR:HG23 | 2.16                     | 0.45              |
| 3:A:267:SER:HA   | 3:A:269:LYS:HE3  | 1.99                     | 0.45              |
| 3:D:162:LEU:HD12 | 3:D:179:GLN:HG3  | 1.98                     | 0.45              |
| 3:A:367:ILE:HD11 | 3:D:364:TYR:HE1  | 1.79                     | 0.45              |
| 3:B:135:LYS:HD2  | 3:B:138:SER:OG   | 2.16                     | 0.45              |
| 3:C:198:VAL:HG22 | 3:C:219:VAL:HG22 | 1.98                     | 0.45              |
| 3:A:227:SER:O    | 3:A:347:ILE:HG21 | 2.17                     | 0.45              |
| 3:D:200:PRO:HA   | 3:D:203:PHE:HE1  | 1.80                     | 0.45              |
| 3:B:400:TYR:OH   | 3:B:415:LEU:HD23 | 2.17                     | 0.45              |
| 3:C:181:LEU:O    | 3:C:184:ALA:HB3  | 2.17                     | 0.45              |
| 3:C:357:LEU:HB2  | 3:C:371:MET:HE1  | 1.99                     | 0.45              |
| 3:B:287:LEU:CD1  | 3:B:291:ALA:HB2  | 2.44                     | 0.45              |
| 3:C:236:ARG:HD3  | 3:C:236:ARG:C    | 2.41                     | 0.45              |
| 3:A:343:TYR:CD2  | 3:C:141:LYS:HE2  | 2.52                     | 0.45              |
| 3:B:269:LYS:HE2  | 3:B:269:LYS:CA   | 2.47                     | 0.45              |
| 3:C:87:THR:O     | 3:C:90:GLU:HB2   | 2.16                     | 0.45              |
| 3:D:33:LEU:C     | 3:D:35:ALA:H     | 2.25                     | 0.45              |
| 3:D:64:ILE:O     | 3:D:65:SER:C     | 2.60                     | 0.45              |
| 3:D:385:GLN:O    | 3:D:389:GLN:HG3  | 2.17                     | 0.45              |
| 2:F:-3:DT:H2''   | 2:F:-2:DT:H5'    | 1.98                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:4:DA:H2''    | 2:F:5:DG:H5'    | 1.99                     | 0.45              |
| 3:D:286:ALA:O    | 3:D:290:ASN:HB3 | 2.17                     | 0.45              |
| 3:A:291:ALA:CB   | 3:A:296:PHE:CD1 | 3.01                     | 0.44              |
| 3:C:22:ARG:HA    | 3:C:30:LYS:CD   | 2.42                     | 0.44              |
| 2:L:7:DA:H2''    | 2:L:8:DT:C6     | 2.53                     | 0.44              |
| 3:B:334:ARG:HD3  | 3:B:334:ARG:N   | 2.31                     | 0.44              |
| 3:C:175:LYS:O    | 3:C:179:GLN:HB2 | 2.17                     | 0.44              |
| 3:D:168:THR:HG21 | 3:D:290:ASN:CG  | 2.42                     | 0.44              |
| 3:D:185:THR:O    | 3:D:189:CYS:N   | 2.51                     | 0.44              |
| 2:H:-2:DT:H2''   | 2:H:-1:DT:C5'   | 2.45                     | 0.44              |
| 2:J:9:DA:H5'     | 3:C:303:LYS:HB2 | 1.99                     | 0.44              |
| 3:B:127:PHE:CE2  | 3:C:11:PRO:HG3  | 2.50                     | 0.44              |
| 3:C:60:TYR:CE1   | 3:C:82:LYS:HD2  | 2.53                     | 0.44              |
| 3:D:75:LYS:O     | 3:D:76:SER:HB3  | 2.17                     | 0.44              |
| 3:A:254:PRO:HG3  | 3:A:403:TRP:CZ3 | 2.52                     | 0.44              |
| 3:B:24:GLU:O     | 3:B:25:ARG:CB   | 2.66                     | 0.44              |
| 3:A:346:GLN:O    | 3:A:346:GLN:NE2 | 2.50                     | 0.44              |
| 3:C:177:LEU:O    | 3:C:178:TYR:C   | 2.60                     | 0.44              |
| 3:D:14:VAL:O     | 3:D:18:GLN:HG3  | 2.18                     | 0.44              |
| 3:D:83:THR:HG22  | 3:D:84:GLN:N    | 2.33                     | 0.44              |
| 3:D:177:LEU:O    | 3:D:178:TYR:C   | 2.60                     | 0.44              |
| 2:L:15:DT:H2''   | 2:L:16:DT:C6    | 2.52                     | 0.44              |
| 3:B:135:LYS:O    | 3:B:139:HIS:HB2 | 2.18                     | 0.44              |
| 3:C:153:SER:OG   | 3:C:156:GLU:HG3 | 2.18                     | 0.44              |
| 3:C:206:VAL:HG12 | 3:C:207:GLN:N   | 2.32                     | 0.44              |
| 3:C:306:ILE:HG23 | 3:C:307:GLY:N   | 2.33                     | 0.44              |
| 3:D:96:LEU:C     | 3:D:97:ILE:HD12 | 2.42                     | 0.44              |
| 1:E:-8:DA:H1'    | 1:E:-7:DT:H5''  | 1.99                     | 0.44              |
| 2:J:6:DA:H2''    | 2:J:7:DA:OP2    | 2.17                     | 0.44              |
| 3:D:97:ILE:HD12  | 3:D:97:ILE:N    | 2.32                     | 0.44              |
| 3:B:23:PHE:CG    | 3:B:97:ILE:HD13 | 2.53                     | 0.44              |
| 3:C:74:ASN:O     | 3:C:75:LYS:HB2  | 2.18                     | 0.44              |
| 3:C:401:PRO:O    | 3:C:402:ALA:CB  | 2.66                     | 0.44              |
| 1:I:-15:DA:OP2   | 1:I:-15:DA:C8   | 2.71                     | 0.43              |
| 3:B:10:THR:HA    | 3:B:11:PRO:HD3  | 1.89                     | 0.43              |
| 3:B:143:MET:HE3  | 3:B:294:SER:OG  | 2.17                     | 0.43              |
| 3:C:178:TYR:HD1  | 3:C:178:TYR:N   | 2.09                     | 0.43              |
| 3:D:4:PHE:CD2    | 3:D:54:ARG:NH1  | 2.86                     | 0.43              |
| 1:E:-14:DG:H2''  | 1:E:-13:DT:C5'  | 2.47                     | 0.43              |
| 1:K:-17:DT:H2'   | 1:K:-16:DA:C5   | 2.54                     | 0.43              |
| 3:A:75:LYS:C     | 3:A:100:TRP:CE3 | 2.96                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:B:141:LYS:O    | 3:B:142:LYS:C    | 2.62                     | 0.43              |
| 3:D:174:THR:HB   | 3:D:178:TYR:CE1  | 2.53                     | 0.43              |
| 3:D:361:TYR:CE2  | 3:D:380:PRO:HG3  | 2.54                     | 0.43              |
| 3:C:361:TYR:CD2  | 3:C:380:PRO:HD3  | 2.54                     | 0.43              |
| 3:D:361:TYR:CD2  | 3:D:380:PRO:HG3  | 2.53                     | 0.43              |
| 3:C:71:ASP:HB2   | 3:C:76:SER:HG    | 1.77                     | 0.43              |
| 3:D:23:PHE:N     | 3:D:23:PHE:CD1   | 2.86                     | 0.43              |
| 2:L:9:DA:OP2     | 3:D:304:SER:OG   | 2.36                     | 0.43              |
| 3:A:115:ASP:O    | 3:A:119:ILE:HG13 | 2.18                     | 0.43              |
| 3:C:254:PRO:HG3  | 3:C:403:TRP:CE3  | 2.54                     | 0.43              |
| 2:F:4:DA:H1'     | 2:F:5:DG:H5''    | 2.00                     | 0.43              |
| 3:B:163:ASN:C    | 3:B:165:PHE:H    | 2.26                     | 0.43              |
| 3:C:279:LEU:HD12 | 3:C:279:LEU:O    | 2.18                     | 0.43              |
| 3:C:387:ILE:HG23 | 3:C:421:ARG:HG3  | 2.00                     | 0.43              |
| 2:J:1:DA:H2''    | 2:J:2:DA:OP2     | 2.18                     | 0.43              |
| 3:C:199:ASP:HB2  | 3:C:270:GLN:HE21 | 1.82                     | 0.43              |
| 3:D:206:VAL:HG12 | 3:D:207:GLN:N    | 2.33                     | 0.43              |
| 3:A:191:ARG:HG2  | 3:A:305:HIS:HE1  | 1.83                     | 0.43              |
| 3:C:11:PRO:HB2   | 3:C:14:VAL:CG2   | 2.49                     | 0.43              |
| 3:C:34:CYS:O     | 3:C:35:ALA:C     | 2.62                     | 0.43              |
| 3:C:168:THR:N    | 5:C:432:HOH:O    | 2.52                     | 0.43              |
| 2:J:9:DA:OP2     | 3:C:304:SER:OG   | 2.37                     | 0.42              |
| 3:C:164:SER:O    | 3:C:290:ASN:ND2  | 2.52                     | 0.42              |
| 3:C:192:PHE:CZ   | 3:C:280:VAL:HB   | 2.54                     | 0.42              |
| 3:C:409:GLN:HG3  | 3:C:413:ASP:OD2  | 2.19                     | 0.42              |
| 3:C:25:ARG:O     | 3:C:25:ARG:HG3   | 2.18                     | 0.42              |
| 3:A:72:ILE:HG13  | 5:A:503:HOH:O    | 2.19                     | 0.42              |
| 3:A:299:LYS:O    | 3:A:300:ASN:HB2  | 2.19                     | 0.42              |
| 3:A:397:SER:HB2  | 3:A:409:GLN:HE22 | 1.84                     | 0.42              |
| 3:B:188:ASN:HB3  | 3:B:228:ARG:NH2  | 2.34                     | 0.42              |
| 3:C:213:VAL:C    | 3:C:214:ILE:HG13 | 2.45                     | 0.42              |
| 3:A:141:LYS:O    | 3:A:142:LYS:C    | 2.62                     | 0.42              |
| 3:A:199:ASP:HA   | 3:A:200:PRO:HD3  | 1.85                     | 0.42              |
| 3:B:12:PRO:O     | 3:B:16:VAL:HG23  | 2.19                     | 0.42              |
| 3:B:116:ILE:HD12 | 3:C:96:LEU:HG    | 2.02                     | 0.42              |
| 3:D:182:PHE:HB2  | 3:D:283:TYR:OH   | 2.19                     | 0.42              |
| 3:A:163:ASN:C    | 3:A:165:PHE:H    | 2.27                     | 0.42              |
| 3:B:20:VAL:HA    | 3:B:97:ILE:HD11  | 2.00                     | 0.42              |
| 3:D:420:ASN:O    | 3:D:421:ARG:C    | 2.63                     | 0.42              |
| 3:A:146:ALA:C    | 3:A:148:LEU:N    | 2.78                     | 0.42              |
| 3:C:105:ILE:HA   | 3:C:106:PRO:HD3  | 1.88                     | 0.42              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:260:ASN:O    | 3:C:261:ARG:CB   | 2.65                     | 0.42              |
| 3:D:208:ASN:C    | 3:D:210:TYR:H    | 2.27                     | 0.42              |
| 3:D:234:SER:HB2  | 3:D:242:LEU:HD12 | 2.01                     | 0.42              |
| 3:B:236:ARG:HD3  | 3:B:236:ARG:O    | 2.20                     | 0.42              |
| 3:C:109:GLY:O    | 3:C:112:HIS:NE2  | 2.53                     | 0.42              |
| 3:C:178:TYR:OH   | 3:C:282:SER:HB2  | 2.19                     | 0.42              |
| 3:D:11:PRO:HA    | 3:D:12:PRO:HD3   | 1.97                     | 0.42              |
| 3:D:105:ILE:HA   | 3:D:106:PRO:HD3  | 1.93                     | 0.42              |
| 3:A:120:VAL:CG1  | 3:D:16:VAL:HG11  | 2.48                     | 0.42              |
| 3:B:317:MET:HE2  | 3:B:318:LYS:HG2  | 2.01                     | 0.42              |
| 3:A:287:LEU:CD1  | 3:A:291:ALA:HB2  | 2.48                     | 0.42              |
| 3:D:420:ASN:C    | 3:D:422:ARG:N    | 2.74                     | 0.42              |
| 1:E:-8:DA:C2     | 2:F:9:DA:C2      | 3.08                     | 0.42              |
| 3:B:70:PHE:CE1   | 3:B:72:ILE:HD11  | 2.53                     | 0.42              |
| 3:C:110:GLN:C    | 3:C:111:LYS:HG2  | 2.43                     | 0.42              |
| 3:D:22:ARG:NH1   | 3:D:30:LYS:O     | 2.52                     | 0.42              |
| 3:A:317:MET:HE2  | 3:A:318:LYS:N    | 2.35                     | 0.41              |
| 3:C:23:PHE:N     | 3:C:23:PHE:CD1   | 2.88                     | 0.41              |
| 3:D:108:TYR:O    | 3:D:109:GLY:C    | 2.63                     | 0.41              |
| 3:D:173:LYS:HG3  | 3:D:251:ASN:O    | 2.20                     | 0.41              |
| 3:D:246:ASP:OD1  | 3:D:399:ARG:NH2  | 2.53                     | 0.41              |
| 3:B:119:ILE:O    | 3:B:123:LEU:HG   | 2.20                     | 0.41              |
| 3:B:199:ASP:OD2  | 3:B:199:ASP:C    | 2.63                     | 0.41              |
| 3:C:211:LEU:N    | 3:C:211:LEU:CD1  | 2.83                     | 0.41              |
| 3:D:97:ILE:N     | 3:D:98:PRO:HD3   | 2.35                     | 0.41              |
| 2:L:15:DT:H2'    | 2:L:16:DT:C7     | 2.49                     | 0.41              |
| 3:A:263:GLY:O    | 3:A:264:ASN:C    | 2.63                     | 0.41              |
| 3:B:267:SER:HA   | 3:B:269:LYS:HE3  | 2.00                     | 0.41              |
| 3:C:22:ARG:NH2   | 3:C:37:GLU:OE2   | 2.40                     | 0.41              |
| 3:C:116:ILE:CD1  | 5:C:438:HOH:O    | 2.68                     | 0.41              |
| 3:D:188:ASN:O    | 3:D:189:CYS:C    | 2.63                     | 0.41              |
| 3:A:120:VAL:HG21 | 3:D:16:VAL:HG11  | 2.03                     | 0.41              |
| 3:B:345:HIS:ND1  | 3:B:345:HIS:C    | 2.74                     | 0.41              |
| 3:D:166:GLU:HA   | 3:D:175:LYS:HD2  | 2.02                     | 0.41              |
| 3:D:235:ALA:HB3  | 3:D:241:PRO:HD3  | 2.01                     | 0.41              |
| 3:D:246:ASP:O    | 3:D:250:ARG:HG3  | 2.19                     | 0.41              |
| 3:D:314:PHE:O    | 3:D:318:LYS:HG2  | 2.20                     | 0.41              |
| 1:G:-14:DG:H2''  | 1:G:-13:DT:C5'   | 2.50                     | 0.41              |
| 3:A:74:ASN:O     | 3:A:75:LYS:HB2   | 2.21                     | 0.41              |
| 3:A:108:TYR:C    | 3:A:108:TYR:CD2  | 2.99                     | 0.41              |
| 3:B:236:ARG:HD2  | 3:B:360:ARG:O    | 2.18                     | 0.41              |

*Continued on next page...*



*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:A:291:ALA:HB1  | 3:A:296:PHE:CD1  | 2.56                     | 0.41              |
| 3:A:352:ASP:OD2  | 3:A:352:ASP:N    | 2.52                     | 0.41              |
| 3:C:182:PHE:HB2  | 3:C:283:TYR:OH   | 2.21                     | 0.41              |
| 3:D:257:LYS:HA   | 3:D:273:GLN:OE1  | 2.21                     | 0.41              |
| 2:J:9:DA:H2''    | 2:J:10:DG:C5'    | 2.39                     | 0.41              |
| 3:B:214:ILE:HD13 | 3:B:214:ILE:HA   | 1.87                     | 0.41              |
| 3:D:25:ARG:HG3   | 3:D:25:ARG:O     | 2.21                     | 0.41              |
| 1:G:-10:DC:H2''  | 1:G:-9:DT:C6     | 2.55                     | 0.41              |
| 3:A:16:VAL:HG21  | 3:C:120:VAL:HG11 | 2.02                     | 0.41              |
| 3:A:181:LEU:O    | 3:A:185:THR:HG23 | 2.21                     | 0.41              |
| 3:A:343:TYR:O    | 3:A:344:THR:OG1  | 2.36                     | 0.41              |
| 3:B:400:TYR:HD1  | 3:B:412:LEU:HB3  | 1.86                     | 0.41              |
| 3:C:15:LEU:HD23  | 3:C:40:TYR:CD2   | 2.56                     | 0.41              |
| 3:C:309:HIS:CE1  | 5:C:427:HOH:O    | 2.64                     | 0.41              |
| 3:C:369:LYS:C    | 3:C:370:GLU:HG2  | 2.46                     | 0.41              |
| 3:D:299:LYS:O    | 3:D:300:ASN:HB2  | 2.21                     | 0.41              |
| 2:H:4:DA:H2''    | 2:H:5:DG:H5'     | 2.03                     | 0.41              |
| 3:A:54:ARG:NH1   | 3:A:259:VAL:O    | 2.54                     | 0.41              |
| 3:B:291:ALA:CB   | 3:B:296:PHE:CD1  | 3.04                     | 0.41              |
| 3:C:24:GLU:O     | 3:C:26:PRO:HD3   | 2.20                     | 0.41              |
| 3:D:303:LYS:O    | 3:D:306:ILE:HG22 | 2.21                     | 0.41              |
| 3:A:47:HIS:HB3   | 3:A:50:THR:HB    | 2.03                     | 0.40              |
| 3:A:93:LEU:HD23  | 3:A:93:LEU:HA    | 1.96                     | 0.40              |
| 3:A:127:PHE:CE2  | 3:D:11:PRO:HG3   | 2.52                     | 0.40              |
| 3:A:146:ALA:O    | 3:A:148:LEU:N    | 2.54                     | 0.40              |
| 3:A:198:VAL:CG2  | 3:A:219:VAL:CG2  | 2.99                     | 0.40              |
| 3:D:245:LEU:O    | 3:D:248:PHE:HB3  | 2.21                     | 0.40              |
| 3:A:158:THR:HG23 | 3:A:182:PHE:HE2  | 1.86                     | 0.40              |
| 3:A:214:ILE:HD13 | 3:A:214:ILE:HA   | 1.78                     | 0.40              |
| 3:C:3:GLN:O      | 3:C:6:ILE:HB     | 2.21                     | 0.40              |
| 3:C:381:ILE:O    | 3:C:384:TRP:HB3  | 2.21                     | 0.40              |
| 3:D:205:LEU:HA   | 3:D:214:ILE:O    | 2.21                     | 0.40              |
| 3:D:224:THR:O    | 3:D:225:SER:HB2  | 2.21                     | 0.40              |
| 3:A:23:PHE:CD1   | 3:A:97:ILE:HD13  | 2.57                     | 0.40              |
| 3:B:115:ASP:HB3  | 3:B:118:ASP:HB2  | 2.02                     | 0.40              |
| 3:C:37:GLU:O     | 3:C:41:LEU:HG    | 2.22                     | 0.40              |
| 3:C:97:ILE:O     | 3:C:97:ILE:HG22  | 2.21                     | 0.40              |
| 3:D:409:GLN:HG3  | 3:D:413:ASP:OD2  | 2.21                     | 0.40              |
| 3:B:11:PRO:HA    | 3:B:12:PRO:HD3   | 1.99                     | 0.40              |
| 3:B:115:ASP:OD2  | 3:B:117:THR:HB   | 2.21                     | 0.40              |
| 3:B:116:ILE:HG13 | 3:B:117:THR:N    | 2.36                     | 0.40              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 3:C:159:GLU:HG3 | 3:C:163:ASN:HD21 | 1.87                     | 0.40              |
| 3:D:160:LYS:HD2 | 3:D:160:LYS:N    | 2.36                     | 0.40              |
| 3:B:171:PHE:CD1 | 3:B:171:PHE:N    | 2.90                     | 0.40              |
| 3:B:393:SER:C   | 3:B:395:GLU:N    | 2.79                     | 0.40              |
| 3:D:141:LYS:O   | 3:D:145:LYS:HB2  | 2.22                     | 0.40              |
| 3:D:171:PHE:N   | 3:D:171:PHE:CD2  | 2.87                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|-----------|----------|-------------|----|
| 3   | A     | 397/422 (94%)   | 361 (91%)  | 30 (8%)   | 6 (2%)   | 8           | 13 |
| 3   | B     | 402/422 (95%)   | 362 (90%)  | 34 (8%)   | 6 (2%)   | 8           | 13 |
| 3   | C     | 396/422 (94%)   | 344 (87%)  | 41 (10%)  | 11 (3%)  | 4           | 6  |
| 3   | D     | 397/422 (94%)   | 327 (82%)  | 55 (14%)  | 15 (4%)  | 2           | 3  |
| All | All   | 1592/1688 (94%) | 1394 (88%) | 160 (10%) | 38 (2%)  | 4           | 7  |

All (38) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 150 | GLU  |
| 3   | A     | 377 | GLU  |
| 3   | A     | 389 | GLN  |
| 3   | B     | 114 | SER  |
| 3   | B     | 150 | GLU  |
| 3   | B     | 377 | GLU  |
| 3   | B     | 389 | GLN  |
| 3   | C     | 151 | GLY  |
| 3   | C     | 270 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 151 | GLY  |
| 3   | D     | 270 | GLN  |
| 3   | A     | 26  | PRO  |
| 3   | B     | 113 | GLN  |
| 3   | C     | 82  | LYS  |
| 3   | C     | 95  | LYS  |
| 3   | C     | 109 | GLY  |
| 3   | D     | 82  | LYS  |
| 3   | D     | 95  | LYS  |
| 3   | A     | 147 | LEU  |
| 3   | B     | 25  | ARG  |
| 3   | C     | 98  | PRO  |
| 3   | C     | 261 | ARG  |
| 3   | D     | 75  | LYS  |
| 3   | D     | 261 | ARG  |
| 3   | C     | 290 | ASN  |
| 3   | D     | 113 | GLN  |
| 3   | D     | 114 | SER  |
| 3   | D     | 171 | PHE  |
| 3   | D     | 209 | LYS  |
| 3   | D     | 274 | LEU  |
| 3   | D     | 290 | ASN  |
| 3   | D     | 110 | GLN  |
| 3   | A     | 73  | VAL  |
| 3   | C     | 367 | ILE  |
| 3   | D     | 98  | PRO  |
| 3   | D     | 367 | ILE  |
| 3   | C     | 72  | ILE  |
| 3   | C     | 12  | PRO  |

### 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 |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 3   | A     | 370/382 (97%) | 356 (96%) | 14 (4%)  | 29          | 49 |
| 3   | B     | 372/382 (97%) | 360 (97%) | 12 (3%)  | 34          | 55 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | C     | 369/382 (97%)   | 363 (98%)  | 6 (2%)   | 55          | 74 |
| 3   | D     | 370/382 (97%)   | 362 (98%)  | 8 (2%)   | 45          | 67 |
| All | All   | 1481/1528 (97%) | 1441 (97%) | 40 (3%)  | 39          | 61 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 26  | PRO  |
| 3   | A     | 58  | MET  |
| 3   | A     | 85  | LYS  |
| 3   | A     | 108 | TYR  |
| 3   | A     | 187 | ILE  |
| 3   | A     | 236 | ARG  |
| 3   | A     | 241 | PRO  |
| 3   | A     | 280 | VAL  |
| 3   | A     | 287 | LEU  |
| 3   | A     | 305 | HIS  |
| 3   | A     | 345 | HIS  |
| 3   | A     | 346 | GLN  |
| 3   | A     | 353 | HIS  |
| 3   | A     | 382 | GLU  |
| 3   | B     | 58  | MET  |
| 3   | B     | 72  | ILE  |
| 3   | B     | 85  | LYS  |
| 3   | B     | 108 | TYR  |
| 3   | B     | 198 | VAL  |
| 3   | B     | 236 | ARG  |
| 3   | B     | 280 | VAL  |
| 3   | B     | 287 | LEU  |
| 3   | B     | 305 | HIS  |
| 3   | B     | 345 | HIS  |
| 3   | B     | 346 | GLN  |
| 3   | B     | 353 | HIS  |
| 3   | C     | 103 | THR  |
| 3   | C     | 116 | ILE  |
| 3   | C     | 178 | TYR  |
| 3   | C     | 253 | GLU  |
| 3   | C     | 305 | HIS  |
| 3   | C     | 341 | THR  |
| 3   | D     | 103 | THR  |
| 3   | D     | 116 | ILE  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 178 | TYR  |
| 3   | D     | 253 | GLU  |
| 3   | D     | 268 | ASN  |
| 3   | D     | 305 | HIS  |
| 3   | D     | 315 | LEU  |
| 3   | D     | 341 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | A     | 48  | ASN  |
| 3   | A     | 74  | ASN  |
| 3   | A     | 126 | GLN  |
| 3   | A     | 137 | ASN  |
| 3   | A     | 163 | ASN  |
| 3   | A     | 179 | GLN  |
| 3   | A     | 188 | ASN  |
| 3   | A     | 197 | ASN  |
| 3   | A     | 216 | GLN  |
| 3   | A     | 229 | HIS  |
| 3   | A     | 260 | ASN  |
| 3   | A     | 264 | ASN  |
| 3   | A     | 268 | ASN  |
| 3   | A     | 300 | ASN  |
| 3   | A     | 309 | HIS  |
| 3   | A     | 345 | HIS  |
| 3   | A     | 346 | GLN  |
| 3   | A     | 353 | HIS  |
| 3   | A     | 385 | GLN  |
| 3   | A     | 404 | ASN  |
| 3   | A     | 409 | GLN  |
| 3   | B     | 3   | GLN  |
| 3   | B     | 48  | ASN  |
| 3   | B     | 112 | HIS  |
| 3   | B     | 137 | ASN  |
| 3   | B     | 163 | ASN  |
| 3   | B     | 179 | GLN  |
| 3   | B     | 188 | ASN  |
| 3   | B     | 197 | ASN  |
| 3   | B     | 229 | HIS  |
| 3   | B     | 260 | ASN  |
| 3   | B     | 264 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 268 | ASN  |
| 3   | B     | 300 | ASN  |
| 3   | B     | 309 | HIS  |
| 3   | B     | 345 | HIS  |
| 3   | B     | 346 | GLN  |
| 3   | B     | 353 | HIS  |
| 3   | B     | 385 | GLN  |
| 3   | B     | 409 | GLN  |
| 3   | C     | 18  | GLN  |
| 3   | C     | 48  | ASN  |
| 3   | C     | 112 | HIS  |
| 3   | C     | 113 | GLN  |
| 3   | C     | 137 | ASN  |
| 3   | C     | 163 | ASN  |
| 3   | C     | 179 | GLN  |
| 3   | C     | 325 | ASN  |
| 3   | C     | 329 | ASN  |
| 3   | C     | 346 | GLN  |
| 3   | C     | 379 | ASN  |
| 3   | C     | 404 | ASN  |
| 3   | C     | 409 | GLN  |
| 3   | D     | 18  | GLN  |
| 3   | D     | 74  | ASN  |
| 3   | D     | 110 | GLN  |
| 3   | D     | 163 | ASN  |
| 3   | D     | 216 | GLN  |
| 3   | D     | 251 | ASN  |
| 3   | D     | 270 | GLN  |
| 3   | D     | 325 | ASN  |
| 3   | D     | 329 | ASN  |
| 3   | D     | 353 | HIS  |
| 3   | D     | 379 | ASN  |
| 3   | D     | 420 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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 | $\# Z  > 2$ |
| 4   | PHS  | E     | -4  | 1    | 0,3,3        | -    | -           | 0,3,3       | -    | -           |
| 4   | PHS  | I     | -4  | 1    | 0,3,3        | -    | -           | 0,3,3       | -    | -           |
| 4   | PHS  | K     | -4  | 1    | 0,3,3        | -    | -           | 0,3,3       | -    | -           |
| 4   | PHS  | G     | -4  | 1    | 0,3,3        | -    | -           | 0,3,3       | -    | -           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | E     | -4  | PHS  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | E     | 13/13 (100%)    | -0.59  | 0 100 100     | 33, 38, 50, 51        | 0     |
| 1   | G     | 13/13 (100%)    | -0.50  | 0 100 100     | 50, 57, 69, 83        | 0     |
| 1   | I     | 13/13 (100%)    | 0.20   | 0 100 100     | 58, 75, 85, 99        | 0     |
| 1   | K     | 13/13 (100%)    | 0.69   | 0 100 100     | 65, 88, 98, 100       | 0     |
| 2   | F     | 20/20 (100%)    | -0.54  | 0 100 100     | 25, 48, 79, 89        | 0     |
| 2   | H     | 20/20 (100%)    | -0.22  | 0 100 100     | 46, 58, 84, 100       | 0     |
| 2   | J     | 19/20 (95%)     | 0.32   | 0 100 100     | 39, 72, 98, 99        | 0     |
| 2   | L     | 19/20 (95%)     | 0.75   | 1 (5%) 32 25  | 57, 80, 101, 101      | 0     |
| 3   | A     | 405/422 (95%)   | -0.21  | 7 (1%) 69 64  | 13, 47, 100, 103      | 0     |
| 3   | B     | 408/422 (96%)   | 0.14   | 15 (3%) 45 37 | 32, 66, 102, 103      | 0     |
| 3   | C     | 404/422 (95%)   | 0.35   | 14 (3%) 47 38 | 40, 77, 102, 103      | 0     |
| 3   | D     | 405/422 (95%)   | 0.74   | 29 (7%) 21 16 | 35, 94, 103, 103      | 0     |
| All | All   | 1752/1820 (96%) | 0.24   | 66 (3%) 44 36 | 13, 73, 102, 103      | 0     |

All (66) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | B     | 109 | GLY  | 9.6  |
| 3   | B     | 392 | GLY  | 6.4  |
| 3   | A     | 136 | GLY  | 5.7  |
| 3   | D     | 272 | TYR  | 3.4  |
| 3   | D     | 404 | ASN  | 3.4  |
| 3   | B     | 423 | ILE  | 3.2  |
| 3   | B     | 136 | GLY  | 3.1  |
| 3   | D     | 422 | ARG  | 3.1  |
| 3   | B     | 111 | LYS  | 3.0  |
| 3   | D     | 30  | LYS  | 3.0  |
| 3   | B     | 334 | ARG  | 3.0  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 384 | TRP  | 3.0  |
| 3   | D     | 149 | SER  | 3.0  |
| 3   | D     | 69  | SER  | 2.9  |
| 3   | D     | 378 | THR  | 2.9  |
| 3   | D     | 28  | GLY  | 2.8  |
| 3   | C     | 268 | ASN  | 2.7  |
| 3   | B     | 375 | LYS  | 2.7  |
| 3   | B     | 112 | HIS  | 2.6  |
| 3   | A     | 138 | SER  | 2.6  |
| 3   | D     | 198 | VAL  | 2.6  |
| 3   | D     | 363 | ALA  | 2.6  |
| 3   | D     | 268 | ASN  | 2.5  |
| 3   | C     | 139 | HIS  | 2.5  |
| 3   | D     | 23  | PHE  | 2.5  |
| 3   | D     | 71  | ASP  | 2.5  |
| 3   | D     | 244 | TYR  | 2.5  |
| 3   | D     | 73  | VAL  | 2.5  |
| 3   | B     | 268 | ASN  | 2.4  |
| 3   | D     | 423 | ILE  | 2.4  |
| 3   | D     | 387 | ILE  | 2.4  |
| 3   | C     | 151 | GLY  | 2.4  |
| 3   | A     | 129 | SER  | 2.3  |
| 3   | D     | 292 | PRO  | 2.3  |
| 3   | C     | 398 | ILE  | 2.3  |
| 3   | D     | 416 | SER  | 2.3  |
| 3   | B     | 108 | TYR  | 2.2  |
| 3   | C     | 26  | PRO  | 2.2  |
| 3   | B     | 393 | SER  | 2.2  |
| 3   | D     | 31  | ILE  | 2.2  |
| 3   | D     | 36  | ALA  | 2.2  |
| 3   | C     | 386 | HIS  | 2.2  |
| 3   | D     | 8   | CYS  | 2.2  |
| 3   | C     | 380 | PRO  | 2.2  |
| 3   | A     | 392 | GLY  | 2.2  |
| 3   | D     | 27  | SER  | 2.2  |
| 3   | D     | 65  | SER  | 2.2  |
| 3   | C     | 113 | GLN  | 2.1  |
| 3   | C     | 290 | ASN  | 2.1  |
| 3   | C     | 114 | SER  | 2.1  |
| 3   | D     | 370 | GLU  | 2.1  |
| 3   | A     | 344 | THR  | 2.1  |
| 3   | B     | 110 | GLN  | 2.1  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | A     | 267 | SER  | 2.1  |
| 3   | A     | 116 | ILE  | 2.1  |
| 3   | B     | 387 | ILE  | 2.1  |
| 3   | D     | 411 | VAL  | 2.1  |
| 3   | C     | 101 | GLU  | 2.1  |
| 2   | L     | 14  | DC   | 2.1  |
| 3   | C     | 263 | GLY  | 2.1  |
| 3   | B     | 331 | SER  | 2.0  |
| 3   | B     | 99  | ALA  | 2.0  |
| 3   | C     | 30  | LYS  | 2.0  |
| 3   | D     | 26  | PRO  | 2.0  |
| 3   | D     | 96  | LEU  | 2.0  |
| 3   | D     | 72  | ILE  | 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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | PHS  | E     | -4  | 4/4   | 0.97 | 0.10 | 26,34,48,50                 | 0     |
| 4   | PHS  | G     | -4  | 4/4   | 0.98 | 0.04 | 42,43,60,61                 | 0     |
| 4   | PHS  | I     | -4  | 4/4   | 0.98 | 0.06 | 53,55,56,63                 | 0     |
| 4   | PHS  | K     | -4  | 4/4   | 0.99 | 0.04 | 51,57,60,64                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.