

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 17, 2021 – 05:50 AM EDT

| PDB ID       | : | 1N5Y   |
|--------------|---|--|
| Title        | : | HIV-1 Reverse Transcriptase Crosslinked to Post-Translocation AZTMP-           |
|              |   | Terminated DNA (Complex P)   |
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|              |   | S.H.; Arnold, E.   |
| Deposited on | : | 2002-11-07   |
| Resolution   | : | 3.10 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

| MolProbity                     | : | 4.02b-467  |
|--------------------------------|---|--|
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.23.2   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2   |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 3.10 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                | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$ |
|-----------------------|--|---|
| R <sub>free</sub>     | 130704   | 1094 (3.10-3.10)  |
| Clashscore            | 141614   | 1184 (3.10-3.10)  |
| Ramachandran outliers | 138981   | 1141 (3.10-3.10)  |
| Sidechain outliers    | 138945   | 1141 (3.10-3.10)  |
| RSRZ outliers         | 127900   | 1067 (3.10-3.10)  |

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 >=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 <=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 | Q      | uality of chain |       |
|-----|-------|--------|--------|-----------------|-------|
| 1   | Т     | 27     | • 37%  | 37%             | 22%   |
| 2   | Р     | 21     | 33%    | 62%             | 5%    |
| 3   | А     | 558    | 2%<br> | 48%             | 13% • |
| 4   | В     | 430    | .%     | 52%             | 13% • |
| 5   | L     | 211    | 36%    | 55%             | 9%    |



| Mol | Chain | Length | Quality | of chain |      |
|-----|-------|--------|---------|----------|------|
| 6   | Н     | 225    | 46%     | 47%      | 6% • |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | MRG  | Р     | 817 | -         | -        | Х       | -                |



# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12185 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 5'-D(\*AP\*TP\*GP\*C\*TP\*AP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*CP\*CP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3'.

| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 1   | Т     | 21       | Total<br>432 | C<br>204 | N<br>87 | 0<br>121 | Р<br>20 | 0       | 0       | 0     |

• Molecule 2 is a DNA chain called 5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*CP\*TP\*GP\*TP\*TP\* CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*(ATM))-3'.

| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|---|
| 2   | Р     | 20       | Total<br>408 | C<br>195 | N<br>72 | 0<br>121 | Р<br>19 | S<br>1  | 0       | 0     | 0 |

• Molecule 3 is a protein called REVERSE TRANSCRIPTASE.

| Mol | Chain | Residues |               | Atoms     |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 3   | А     | 558      | Total<br>4482 | C<br>2901 | N<br>741 | O<br>832 | S<br>8 | 15      | 0       | 0     |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue Modelled A |     | Actual | Comment             | Reference  |
|-------|--------------------|-----|--------|---------------------|------------|
| А     | 258                | CYS | GLN    | engineered mutation | UNP P03366 |
| А     | 280                | SER | CYS    | engineered mutation | UNP P03366 |

• Molecule 4 is a protein called REVERSE TRANSCRIPTASE.

| Mol | Chain | Residues |               | Ate       | oms      |          |            | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|------------|---------|---------|-------|
| 4   | В     | 429      | Total<br>3534 | C<br>2304 | N<br>586 | O<br>637 | ${f S}{7}$ | 18      | 0       | 0     |

There is a discrepancy between the modelled and reference sequences:



| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| В     | 280     | SER      | CYS    | engineered mutation | UNP P03366 |

• Molecule 5 is a protein called monoclonal antibody (light chain).

| Mol | Chain | Residues | Atoms         |           |          |          | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|---|
| 5   | L     | 211      | Total<br>1643 | C<br>1025 | N<br>270 | 0<br>342 | S<br>6  | 0       | 0     | 0 |

• Molecule 6 is a protein called monoclonal antibody (heavy chain).

| Mol | Chain | Residues | Atoms         |           |          |          | ZeroOcc | AltConf | Trace |   |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|---|
| 6   | Н     | 225      | Total<br>1685 | C<br>1060 | N<br>276 | O<br>340 | S<br>9  | 0       | 0     | 0 |

• Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | А     | 1        | Total Mg<br>1 1 | 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: 5'-D(\*AP\*TP\*GP\*C\*TP\*AP\*GP\*GP\*CP\*GP\*CP\*CP\*CP\*CP\*GP\*AP\*AP\*CP\*AP \*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3'





• Molecule 5: monoclonal antibody (light chain)







• Molecule 6: monoclonal antibody (heavy chain)



# 4 Data and refinement statistics (i)

| Property  | Value  | Source    |
|---|--|-----------|
| Space group                                       | P 32 1 2   | Depositor |
| Cell constants                                    | 166.70Å 166.70Å 221.12Å                          | Deperitor |
| a, b, c, $\alpha$ , $\beta$ , $\gamma$            | $90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$ | Depositor |
| $\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$ | 20.00 - 3.10                                     | Depositor |
| Resolution (A)                                    | 34.36 - 3.10                                     | EDS       |
| % Data completeness                               | 91.8 (20.00-3.10)                                | Depositor |
| (in resolution range)                             | 91.7 (34.36-3.10)                                | EDS       |
| R <sub>merge</sub>                                | (Not available)                                  | Depositor |
| $R_{sym}$   | 0.11   | Depositor |
| $< I/\sigma(I) > 1$                               | $1.54 (at 3.12 \text{\AA})$                      | Xtriage   |
| Refinement program                                | CNS 1.0  | Depositor |
| D D.  | 0.255 , $0.285$                                  | Depositor |
| $\Pi, \Pi_{free}$                                 | 0.238 , $0.270$                                  | DCC       |
| $R_{free}$ test set                               | 2502 reflections $(4.05%)$                       | wwPDB-VP  |
| Wilson B-factor $(Å^2)$                           | 85.4   | Xtriage   |
| Anisotropy  | 0.042  | Xtriage   |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$       | 0.31, 56.2                                       | EDS       |
| L-test for twinning <sup>2</sup>                  | $< L >=0.44, < L^2>=0.27$                        | Xtriage   |
| Estimated twinning fraction                       | 0.054 for -h,-k,l                                | Xtriage   |
| $F_o, F_c$ correlation                            | 0.91   | EDS       |
| Total number of atoms                             | 12185  | wwPDB-VP  |
| Average B, all atoms $(Å^2)$                      | 83.0   | wwPDB-VP  |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mal | Chain | Bo   | ond lengths     | B    | ond angles      |
|-----|-------|------|-----------------|------|-----------------|
|     |       | RMSZ | # Z  > 5        | RMSZ | # Z  > 5        |
| 1   | Т     | 2.09 | 16/486~(3.3%)   | 1.80 | 20/749~(2.7%)   |
| 2   | Р     | 2.68 | 28/400~(7.0%)   | 2.60 | 44/612~(7.2%)   |
| 3   | А     | 0.62 | 1/4600~(0.0%)   | 0.77 | 1/6259~(0.0%)   |
| 4   | В     | 0.69 | 0/3639          | 0.83 | 3/4949~(0.1%)   |
| 5   | L     | 0.58 | 0/1681          | 0.78 | 0/2283          |
| 6   | Н     | 0.63 | 0/1729          | 0.84 | 1/2372~(0.0%)   |
| All | All   | 0.88 | 45/12535~(0.4%) | 0.98 | 69/17224~(0.4%) |

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   | Р     | 1                   | 0                   |
| 3   | А     | 0                   | 1                   |
| 5   | L     | 0                   | 1                   |
| All | All   | 1                   | 2                   |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | Р     | 812 | DT   | C4-C5 | 19.16 | 1.62        | 1.45     |
| 2   | Р     | 806 | DT   | C4-C5 | 18.46 | 1.61        | 1.45     |
| 1   | Т     | 720 | DG   | C5-C6 | 15.98 | 1.58        | 1.42     |
| 1   | Т     | 721 | DG   | C5-C6 | 11.98 | 1.54        | 1.42     |
| 2   | Р     | 813 | DT   | C4-C5 | 10.86 | 1.54        | 1.45     |
| 2   | Р     | 818 | DC   | N3-C4 | 10.35 | 1.41        | 1.33     |
| 2   | Р     | 806 | DT   | C2-N3 | -9.41 | 1.30        | 1.37     |
| 2   | Р     | 816 | DG   | C5-C6 | 9.41  | 1.51        | 1.42     |
| 2   | Р     | 808 | DC   | N1-C2 | 8.34  | 1.48        | 1.40     |



| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Р     | 809 | DC   | N1-C2   | 8.25  | 1.48        | 1.40     |
| 1   | Т     | 724 | DT   | N1-C2   | 7.90  | 1.44        | 1.38     |
| 2   | Р     | 820 | DC   | N3-C4   | 7.87  | 1.39        | 1.33     |
| 2   | Р     | 821 | DC   | C3'-O3' | 7.82  | 1.54        | 1.44     |
| 2   | Р     | 818 | DC   | N1-C6   | -7.66 | 1.32        | 1.37     |
| 3   | А     | 248 | GLU  | CD-OE2  | 7.58  | 1.33        | 1.25     |
| 1   | Т     | 711 | DC   | N1-C2   | -7.27 | 1.32        | 1.40     |
| 2   | Р     | 818 | DC   | C2'-C1' | 7.20  | 1.59        | 1.52     |
| 2   | Р     | 809 | DC   | C4-C5   | 6.98  | 1.48        | 1.43     |
| 2   | Р     | 818 | DC   | P-OP1   | -6.83 | 1.37        | 1.49     |
| 2   | Р     | 818 | DC   | O3'-P   | 6.68  | 1.69        | 1.61     |
| 2   | Р     | 808 | DC   | C4-C5   | 6.54  | 1.48        | 1.43     |
| 1   | Т     | 716 | DA   | C5-C6   | 6.44  | 1.46        | 1.41     |
| 2   | Р     | 818 | DC   | C3'-O3' | 6.37  | 1.52        | 1.44     |
| 1   | Т     | 720 | DG   | C6-O6   | 6.36  | 1.29        | 1.24     |
| 1   | Т     | 723 | DC   | N1-C2   | -6.34 | 1.33        | 1.40     |
| 1   | Т     | 709 | DC   | N1-C2   | -6.31 | 1.33        | 1.40     |
| 2   | Р     | 818 | DC   | C2-N3   | 6.07  | 1.40        | 1.35     |
| 2   | Р     | 810 | DT   | C4-C5   | 6.03  | 1.50        | 1.45     |
| 1   | Т     | 720 | DG   | N9-C4   | 5.96  | 1.42        | 1.38     |
| 1   | Т     | 721 | DG   | N1-C2   | -5.67 | 1.33        | 1.37     |
| 1   | Т     | 717 | DC   | N1-C2   | -5.65 | 1.34        | 1.40     |
| 1   | Т     | 723 | DC   | N3-C4   | 5.57  | 1.37        | 1.33     |
| 2   | Р     | 804 | DA   | C6-N1   | 5.57  | 1.39        | 1.35     |
| 1   | Т     | 724 | DT   | C1'-N1  | 5.54  | 1.56        | 1.49     |
| 2   | Р     | 806 | DT   | N1-C2   | 5.50  | 1.42        | 1.38     |
| 1   | Т     | 723 | DC   | C5-C6   | -5.46 | 1.29        | 1.34     |
| 2   | Р     | 816 | DG   | N1-C2   | -5.45 | 1.33        | 1.37     |
| 2   | Р     | 816 | DG   | C8-N7   | 5.35  | 1.34        | 1.30     |
| 2   | Р     | 816 | DG   | N9-C8   | 5.20  | 1.41        | 1.37     |
| 2   | Р     | 809 | DC   | C5-C6   | 5.17  | 1.38        | 1.34     |
| 1   | Т     | 717 | DC   | N3-C4   | 5.15  | 1.37        | 1.33     |
| 1   | Т     | 723 | DC   | C4-C5   | -5.07 | 1.38        | 1.43     |
| 2   | Р     | 808 | DC   | N3-C4   | -5.05 | 1.30        | 1.33     |
| 2   | Р     | 812 | DT   | C4-O4   | 5.03  | 1.27        | 1.23     |
| 2   | Р     | 812 | DT   | N1-C2   | 5.01  | 1.42        | 1.38     |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|----------|--------|------------------|---------------|
| 2   | Р     | 806 | DT   | N3-C4-O4 | -17.47 | 109.42           | 119.90        |
| 2   | Р     | 806 | DT   | C5-C4-O4 | 15.05  | 135.44           | 124.90        |



| Mol | Chain | Res | Type | Atoms       | Z      | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-------------|--------|------------------|---------------|
| 2   | Р     | 812 | DT   | N3-C4-O4    | -13.97 | 111.52           | 119.90        |
| 2   | Р     | 812 | DT   | C5-C4-O4    | 12.77  | 133.84           | 124.90        |
| 2   | Р     | 816 | DG   | N9-C1'-C2'  | 12.07  | 135.53           | 112.60        |
| 2   | Р     | 815 | DG   | N9-C1'-C2'  | 11.90  | 135.22           | 112.60        |
| 2   | Р     | 812 | DT   | C4-C5-C7    | 11.06  | 125.63           | 119.00        |
| 2   | Р     | 806 | DT   | C4-C5-C7    | 10.71  | 125.43           | 119.00        |
| 2   | Р     | 818 | DC   | O4'-C1'-N1  | 8.74   | 114.12           | 108.00        |
| 2   | Р     | 806 | DT   | N3-C2-O2    | -8.39  | 117.26           | 122.30        |
| 2   | Р     | 808 | DC   | N3-C4-N4    | -8.34  | 112.16           | 118.00        |
| 1   | Т     | 720 | DG   | C5-C6-O6    | 8.32   | 133.59           | 128.60        |
| 2   | Р     | 813 | DT   | C5-C4-O4    | 8.30   | 130.71           | 124.90        |
| 1   | Т     | 713 | DC   | N1-C1'-C2'  | 8.17   | 128.12           | 112.60        |
| 2   | Р     | 809 | DC   | N3-C4-N4    | -8.00  | 112.40           | 118.00        |
| 1   | Т     | 723 | DC   | O4'-C1'-N1  | 7.89   | 113.53           | 108.00        |
| 1   | Т     | 711 | DC   | N1-C1'-C2'  | 7.87   | 127.56           | 112.60        |
| 2   | Р     | 808 | DC   | C5-C4-N4    | 7.87   | 125.71           | 120.20        |
| 1   | Т     | 721 | DG   | C5-C6-O6    | 7.73   | 133.24           | 128.60        |
| 2   | Р     | 812 | DT   | C6-C5-C7    | -7.64  | 118.31           | 122.90        |
| 2   | Р     | 813 | DT   | N3-C4-O4    | -7.57  | 115.36           | 119.90        |
| 2   | Р     | 809 | DC   | C5-C4-N4    | 7.55   | 125.48           | 120.20        |
| 4   | В     | 427 | TYR  | N-CA-C      | 7.47   | 131.16           | 111.00        |
| 1   | Т     | 721 | DG   | N1-C6-O6    | -7.38  | 115.47           | 119.90        |
| 1   | Т     | 712 | DC   | N1-C1'-C2'  | 7.15   | 126.18           | 112.60        |
| 1   | Т     | 720 | DG   | N1-C6-O6    | -7.09  | 115.64           | 119.90        |
| 6   | Н     | 141 | GLN  | N-CA-C      | 6.84   | 129.47           | 111.00        |
| 1   | Т     | 723 | DC   | N3-C4-N4    | 6.74   | 122.72           | 118.00        |
| 2   | Р     | 806 | DT   | C6-C5-C7    | -6.72  | 118.87           | 122.90        |
| 2   | Р     | 813 | DT   | C4-C5-C7    | 6.50   | 122.90           | 119.00        |
| 1   | Т     | 709 | DC   | O4'-C1'-N1  | 6.47   | 112.53           | 108.00        |
| 1   | Т     | 723 | DC   | C5-C4-N4    | -6.42  | 115.71           | 120.20        |
| 2   | Р     | 815 | DG   | O4'-C1'-C2' | 6.40   | 111.02           | 105.90        |
| 2   | Р     | 816 | DG   | N1-C2-N2    | -6.29  | 110.54           | 116.20        |
| 2   | P     | 816 | DG   | O5'-P-OP1   | 6.09   | 118.00           | 110.70        |
| 2   | P     | 808 | DC   | N3-C2-O2    | -6.07  | 117.65           | 121.90        |
| 1   | Т     | 717 | DC   | C5-C4-N4    | -5.93  | 116.05           | 120.20        |
| 2   | P     | 812 | DT   | N1-C1'-C2'  | 5.85   | 123.72           | 112.60        |
| 2   | P     | 816 | DG   | C5-C6-O6    | 5.83   | 132.09           | 128.60        |
| 1   | Т     | 717 | DC   | N3-C4-N4    | 5.82   | 122.07           | 118.00        |
| 2   | P     | 819 | DG   | C5'-C4'-C3' | -5.81  | 103.65           | 114.10        |
| 2   | P     | 818 | DC   | C5-C4-N4    | -5.78  | 116.15           | 120.20        |
| 4   | B     | 225 | PRO  | N-CA-C      | 5.75   | 127.06           | 112.10        |
| 2   | P     | 820 | DC   | C2-N3-C4    | -5.68  | 117.06           | 119.90        |



| Mol | Chain | $\operatorname{Res}$ | Type | Atoms      | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|----------------------|------|------------|-------|------------------|---------------|
| 2   | Р     | 820                  | DC   | C5-C4-N4   | -5.59 | 116.29           | 120.20        |
| 2   | Р     | 808                  | DC   | N1-C2-O2   | 5.57  | 122.24           | 118.90        |
| 1   | Т     | 720                  | DG   | N1-C2-N2   | -5.54 | 111.22           | 116.20        |
| 1   | Т     | 716                  | DA   | N9-C1'-C2' | 5.49  | 123.02           | 112.60        |
| 2   | Р     | 809                  | DC   | N3-C2-O2   | -5.46 | 118.08           | 121.90        |
| 1   | Т     | 717                  | DC   | O4'-C1'-N1 | 5.43  | 111.80           | 108.00        |
| 2   | Р     | 806                  | DT   | O4'-C1'-N1 | -5.37 | 104.24           | 108.00        |
| 2   | Р     | 816                  | DG   | N1-C6-O6   | -5.36 | 116.69           | 119.90        |
| 2   | Р     | 815                  | DG   | O4'-C1'-N9 | 5.33  | 111.73           | 108.00        |
| 2   | Р     | 816                  | DG   | N3-C2-N2   | 5.33  | 123.63           | 119.90        |
| 2   | Р     | 818                  | DC   | OP1-P-O3'  | 5.28  | 116.81           | 105.20        |
| 3   | А     | 365                  | VAL  | N-CA-C     | -5.27 | 96.78            | 111.00        |
| 2   | Р     | 818                  | DC   | N3-C4-N4   | 5.21  | 121.65           | 118.00        |
| 1   | Т     | 721                  | DG   | N1-C2-N2   | -5.16 | 111.56           | 116.20        |
| 1   | Т     | 721                  | DG   | C6-C5-N7   | 5.15  | 133.49           | 130.40        |
| 2   | Р     | 818                  | DC   | C6-N1-C2   | 5.15  | 122.36           | 120.30        |
| 2   | Р     | 813                  | DT   | O4'-C1'-N1 | -5.13 | 104.41           | 108.00        |
| 2   | Р     | 813                  | DT   | N1-C1'-C2' | 5.12  | 122.32           | 112.60        |
| 2   | Р     | 813                  | DT   | C6-C5-C7   | -5.10 | 119.84           | 122.90        |
| 1   | Т     | 720                  | DG   | C6-C5-N7   | 5.08  | 133.45           | 130.40        |
| 4   | В     | 423                  | VAL  | N-CA-C     | -5.06 | 97.33            | 111.00        |
| 2   | Р     | 812                  | DT   | N3-C2-O2   | -5.06 | 119.26           | 122.30        |
| 2   | Р     | 818                  | DC   | P-O5'-C5'  | 5.05  | 128.99           | 120.90        |
| 2   | Р     | 806                  | DT   | N1-C1'-C2' | 5.05  | 122.20           | 112.60        |
| 1   | Т     | 721                  | DG   | N9-C1'-C2' | 5.04  | 122.19           | 112.60        |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2   | Р     | 815 | DG   | C1'  |

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 3   | А     | 354 | TYR  | Sidechain |
| 5   | L     | 49  | TYR  | Sidechain |

#### 5.2 Too-close contacts (i)

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



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Т     | 432   | 0        | 235      | 38      | 0            |
| 2   | Р     | 408   | 0        | 230      | 35      | 0            |
| 3   | А     | 4482  | 0        | 4484     | 419     | 0            |
| 4   | В     | 3534  | 0        | 3568     | 359     | 1            |
| 5   | L     | 1643  | 0        | 1565     | 137     | 0            |
| 6   | Н     | 1685  | 0        | 1640     | 103     | 0            |
| 7   | А     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 12185 | 0        | 11722    | 1038    | 1            |

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.

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 44.

All (1038) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom 1           | Atom 2           | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 5:L:61:ARG:HB2   | 5:L:76:SER:HB3   | 1.25         | 1.17        |
| 6:H:166:SER:H    | 6:H:206:ASN:ND2  | 1.51         | 1.07        |
| 6:H:166:SER:N    | 6:H:206:ASN:HD21 | 1.52         | 1.05        |
| 3:A:441:TYR:CE2  | 3:A:544:GLY:HA3  | 1.91         | 1.05        |
| 4:B:244:ILE:HD13 | 4:B:244:ILE:H    | 1.18         | 1.04        |
| 4:B:12:LEU:HD12  | 4:B:12:LEU:H     | 1.22         | 1.03        |
| 3:A:293:ILE:HD12 | 3:A:294:PRO:HD2  | 1.39         | 1.02        |
| 3:A:439:THR:HG21 | 4:B:289:LEU:H    | 1.19         | 1.01        |
| 3:A:254:VAL:HG13 | 3:A:255:ASN:H    | 1.26         | 1.01        |
| 3:A:279:LEU:HD23 | 3:A:279:LEU:H    | 1.25         | 1.01        |
| 3:A:331:LYS:HB3  | 3:A:421:PRO:HG2  | 1.40         | 1.01        |
| 1:T:712:DC:H2"   | 1:T:713:DC:H5'   | 1.42         | 1.00        |
| 4:B:60:VAL:HG12  | 4:B:75:VAL:HG22  | 1.41         | 1.00        |
| 4:B:371:ALA:O    | 4:B:375:ILE:HG13 | 1.60         | 0.99        |
| 6:H:53:ILE:HB    | 6:H:71:VAL:HG11  | 1.42         | 0.99        |
| 3:A:138:GLU:HG2  | 3:A:139:THR:H    | 1.29         | 0.97        |
| 3:A:246:LEU:HD23 | 3:A:246:LEU:H    | 1.31         | 0.95        |
| 4:B:363:ASN:ND2  | 4:B:366:LYS:H    | 1.66         | 0.94        |
| 1:T:724:DT:H2"   | 1:T:725:DG:C8    | 2.02         | 0.94        |
| 4:B:330:GLN:HE22 | 4:B:340:GLN:HE22 | 1.14         | 0.94        |
| 3:A:354:TYR:CE1  | 3:A:374:LYS:HB3  | 2.02         | 0.93        |
| 5:L:90:GLN:HE21  | 5:L:92:SER:H     | 0.93         | 0.91        |
| 2:P:819:DG:H2"   | 2:P:820:DC:O5'   | 1.70         | 0.91        |
| 5:L:170:ASP:O    | 5:L:172:THR:HG23 | 1.71         | 0.90        |



|                  |                  | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:296:THR:HG22 | 4:B:298:GLU:H    | 1.31         | 0.90        |
| 5:L:90:GLN:HE21  | 5:L:92:SER:N     | 1.69         | 0.89        |
| 3:A:317:VAL:HG22 | 3:A:318:TYR:H    | 1.38         | 0.89        |
| 4:B:363:ASN:O    | 4:B:367:GLN:HG3  | 1.72         | 0.89        |
| 4:B:257:ILE:O    | 4:B:261:VAL:HG23 | 1.73         | 0.89        |
| 3:A:469:LEU:HD21 | 3:A:480:GLN:HG2  | 1.55         | 0.88        |
| 4:B:225:PRO:HB2  | 4:B:226:PRO:HD3  | 1.53         | 0.88        |
| 2:P:820:DC:H2"   | 2:P:821:DC:H5'   | 1.55         | 0.88        |
| 3:A:459:THR:HG22 | 3:A:463:ARG:HB3  | 1.55         | 0.88        |
| 2:P:818:DC:H2"   | 2:P:819:DG:O5'   | 1.72         | 0.87        |
| 3:A:215:THR:O    | 3:A:217:PRO:HD3  | 1.74         | 0.86        |
| 3:A:394:GLN:HG2  | 3:A:416:PHE:CE2  | 2.09         | 0.86        |
| 3:A:279:LEU:H    | 3:A:279:LEU:CD2  | 1.86         | 0.86        |
| 4:B:222:GLN:HG3  | 4:B:224:GLU:H    | 1.40         | 0.86        |
| 4:B:237:ASP:C    | 4:B:239:TRP:H    | 1.76         | 0.86        |
| 1:T:707:DG:H2"   | 1:T:708:DG:H5'   | 1.58         | 0.85        |
| 4:B:225:PRO:CG   | 5:L:92:SER:HA    | 2.07         | 0.85        |
| 3:A:459:THR:CG2  | 3:A:463:ARG:HB3  | 2.07         | 0.84        |
| 5:L:34:ASN:OD1   | 5:L:49:TYR:HA    | 1.77         | 0.84        |
| 3:A:447:ASN:HD22 | 3:A:450:THR:HG23 | 1.41         | 0.84        |
| 3:A:489:SER:HB3  | 3:A:528:LYS:HZ3  | 1.41         | 0.84        |
| 3:A:501:TYR:HE1  | 3:A:505:ILE:HD11 | 1.41         | 0.84        |
| 3:A:366:LYS:O    | 3:A:370:GLU:HG2  | 1.76         | 0.84        |
| 3:A:106:VAL:HB   | 3:A:227:PHE:HE1  | 1.41         | 0.84        |
| 2:P:818:DC:H2'   | 2:P:819:DG:H8    | 1.43         | 0.83        |
| 3:A:22:LYS:H     | 3:A:22:LYS:HD3   | 1.43         | 0.83        |
| 4:B:58:THR:HG23  | 4:B:59:PRO:HD2   | 1.59         | 0.83        |
| 4:B:423:VAL:C    | 4:B:425:LEU:H    | 1.82         | 0.83        |
| 6:H:38:TRP:O     | 6:H:50:LEU:HB2   | 1.79         | 0.83        |
| 3:A:500:GLN:H    | 3:A:500:GLN:NE2  | 1.77         | 0.82        |
| 5:L:182:THR:HG22 | 5:L:183:LYS:H    | 1.43         | 0.82        |
| 5:L:90:GLN:NE2   | 5:L:92:SER:H     | 1.77         | 0.82        |
| 3:A:434:ILE:HG22 | 3:A:494:ASN:HD21 | 1.43         | 0.82        |
| 3:A:90:VAL:HG12  | 4:B:141:GLY:H    | 1.43         | 0.81        |
| 5:L:15:LEU:HD12  | 5:L:15:LEU:H     | 1.44         | 0.81        |
| 5:L:38:GLN:HG3   | 5:L:44:VAL:HG22  | 1.60         | 0.81        |
| 5:L:89:GLN:HB2   | 5:L:98:PHE:CD1   | 2.15         | 0.81        |
| 3:A:439:THR:HG21 | 4:B:289:LEU:N    | 1.96         | 0.80        |
| 5:L:61:ARG:CB    | 5:L:76:SER:HB3   | 2.08         | 0.80        |
| 1:T:722:DA:N6    | 2:P:806:DT:O4    | 2.15         | 0.79        |
| 3:A:143:ARG:HG3  | 3:A:143:ARG:HH11 | 1.45         | 0.79        |



|                  |                  | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 5:L:33:LEU:HD21  | 5:L:88:CYS:HB2   | 1.65         | 0.78        |
| 3:A:441:TYR:CD2  | 3:A:544:GLY:HA3  | 2.17         | 0.78        |
| 2:P:818:DC:H2'   | 2:P:819:DG:C8    | 2.18         | 0.78        |
| 4:B:253:THR:O    | 4:B:257:ILE:HG12 | 1.84         | 0.78        |
| 2:P:819:DG:C2'   | 2:P:820:DC:O5'   | 2.31         | 0.78        |
| 5:L:17:ASP:O     | 5:L:77:ASN:HA    | 1.84         | 0.77        |
| 5:L:34:ASN:HB2   | 5:L:89:GLN:NE2   | 1.98         | 0.77        |
| 5:L:195:GLU:HG3  | 5:L:206:VAL:HG22 | 1.63         | 0.77        |
| 4:B:312:GLU:HB3  | 4:B:313:PRO:HD2  | 1.66         | 0.77        |
| 3:A:209:LEU:HB3  | 3:A:214:LEU:HB2  | 1.66         | 0.77        |
| 1:T:716:DA:N6    | 2:P:812:DT:O4    | 2.16         | 0.77        |
| 4:B:163:SER:O    | 4:B:167:ILE:HG13 | 1.85         | 0.77        |
| 6:H:148:LEU:HD13 | 6:H:220:ILE:HG21 | 1.67         | 0.77        |
| 4:B:393:ILE:HD13 | 4:B:398:TRP:HB2  | 1.66         | 0.76        |
| 3:A:489:SER:HB3  | 3:A:528:LYS:NZ   | 2.00         | 0.76        |
| 1:T:724:DT:H2"   | 1:T:725:DG:H8    | 1.50         | 0.76        |
| 3:A:344:GLU:HB3  | 3:A:345:PRO:HD2  | 1.67         | 0.76        |
| 3:A:405:TYR:HD1  | 3:A:406:TRP:H    | 1.34         | 0.76        |
| 3:A:132:ILE:HG23 | 3:A:142:ILE:HB   | 1.68         | 0.76        |
| 4:B:369:THR:HG22 | 4:B:398:TRP:CZ3  | 2.19         | 0.76        |
| 4:B:363:ASN:HD21 | 4:B:365:VAL:HB   | 1.51         | 0.76        |
| 4:B:423:VAL:O    | 4:B:425:LEU:N    | 2.19         | 0.76        |
| 3:A:371:ALA:O    | 3:A:375:ILE:HG12 | 1.87         | 0.75        |
| 3:A:460:ASN:HA   | 4:B:286:THR:OG1  | 1.87         | 0.75        |
| 2:P:817:MRG:C2'  | 2:P:818:DC:O5'   | 2.35         | 0.74        |
| 3:A:310:LEU:HD23 | 3:A:310:LEU:O    | 1.87         | 0.74        |
| 3:A:136:ASN:O    | 3:A:138:GLU:N    | 2.21         | 0.74        |
| 3:A:397:THR:HG21 | 3:A:424:LYS:HA   | 1.68         | 0.74        |
| 3:A:406:TRP:CZ2  | 4:B:420:PRO:HG3  | 2.22         | 0.74        |
| 4:B:91:GLN:OE1   | 4:B:91:GLN:HA    | 1.85         | 0.74        |
| 4:B:111:VAL:HG23 | 4:B:111:VAL:O    | 1.85         | 0.74        |
| 4:B:12:LEU:HD12  | 4:B:12:LEU:N     | 2.01         | 0.74        |
| 4:B:178:ILE:HD11 | 4:B:201:LYS:HG2  | 1.68         | 0.74        |
| 3:A:279:LEU:HD23 | 3:A:279:LEU:N    | 2.02         | 0.74        |
| 4:B:365:VAL:O    | 4:B:369:THR:HG23 | 1.87         | 0.74        |
| 3:A:297:GLU:HA   | 3:A:300:GLU:HB2  | 1.69         | 0.73        |
| 3:A:50:ILE:CG2   | 3:A:145:GLN:HB3  | 2.18         | 0.73        |
| 3:A:450:THR:O    | 3:A:451:LYS:HG2  | 1.87         | 0.73        |
| 6:H:141:GLN:HE22 | 6:H:199:PRO:HD3  | 1.54         | 0.73        |
| 5:L:120:PRO:HB2  | 5:L:125:LEU:HD21 | 1.71         | 0.73        |
| 4:B:423:VAL:C    | 4:B:425:LEU:N    | 2.40         | 0.73        |



|                  |                  | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:299:ALA:O    | 4:B:301:LEU:N    | 2.22         | 0.73        |
| 2:P:820:DC:H2"   | 2:P:821:DC:C5'   | 2.18         | 0.72        |
| 6:H:53:ILE:HB    | 6:H:71:VAL:CG1   | 2.19         | 0.72        |
| 3:A:254:VAL:HG13 | 3:A:255:ASN:N    | 2.03         | 0.72        |
| 4:B:285:GLY:H    | 4:B:287:LYS:NZ   | 1.87         | 0.72        |
| 4:B:279:LEU:HD11 | 4:B:302:GLU:HB2  | 1.70         | 0.72        |
| 4:B:229:TRP:HA   | 4:B:232:TYR:CE1  | 2.25         | 0.72        |
| 4:B:244:ILE:H    | 4:B:244:ILE:CD1  | 1.98         | 0.72        |
| 3:A:30:LYS:O     | 3:A:33:ALA:HB3   | 1.90         | 0.72        |
| 3:A:406:TRP:HE1  | 4:B:418:ASN:ND2  | 1.87         | 0.72        |
| 3:A:435:VAL:HG22 | 4:B:290:THR:HG21 | 1.72         | 0.72        |
| 3:A:27:THR:HG23  | 3:A:30:LYS:HD2   | 1.70         | 0.71        |
| 3:A:484:LEU:O    | 3:A:486:LEU:N    | 2.23         | 0.71        |
| 4:B:237:ASP:C    | 4:B:239:TRP:N    | 2.43         | 0.71        |
| 4:B:387:PRO:HG2  | 4:B:389:PHE:CE1  | 2.25         | 0.71        |
| 3:A:501:TYR:CD1  | 3:A:501:TYR:C    | 2.62         | 0.71        |
| 4:B:2:ILE:HD12   | 4:B:2:ILE:O      | 1.91         | 0.71        |
| 4:B:426:TRP:HA   | 4:B:426:TRP:CE3  | 2.26         | 0.71        |
| 4:B:162:SER:O    | 4:B:165:THR:HG22 | 1.90         | 0.71        |
| 2:P:817:MRG:H2"  | 2:P:818:DC:C5'   | 2.21         | 0.70        |
| 3:A:440:PHE:HE2  | 3:A:489:SER:HG   | 1.38         | 0.70        |
| 3:A:460:ASN:HD22 | 4:B:288:ALA:HB2  | 1.55         | 0.70        |
| 4:B:225:PRO:HG3  | 5:L:92:SER:HA    | 1.73         | 0.70        |
| 5:L:83:ILE:HG21  | 5:L:106:ILE:HG13 | 1.71         | 0.70        |
| 5:L:162:SER:OG   | 6:H:177:PRO:HG2  | 1.92         | 0.70        |
| 5:L:38:GLN:NE2   | 6:H:41:GLN:HE22  | 1.90         | 0.70        |
| 3:A:317:VAL:HG22 | 3:A:318:TYR:N    | 2.06         | 0.70        |
| 3:A:533:LEU:HD12 | 3:A:533:LEU:N    | 2.05         | 0.70        |
| 6:H:125:LYS:O    | 6:H:127:THR:HG23 | 1.91         | 0.70        |
| 4:B:8:VAL:HG11   | 4:B:159:ILE:HG12 | 1.73         | 0.70        |
| 4:B:206:ARG:NH1  | 4:B:217:PRO:O    | 2.25         | 0.70        |
| 2:P:818:DC:C2'   | 2:P:819:DG:O5'   | 2.39         | 0.69        |
| 3:A:354:TYR:HE1  | 3:A:374:LYS:HB3  | 1.54         | 0.69        |
| 4:B:263:LYS:HA   | 4:B:423:VAL:HG11 | 1.74         | 0.69        |
| 4:B:363:ASN:HD22 | 4:B:366:LYS:H    | 1.41         | 0.69        |
| 5:L:38:GLN:HE22  | 6:H:41:GLN:HE22  | 1.39         | 0.69        |
| 2:P:803:DC:H2"   | 2:P:804:DA:C8    | 2.28         | 0.69        |
| 3:A:376:THR:HG23 | 3:A:386:THR:HG23 | 1.73         | 0.69        |
| 4:B:266:TRP:CH2  | 4:B:422:LEU:HB3  | 2.27         | 0.69        |
| 3:A:138:GLU:HG2  | 3:A:139:THR:N    | 2.06         | 0.69        |
| 3:A:90:VAL:CG1   | 4:B:141:GLY:H    | 2.06         | 0.69        |



|                  | 1                | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:285:GLY:O    | 4:B:287:LYS:HG2  | 1.93         | 0.69        |
| 5:L:86:TYR:O     | 5:L:101:GLY:HA2  | 1.94         | 0.68        |
| 3:A:501:TYR:HE1  | 3:A:505:ILE:CD1  | 2.06         | 0.68        |
| 4:B:299:ALA:C    | 4:B:301:LEU:H    | 1.94         | 0.68        |
| 2:P:817:MRG:H2"  | 2:P:818:DC:H5'   | 1.76         | 0.68        |
| 4:B:178:ILE:CD1  | 4:B:201:LYS:HG2  | 2.24         | 0.68        |
| 3:A:257:ILE:HG21 | 3:A:283:LEU:HD21 | 1.75         | 0.68        |
| 1:T:706:DA:H2'   | 1:T:707:DG:C8    | 2.29         | 0.68        |
| 3:A:9:PRO:HA     | 3:A:121:ASP:OD2  | 1.94         | 0.68        |
| 5:L:113:PRO:HG3  | 5:L:144:ILE:HD11 | 1.76         | 0.67        |
| 4:B:320:ASP:OD2  | 4:B:323:LYS:HG3  | 1.94         | 0.67        |
| 3:A:3:SER:HB3    | 3:A:5:ILE:HG13   | 1.75         | 0.67        |
| 3:A:437:ALA:HB1  | 3:A:493:VAL:HA   | 1.75         | 0.67        |
| 5:L:106:ILE:H    | 5:L:166:GLN:HE22 | 1.42         | 0.67        |
| 4:B:106:VAL:HG13 | 4:B:234:LEU:HB2  | 1.77         | 0.66        |
| 5:L:151:ASP:HA   | 5:L:191:SER:HB3  | 1.78         | 0.66        |
| 3:A:518:VAL:O    | 3:A:522:ILE:HG13 | 1.94         | 0.66        |
| 3:A:246:LEU:H    | 3:A:246:LEU:CD2  | 2.06         | 0.66        |
| 4:B:166:LYS:HA   | 4:B:169:GLU:OE1  | 1.94         | 0.66        |
| 3:A:22:LYS:HD3   | 3:A:22:LYS:N     | 2.09         | 0.66        |
| 4:B:225:PRO:HG2  | 5:L:92:SER:HA    | 1.77         | 0.66        |
| 3:A:420:PRO:HA   | 3:A:421:PRO:C    | 2.17         | 0.66        |
| 3:A:457:TYR:HA   | 3:A:548:VAL:CG1  | 2.24         | 0.66        |
| 4:B:244:ILE:HD11 | 4:B:271:TYR:OH   | 1.95         | 0.66        |
| 6:H:54:TRP:HB3   | 6:H:55:TRP:CE3   | 2.30         | 0.66        |
| 4:B:285:GLY:H    | 4:B:287:LYS:HZ3  | 1.42         | 0.66        |
| 3:A:439:THR:CG2  | 4:B:288:ALA:HA   | 2.26         | 0.65        |
| 5:L:23:CYS:SG    | 5:L:33:LEU:HD11  | 2.37         | 0.65        |
| 6:H:34:ILE:CG2   | 6:H:35:GLY:N     | 2.59         | 0.65        |
| 3:A:354:TYR:CZ   | 3:A:374:LYS:HG2  | 2.30         | 0.65        |
| 4:B:195:ILE:HG23 | 4:B:196:GLY:N    | 2.11         | 0.65        |
| 3:A:293:ILE:CD1  | 3:A:294:PRO:HD2  | 2.21         | 0.65        |
| 3:A:430:GLU:HB2  | 3:A:532:TYR:HB2  | 1.79         | 0.65        |
| 3:A:486:LEU:HA   | 3:A:528:LYS:NZ   | 2.12         | 0.65        |
| 4:B:47:ILE:HD12  | 4:B:146:TYR:HA   | 1.77         | 0.64        |
| 3:A:96:HIS:ND1   | 3:A:97:PRO:HD2   | 2.12         | 0.64        |
| 5:L:11:LEU:HD21  | 5:L:19:VAL:HG11  | 1.78         | 0.64        |
| 3:A:254:VAL:CG1  | 3:A:255:ASN:H    | 2.06         | 0.64        |
| 3:A:486:LEU:HA   | 3:A:528:LYS:HZ2  | 1.60         | 0.64        |
| 4:B:395:LYS:HB2  | 4:B:416:PHE:CD2  | 2.32         | 0.64        |
| 4:B:87:PHE:CD2   | 4:B:88:TRP:N     | 2.65         | 0.64        |



|                  |                  | Interatomic             | Clash       |
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| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 4:B:403:THR:O    | 4:B:405:TYR:N    | 2.31                    | 0.64        |
| 3:A:501:TYR:CE1  | 3:A:505:ILE:HD11 | 2.29                    | 0.64        |
| 5:L:38:GLN:HE22  | 6:H:41:GLN:NE2   | 1.96                    | 0.64        |
| 3:A:271:TYR:CE1  | 3:A:314:VAL:HG22 | 2.33                    | 0.64        |
| 3:A:182:GLN:O    | 3:A:182:GLN:HG3  | 1.97                    | 0.63        |
| 5:L:108:ARG:HG2  | 5:L:109:ALA:N    | 2.13                    | 0.63        |
| 6:H:12:VAL:HG21  | 6:H:18:PHE:HB3   | 1.80                    | 0.63        |
| 6:H:27:PHE:CZ    | 6:H:99:GLN:HG3   | 2.33                    | 0.63        |
| 6:H:34:ILE:HD12  | 6:H:34:ILE:H     | 1.62                    | 0.63        |
| 4:B:224:GLU:HB3  | 4:B:225:PRO:HD2  | 1.80                    | 0.63        |
| 5:L:19:VAL:O     | 5:L:74:THR:HA    | 1.97                    | 0.63        |
| 3:A:501:TYR:C    | 3:A:501:TYR:HD1  | 2.01                    | 0.63        |
| 4:B:393:ILE:HG12 | 4:B:394:GLN:N    | 2.12                    | 0.63        |
| 5:L:38:GLN:HG3   | 5:L:44:VAL:CG2   | 2.28                    | 0.63        |
| 6:H:53:ILE:HD12  | 6:H:71:VAL:HG12  | 1.81                    | 0.63        |
| 3:A:542:ILE:HD11 | 4:B:261:VAL:HG11 | 1.80                    | 0.63        |
| 3:A:463:ARG:HG3  | 3:A:464:GLN:H    | 1.62                    | 0.62        |
| 5:L:35:TRP:HB2   | 5:L:48:ILE:HD12  | 1.80                    | 0.62        |
| 3:A:109:LEU:HD23 | 3:A:220:LYS:HB2  | 1.81                    | 0.62        |
| 3:A:447:ASN:ND2  | 3:A:450:THR:HG23 | 2.13                    | 0.62        |
| 4:B:263:LYS:HG2  | 4:B:423:VAL:CG1  | 2.29                    | 0.62        |
| 3:A:473:THR:HG22 | 3:A:474:ASN:N    | 2.14                    | 0.62        |
| 2:P:812:DT:C6    | 2:P:813:DT:H73   | 2.34                    | 0.62        |
| 4:B:120:LEU:HD12 | 4:B:121:ASP:H    | 1.64                    | 0.62        |
| 5:L:33:LEU:HD23  | 5:L:34:ASN:H     | 1.63                    | 0.62        |
| 5:L:33:LEU:CD2   | 5:L:88:CYS:HB2   | 2.27                    | 0.62        |
| 3:A:111:VAL:HG11 | 3:A:214:LEU:HD12 | 1.81                    | 0.62        |
| 6:H:209:HIS:HD2  | 6:H:212:SER:OG   | 1.83                    | 0.62        |
| 3:A:420:PRO:HG3  | 3:A:422:LEU:HG   | 1.82                    | 0.61        |
| 4:B:227:PHE:O    | 4:B:230:MET:HB2  | 2.00                    | 0.61        |
| 5:L:37:GLN:HB2   | 5:L:47:LEU:HD11  | 1.82                    | 0.61        |
| 6:H:162:VAL:HG22 | 6:H:207:VAL:HG22 | 1.81                    | 0.61        |
| 1:T:715:DA:H2"   | 1:T:716:DA:H8    | 1.65                    | 0.61        |
| 3:A:465:LYS:NZ   | 3:A:488:ASP:OD2  | 2.31                    | 0.61        |
| 3:A:478:GLU:OE1  | 3:A:498:ASP:OD1  | 2.17                    | 0.61        |
| 4:B:260:LEU:HD12 | 4:B:260:LEU:O    | 2.00                    | 0.61        |
| 4:B:260:LEU:O    | 4:B:264:LEU:HD12 | 2.01                    | 0.61        |
| 3:A:219:LYS:O    | 3:A:219:LYS:HG3  | 2.00                    | 0.61        |
| 4:B:43:LYS:C     | 4:B:45:GLY:H     | 2.02                    | 0.61        |
| 4:B:330:GLN:NE2  | 4:B:340:GLN:HE22 | 1.91                    | 0.61        |
| 3:A:344:GLU:CB   | 3:A:345:PRO:HD2  | 2.29                    | 0.61        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:511:ASP:OD2  | 3:A:511:ASP:C    | 2.39         | 0.61        |
| 4:B:293:ILE:HD13 | 4:B:293:ILE:N    | 2.15         | 0.61        |
| 4:B:323:LYS:HB2  | 4:B:343:GLN:NE2  | 2.16         | 0.61        |
| 3:A:104:LYS:HB2  | 3:A:192:ASP:HA   | 1.82         | 0.61        |
| 4:B:299:ALA:C    | 4:B:301:LEU:N    | 2.54         | 0.61        |
| 4:B:330:GLN:HE22 | 4:B:340:GLN:NE2  | 1.94         | 0.61        |
| 5:L:73:LEU:HD12  | 5:L:74:THR:H     | 1.66         | 0.61        |
| 4:B:225:PRO:HB3  | 5:L:32:TYR:CE1   | 2.36         | 0.61        |
| 4:B:306:ASN:HA   | 4:B:309:ILE:HG12 | 1.82         | 0.61        |
| 4:B:340:GLN:HG3  | 4:B:351:THR:HG22 | 1.83         | 0.61        |
| 3:A:162:SER:OG   | 4:B:52:PRO:HD3   | 2.01         | 0.61        |
| 4:B:34:LEU:CD1   | 4:B:73:LYS:HG3   | 2.30         | 0.61        |
| 4:B:262:GLY:O    | 4:B:265:ASN:N    | 2.33         | 0.61        |
| 4:B:302:GLU:HA   | 4:B:305:GLU:HB2  | 1.81         | 0.61        |
| 4:B:79:GLU:OE1   | 4:B:83:ARG:NH1   | 2.34         | 0.60        |
| 6:H:133:PRO:O    | 6:H:134:LEU:HD23 | 2.00         | 0.60        |
| 4:B:60:VAL:CG1   | 4:B:75:VAL:HG22  | 2.24         | 0.60        |
| 5:L:89:GLN:HB2   | 5:L:98:PHE:CE1   | 2.35         | 0.60        |
| 5:L:117:ILE:HD13 | 5:L:194:CYS:HB2  | 1.82         | 0.60        |
| 6:H:183:ASP:O    | 6:H:184:LEU:HG   | 1.99         | 0.60        |
| 3:A:86:ASP:HA    | 3:A:154:LYS:HZ2  | 1.66         | 0.60        |
| 4:B:59:PRO:HG2   | 4:B:76:ASP:HB3   | 1.83         | 0.60        |
| 4:B:314:VAL:HG12 | 4:B:315:HIS:H    | 1.66         | 0.60        |
| 2:P:817:MRG:H2"  | 2:P:818:DC:O5'   | 2.01         | 0.60        |
| 3:A:479:LEU:HD21 | 3:A:518:VAL:CG2  | 2.32         | 0.60        |
| 5:L:6:GLN:OE1    | 5:L:101:GLY:N    | 2.29         | 0.60        |
| 3:A:493:VAL:HG22 | 3:A:494:ASN:N    | 2.15         | 0.60        |
| 4:B:225:PRO:CB   | 4:B:226:PRO:HD3  | 2.28         | 0.60        |
| 3:A:109:LEU:HD23 | 3:A:220:LYS:CB   | 2.32         | 0.60        |
| 4:B:46:LYS:HD2   | 4:B:116:PHE:HB3  | 1.84         | 0.59        |
| 4:B:43:LYS:C     | 4:B:45:GLY:N     | 2.53         | 0.59        |
| 4:B:155:GLY:O    | 4:B:158:ALA:HB3  | 2.02         | 0.59        |
| 6:H:39:ILE:HG22  | 6:H:40:ARG:N     | 2.18         | 0.59        |
| 3:A:257:ILE:O    | 3:A:261:VAL:HG12 | 2.02         | 0.59        |
| 3:A:379:SER:O    | 3:A:382:ILE:N    | 2.31         | 0.59        |
| 3:A:548:VAL:O    | 3:A:552:VAL:HG23 | 2.02         | 0.59        |
| 4:B:34:LEU:HD11  | 4:B:73:LYS:HG3   | 1.84         | 0.59        |
| 3:A:31:ILE:O     | 3:A:35:VAL:HG23  | 2.03         | 0.59        |
| 5:L:173:TYR:N    | 5:L:173:TYR:CD1  | 2.70         | 0.59        |
| 1:T:713:DC:H2"   | 1:T:714:DG:O5'   | 2.03         | 0.59        |
| 4:B:314:VAL:HG12 | 4:B:315:HIS:N    | 2.17         | 0.59        |



|                  |                  | Interatomic    | Clash       |
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| Atom-1           | Atom-2           | distance $(Å)$ | overlap (Å) |
| 6:H:55:TRP:HE3   | 6:H:55:TRP:H     | 1.50           | 0.59        |
| 3:A:373:GLN:NE2  | 4:B:397:THR:HG23 | 2.17           | 0.59        |
| 3:A:494:ASN:OD1  | 4:B:289:LEU:HD12 | 2.03           | 0.59        |
| 5:L:21:ILE:HD13  | 5:L:102:THR:HB   | 1.85           | 0.59        |
| 6:H:62:ASN:HD22  | 6:H:63:PRO:HD2   | 1.66           | 0.59        |
| 3:A:497:THR:HG22 | 3:A:498:ASP:H    | 1.68           | 0.59        |
| 3:A:175:ASN:OD1  | 3:A:201:LYS:HE3  | 2.03           | 0.58        |
| 3:A:361:HIS:CD2  | 3:A:505:ILE:HD13 | 2.38           | 0.58        |
| 4:B:43:LYS:O     | 4:B:45:GLY:N     | 2.35           | 0.58        |
| 4:B:87:PHE:HE2   | 4:B:155:GLY:HA2  | 1.68           | 0.58        |
| 5:L:66:GLY:HA3   | 5:L:71:TYR:CD2   | 2.38           | 0.58        |
| 3:A:500:GLN:H    | 3:A:500:GLN:HE21 | 1.49           | 0.58        |
| 4:B:168:LEU:HD13 | 4:B:180:ILE:HG21 | 1.84           | 0.58        |
| 5:L:190:ASN:CG   | 5:L:210:ASN:HD22 | 2.07           | 0.58        |
| 3:A:429:LEU:HD22 | 3:A:533:LEU:HD13 | 1.85           | 0.58        |
| 5:L:34:ASN:O     | 5:L:88:CYS:HA    | 2.03           | 0.58        |
| 3:A:543:GLY:O    | 3:A:545:ASN:N    | 2.37           | 0.58        |
| 4:B:113:ASP:O    | 4:B:115:TYR:N    | 2.37           | 0.58        |
| 1:T:707:DG:C2'   | 1:T:708:DG:H5'   | 2.32           | 0.58        |
| 4:B:100:LEU:HD23 | 4:B:100:LEU:O    | 2.04           | 0.58        |
| 6:H:209:HIS:CD2  | 6:H:212:SER:OG   | 2.56           | 0.58        |
| 3:A:166:LYS:O    | 3:A:169:GLU:HB3  | 2.02           | 0.58        |
| 3:A:317:VAL:CG2  | 3:A:318:TYR:H    | 2.15           | 0.58        |
| 5:L:33:LEU:HD23  | 5:L:89:GLN:O     | 2.03           | 0.58        |
| 3:A:280:SER:O    | 3:A:283:LEU:HG   | 2.04           | 0.58        |
| 3:A:363:ASN:OD1  | 3:A:364:ASP:N    | 2.37           | 0.58        |
| 4:B:112:GLY:HA3  | 4:B:151:GLN:HE21 | 1.68           | 0.58        |
| 3:A:475:GLN:HB3  | 3:A:501:TYR:CE2  | 2.39           | 0.58        |
| 3:A:5:ILE:CD1    | 3:A:167:ILE:HD11 | 2.34           | 0.58        |
| 3:A:34:LEU:HA    | 3:A:37:ILE:HD12  | 1.86           | 0.58        |
| 3:A:354:TYR:OH   | 3:A:374:LYS:HG2  | 2.03           | 0.58        |
| 4:B:58:THR:HG23  | 4:B:59:PRO:CD    | 2.33           | 0.57        |
| 4:B:58:THR:CG2   | 4:B:59:PRO:N     | 2.66           | 0.57        |
| 3:A:499:SER:OG   | 3:A:502:ALA:HB3  | 2.03           | 0.57        |
| 4:B:171:PHE:HE1  | 4:B:205:LEU:HA   | 1.68           | 0.57        |
| 6:H:40:ARG:HB2   | 6:H:50:LEU:HD11  | 1.86           | 0.57        |
| 3:A:439:THR:HG1  | 3:A:441:TYR:HE1  | 1.51           | 0.57        |
| 4:B:171:PHE:CE1  | 4:B:205:LEU:HA   | 2.39           | 0.57        |
| 5:L:61:ARG:HG2   | 5:L:61:ARG:HH11  | 1.70           | 0.57        |
| 3:A:416:PHE:CD1  | 3:A:416:PHE:C    | 2.76           | 0.57        |
| 4:B:205:LEU:O    | 4:B:205:LEU:HD12 | 2.05           | 0.57        |



|                  | A L O            | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:11:LYS:O     | 3:A:85:GLN:HG2   | 2.05         | 0.57        |
| 3:A:17:ASP:O     | 3:A:83:ARG:NH1   | 2.37         | 0.57        |
| 3:A:417:VAL:O    | 3:A:417:VAL:HG13 | 2.05         | 0.57        |
| 3:A:463:ARG:HG3  | 3:A:464:GLN:N    | 2.20         | 0.57        |
| 3:A:521:ILE:O    | 3:A:525:LEU:HD13 | 2.05         | 0.57        |
| 5:L:73:LEU:HD12  | 5:L:74:THR:N     | 2.20         | 0.57        |
| 5:L:120:PRO:CB   | 5:L:125:LEU:HD21 | 2.34         | 0.57        |
| 5:L:135:PHE:C    | 5:L:136:LEU:HD12 | 2.25         | 0.57        |
| 6:H:27:PHE:CE2   | 6:H:99:GLN:HG3   | 2.39         | 0.57        |
| 3:A:466:VAL:HG21 | 3:A:551:LEU:HG   | 1.87         | 0.57        |
| 5:L:154:GLU:HG2  | 5:L:155:ARG:N    | 2.20         | 0.57        |
| 3:A:338:THR:HG22 | 3:A:339:TYR:N    | 2.20         | 0.57        |
| 4:B:234:LEU:HD21 | 4:B:377:THR:HG21 | 1.87         | 0.57        |
| 6:H:6:GLU:OE1    | 6:H:116:GLY:N    | 2.34         | 0.56        |
| 1:T:713:DC:H2'   | 1:T:714:DG:C8    | 2.39         | 0.56        |
| 4:B:58:THR:HG22  | 4:B:59:PRO:N     | 2.20         | 0.56        |
| 4:B:106:VAL:HA   | 4:B:190:GLY:HA2  | 1.87         | 0.56        |
| 4:B:112:GLY:HA3  | 4:B:151:GLN:NE2  | 2.19         | 0.56        |
| 3:A:459:THR:HG22 | 3:A:463:ARG:CB   | 2.32         | 0.56        |
| 3:A:518:VAL:O    | 3:A:518:VAL:HG12 | 2.04         | 0.56        |
| 4:B:120:LEU:HD12 | 4:B:121:ASP:N    | 2.20         | 0.56        |
| 5:L:81:GLU:N     | 5:L:81:GLU:OE1   | 2.37         | 0.56        |
| 3:A:261:VAL:HG13 | 3:A:262:GLY:H    | 1.70         | 0.56        |
| 5:L:61:ARG:CZ    | 5:L:79:GLU:HG3   | 2.35         | 0.56        |
| 3:A:460:ASN:HA   | 4:B:286:THR:O    | 2.05         | 0.56        |
| 5:L:35:TRP:CZ3   | 5:L:88:CYS:HB3   | 2.40         | 0.56        |
| 6:H:95:TYR:O     | 6:H:116:GLY:HA2  | 2.04         | 0.56        |
| 3:A:194:GLU:O    | 3:A:196:GLY:N    | 2.39         | 0.56        |
| 3:A:438:GLU:HB3  | 3:A:459:THR:OG1  | 2.05         | 0.56        |
| 5:L:182:THR:HG22 | 5:L:183:LYS:N    | 2.15         | 0.56        |
| 6:H:134:LEU:HD12 | 6:H:149:GLY:HA3  | 1.87         | 0.56        |
| 1:T:715:DA:C2    | 1:T:716:DA:C6    | 2.94         | 0.56        |
| 3:A:443:ASP:O    | 3:A:481:ALA:HB2  | 2.04         | 0.56        |
| 4:B:78:ARG:HD3   | 4:B:411:ILE:HG22 | 1.87         | 0.56        |
| 4:B:210:LEU:C    | 4:B:212:TRP:H    | 2.09         | 0.56        |
| 4:B:223:LYS:HD2  | 4:B:223:LYS:N    | 2.21         | 0.56        |
| 5:L:106:ILE:N    | 5:L:166:GLN:HE22 | 2.04         | 0.56        |
| 4:B:34:LEU:O     | 4:B:38:CYS:HB2   | 2.05         | 0.56        |
| 5:L:46:LEU:HD23  | 5:L:55:HIS:CG    | 2.40         | 0.56        |
| 3:A:108:VAL:HG22 | 3:A:188:TYR:HA   | 1.88         | 0.56        |
| 6:H:34:ILE:HG22  | 6:H:35:GLY:N     | 2.20         | 0.56        |



|                  | is as pagem      | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 6:H:65:LEU:HD22  | 6:H:68:ARG:HH21  | 1.70         | 0.56        |
| 3:A:264:LEU:O    | 3:A:267:ALA:HB3  | 2.06         | 0.56        |
| 6:H:164:TRP:CZ3  | 6:H:205:CYS:HB2  | 2.41         | 0.56        |
| 3:A:115:TYR:C    | 3:A:117:SER:H    | 2.10         | 0.55        |
| 3:A:439:THR:HG23 | 4:B:288:ALA:HA   | 1.87         | 0.55        |
| 3:A:502:ALA:O    | 3:A:506:ILE:HG12 | 2.06         | 0.55        |
| 3:A:536:VAL:HG13 | 3:A:537:PRO:HD2  | 1.88         | 0.55        |
| 4:B:47:ILE:HG23  | 4:B:144:TYR:HD1  | 1.70         | 0.55        |
| 4:B:252:TRP:CD1  | 4:B:252:TRP:N    | 2.75         | 0.55        |
| 3:A:457:TYR:CZ   | 3:A:465:LYS:HB3  | 2.41         | 0.55        |
| 4:B:171:PHE:CD1  | 4:B:205:LEU:HD13 | 2.41         | 0.55        |
| 4:B:263:LYS:HG2  | 4:B:423:VAL:HG12 | 1.88         | 0.55        |
| 4:B:356:ARG:HG2  | 4:B:357:MET:N    | 2.22         | 0.55        |
| 5:L:11:LEU:HG    | 5:L:11:LEU:O     | 2.05         | 0.55        |
| 3:A:466:VAL:HG12 | 3:A:466:VAL:O    | 2.06         | 0.55        |
| 4:B:302:GLU:HA   | 4:B:302:GLU:OE1  | 2.05         | 0.55        |
| 2:P:807:DC:H4'   | 3:A:448:ARG:HD2  | 1.88         | 0.55        |
| 3:A:405:TYR:HD1  | 3:A:406:TRP:N    | 2.04         | 0.55        |
| 3:A:442:VAL:CG2  | 3:A:495:ILE:HG22 | 2.37         | 0.55        |
| 4:B:175:ASN:HD21 | 4:B:201:LYS:NZ   | 2.04         | 0.55        |
| 6:H:4:LEU:HD23   | 6:H:24:PHE:HB3   | 1.89         | 0.55        |
| 3:A:363:ASN:OD1  | 3:A:363:ASN:C    | 2.45         | 0.55        |
| 3:A:394:GLN:HG2  | 3:A:416:PHE:CD2  | 2.42         | 0.55        |
| 3:A:429:LEU:HD22 | 3:A:533:LEU:CD1  | 2.36         | 0.55        |
| 4:B:237:ASP:O    | 4:B:239:TRP:N    | 2.40         | 0.55        |
| 1:T:720:DG:H2"   | 1:T:721:DG:OP2   | 2.07         | 0.55        |
| 3:A:427:TYR:CE2  | 3:A:525:LEU:HD23 | 2.42         | 0.55        |
| 4:B:118:VAL:O    | 4:B:148:VAL:HG23 | 2.06         | 0.55        |
| 4:B:312:GLU:CB   | 4:B:313:PRO:HD2  | 2.35         | 0.55        |
| 5:L:33:LEU:HD23  | 5:L:34:ASN:N     | 2.22         | 0.55        |
| 3:A:447:ASN:HD22 | 3:A:450:THR:CG2  | 2.18         | 0.55        |
| 4:B:116:PHE:C    | 4:B:148:VAL:HG21 | 2.27         | 0.55        |
| 6:H:40:ARG:HD3   | 6:H:50:LEU:HD11  | 1.89         | 0.55        |
| 3:A:136:ASN:C    | 3:A:138:GLU:H    | 2.09         | 0.55        |
| 4:B:328:GLU:O    | 4:B:339:TYR:HA   | 2.07         | 0.55        |
| 2:P:819:DG:OP1   | 3:A:259:LYS:HG3  | 2.07         | 0.55        |
| 3:A:244:ILE:HG13 | 3:A:263:LYS:HD3  | 1.89         | 0.55        |
| 3:A:469:LEU:CD2  | 3:A:480:GLN:HG2  | 2.32         | 0.55        |
| 4:B:91:GLN:OE1   | 4:B:91:GLN:CA    | 2.53         | 0.55        |
| 4:B:131:THR:HG22 | 4:B:132:ILE:N    | 2.21         | 0.55        |
| 3:A:279:LEU:HA   | 3:A:282:LEU:HG   | 1.88         | 0.54        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:500:GLN:HE21 | 3:A:500:GLN:N    | 2.04         | 0.54        |
| 5:L:137:ASN:HB3  | 5:L:138:ASN:ND2  | 2.21         | 0.54        |
| 1:T:709:DC:C2'   | 1:T:710:DG:O5'   | 2.55         | 0.54        |
| 1:T:724:DT:C2'   | 1:T:725:DG:C8    | 2.86         | 0.54        |
| 4:B:101:LYS:O    | 4:B:236:PRO:HB2  | 2.08         | 0.54        |
| 5:L:161:ASN:HB2  | 5:L:163:TRP:CH2  | 2.42         | 0.54        |
| 3:A:5:ILE:HD11   | 3:A:167:ILE:HD11 | 1.88         | 0.54        |
| 3:A:61:PHE:H     | 3:A:61:PHE:HD2   | 1.55         | 0.54        |
| 3:A:278:GLN:HG3  | 3:A:302:GLU:CB   | 2.38         | 0.54        |
| 3:A:479:LEU:HD21 | 3:A:518:VAL:HG22 | 1.88         | 0.54        |
| 3:A:49:LYS:HB2   | 3:A:49:LYS:NZ    | 2.22         | 0.54        |
| 4:B:425:LEU:O    | 4:B:427:TYR:N    | 2.38         | 0.54        |
| 2:P:812:DT:C6    | 2:P:813:DT:C7    | 2.91         | 0.54        |
| 3:A:479:LEU:O    | 3:A:521:ILE:HD11 | 2.08         | 0.54        |
| 3:A:512:LYS:HD2  | 3:A:513:SER:H    | 1.72         | 0.54        |
| 3:A:27:THR:OG1   | 3:A:29:GLU:HB3   | 2.07         | 0.54        |
| 3:A:440:PHE:CZ   | 3:A:488:ASP:O    | 2.60         | 0.54        |
| 3:A:451:LYS:O    | 3:A:471:ASN:N    | 2.39         | 0.54        |
| 5:L:23:CYS:HB2   | 5:L:35:TRP:CH2   | 2.43         | 0.54        |
| 1:T:712:DC:OP1   | 3:A:353:LYS:NZ   | 2.41         | 0.54        |
| 3:A:50:ILE:HG21  | 3:A:145:GLN:HB3  | 1.89         | 0.54        |
| 4:B:75:VAL:HG11  | 4:B:77:PHE:CZ    | 2.43         | 0.54        |
| 6:H:104:SER:O    | 6:H:106:THR:N    | 2.41         | 0.54        |
| 3:A:160:PHE:C    | 3:A:160:PHE:CD2  | 2.82         | 0.54        |
| 4:B:377:THR:O    | 4:B:381:VAL:HG23 | 2.07         | 0.54        |
| 5:L:107:LYS:HA   | 5:L:140:TYR:OH   | 2.08         | 0.54        |
| 3:A:156:SER:HB2  | 3:A:157:PRO:HD3  | 1.89         | 0.53        |
| 3:A:484:LEU:O    | 3:A:487:GLN:N    | 2.40         | 0.53        |
| 3:A:435:VAL:HG22 | 4:B:290:THR:CG2  | 2.37         | 0.53        |
| 6:H:16:GLN:O     | 6:H:87:VAL:HG22  | 2.08         | 0.53        |
| 3:A:272:PRO:O    | 3:A:273:GLY:O    | 2.26         | 0.53        |
| 3:A:493:VAL:CG2  | 3:A:494:ASN:N    | 2.71         | 0.53        |
| 4:B:112:GLY:CA   | 4:B:151:GLN:HE21 | 2.20         | 0.53        |
| 6:H:20:LEU:HD12  | 6:H:82:LEU:HD23  | 1.89         | 0.53        |
| 3:A:138:GLU:OE1  | 3:A:139:THR:HG22 | 2.08         | 0.53        |
| 4:B:368:LEU:O    | 4:B:372:VAL:HG23 | 2.09         | 0.53        |
| 1:T:715:DA:H2"   | 1:T:716:DA:C8    | 2.43         | 0.53        |
| 3:A:416:PHE:CD1  | 3:A:417:VAL:N    | 2.77         | 0.53        |
| 3:A:438:GLU:OE2  | 3:A:463:ARG:NH2  | 2.42         | 0.53        |
| 4:B:332:GLN:HA   | 4:B:332:GLN:OE1  | 2.08         | 0.53        |
| 6:H:69:LEU:HD22  | 6:H:82:LEU:HD11  | 1.90         | 0.53        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:261:VAL:O    | 3:A:264:LEU:HB2  | 2.09         | 0.53        |
| 3:A:473:THR:HG22 | 3:A:474:ASN:H    | 1.74         | 0.53        |
| 4:B:149:LEU:HD13 | 4:B:156:SER:HA   | 1.91         | 0.53        |
| 3:A:513:SER:OG   | 3:A:514:GLU:N    | 2.42         | 0.53        |
| 5:L:19:VAL:HG12  | 5:L:20:THR:N     | 2.24         | 0.53        |
| 6:H:198:TRP:CD1  | 6:H:199:PRO:HA   | 2.44         | 0.53        |
| 5:L:184:ASP:O    | 5:L:188:ARG:HD3  | 2.09         | 0.53        |
| 6:H:38:TRP:CZ3   | 6:H:97:CYS:HB3   | 2.44         | 0.53        |
| 1:T:722:DA:C4    | 1:T:723:DC:C5    | 2.97         | 0.53        |
| 3:A:450:THR:O    | 3:A:451:LYS:CG   | 2.57         | 0.53        |
| 3:A:523:GLU:HA   | 3:A:523:GLU:OE2  | 2.08         | 0.53        |
| 4:B:75:VAL:HG11  | 4:B:77:PHE:CE2   | 2.44         | 0.53        |
| 4:B:226:PRO:O    | 4:B:228:LEU:HG   | 2.08         | 0.53        |
| 4:B:260:LEU:HD21 | 4:B:303:LEU:HD13 | 1.91         | 0.53        |
| 4:B:79:GLU:O     | 4:B:83:ARG:HG2   | 2.10         | 0.52        |
| 4:B:144:TYR:N    | 4:B:144:TYR:CD2  | 2.76         | 0.52        |
| 5:L:46:LEU:HD23  | 5:L:55:HIS:ND1   | 2.23         | 0.52        |
| 1:T:711:DC:H2'   | 1:T:712:DC:C6    | 2.43         | 0.52        |
| 1:T:712:DC:H2"   | 1:T:713:DC:C5'   | 2.27         | 0.52        |
| 4:B:97:PRO:HD3   | 4:B:181:TYR:CD1  | 2.44         | 0.52        |
| 4:B:389:PHE:HB3  | 4:B:391:LEU:HD23 | 1.91         | 0.52        |
| 3:A:434:ILE:HG22 | 3:A:494:ASN:ND2  | 2.18         | 0.52        |
| 5:L:117:ILE:HD12 | 5:L:134:CYS:HB2  | 1.92         | 0.52        |
| 5:L:3:GLN:O      | 5:L:26:SER:HB2   | 2.10         | 0.52        |
| 5:L:137:ASN:HB3  | 5:L:138:ASN:HD22 | 1.75         | 0.52        |
| 3:A:439:THR:HG21 | 4:B:288:ALA:HA   | 1.91         | 0.52        |
| 3:A:69:THR:O     | 3:A:69:THR:HG22  | 2.10         | 0.52        |
| 3:A:96:HIS:ND1   | 3:A:97:PRO:CD    | 2.72         | 0.52        |
| 3:A:503:LEU:CD2  | 3:A:535:TRP:HB2  | 2.40         | 0.52        |
| 4:B:312:GLU:HB3  | 4:B:313:PRO:CD   | 2.36         | 0.52        |
| 3:A:440:PHE:HE2  | 3:A:489:SER:OG   | 1.91         | 0.52        |
| 3:A:486:LEU:CD2  | 3:A:495:ILE:HD11 | 2.39         | 0.52        |
| 5:L:159:VAL:HG22 | 5:L:179:LEU:HD12 | 1.91         | 0.52        |
| 6:H:50:LEU:O     | 6:H:51:ALA:HB2   | 2.09         | 0.52        |
| 6:H:73:LYS:HG3   | 6:H:73:LYS:O     | 2.08         | 0.52        |
| 3:A:106:VAL:CB   | 3:A:227:PHE:HE1  | 2.19         | 0.52        |
| 3:A:329:ILE:CG1  | 3:A:391:LEU:HD22 | 2.39         | 0.52        |
| 3:A:372:VAL:HG13 | 3:A:389:PHE:CE2  | 2.44         | 0.52        |
| 3:A:84:THR:HG22  | 3:A:85:GLN:O     | 2.10         | 0.52        |
| 4:B:195:ILE:HG12 | 4:B:199:ARG:CD   | 2.40         | 0.52        |
| 4:B:380:ILE:O    | 4:B:384:GLY:HA2  | 2.10         | 0.52        |



|                  | ti a             | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:10:VAL:HG13  | 4:B:87:PHE:CD1   | 2.45         | 0.51        |
| 4:B:195:ILE:CG2  | 4:B:196:GLY:N    | 2.72         | 0.51        |
| 5:L:20:THR:HA    | 5:L:73:LEU:O     | 2.09         | 0.51        |
| 3:A:101:LYS:O    | 3:A:103:LYS:HG2  | 2.10         | 0.51        |
| 4:B:121:ASP:OD1  | 4:B:121:ASP:C    | 2.49         | 0.51        |
| 4:B:295:LEU:HD22 | 4:B:300:GLU:N    | 2.25         | 0.51        |
| 3:A:368:LEU:CD2  | 3:A:393:ILE:HG21 | 2.40         | 0.51        |
| 3:A:379:SER:O    | 3:A:380:ILE:C    | 2.49         | 0.51        |
| 4:B:160:PHE:CD2  | 4:B:164:MET:HB2  | 2.45         | 0.51        |
| 4:B:306:ASN:O    | 4:B:309:ILE:HG12 | 2.11         | 0.51        |
| 5:L:60:SER:C     | 5:L:62:PHE:H     | 2.13         | 0.51        |
| 5:L:90:GLN:NE2   | 5:L:92:SER:N     | 2.46         | 0.51        |
| 3:A:258:CYS:HA   | 3:A:261:VAL:CG1  | 2.40         | 0.51        |
| 4:B:422:LEU:O    | 4:B:423:VAL:HG23 | 2.09         | 0.51        |
| 2:P:817:MRG:H2'  | 2:P:818:DC:O5'   | 2.08         | 0.51        |
| 3:A:440:PHE:HD2  | 3:A:493:VAL:HG21 | 1.76         | 0.51        |
| 4:B:195:ILE:HG12 | 4:B:199:ARG:NE   | 2.26         | 0.51        |
| 4:B:342:TYR:HB3  | 4:B:348:ASN:HA   | 1.93         | 0.51        |
| 2:P:807:DC:C4    | 2:P:808:DC:N4    | 2.79         | 0.51        |
| 3:A:27:THR:CG2   | 3:A:30:LYS:HD2   | 2.41         | 0.51        |
| 3:A:427:TYR:CZ   | 3:A:525:LEU:HD23 | 2.45         | 0.51        |
| 4:B:175:ASN:ND2  | 4:B:201:LYS:HD2  | 2.26         | 0.51        |
| 3:A:254:VAL:O    | 3:A:257:ILE:HG13 | 2.11         | 0.51        |
| 3:A:441:TYR:CD2  | 3:A:544:GLY:CA   | 2.91         | 0.51        |
| 4:B:107:THR:HG22 | 4:B:108:VAL:N    | 2.25         | 0.51        |
| 6:H:166:SER:N    | 6:H:206:ASN:ND2  | 2.29         | 0.51        |
| 3:A:27:THR:OG1   | 3:A:30:LYS:HG3   | 2.11         | 0.51        |
| 3:A:457:TYR:HA   | 3:A:548:VAL:HG13 | 1.91         | 0.51        |
| 4:B:49:LYS:O     | 4:B:50:ILE:HG23  | 2.11         | 0.51        |
| 4:B:61:PHE:CZ    | 4:B:74:LEU:HD13  | 2.46         | 0.51        |
| 6:H:68:ARG:O     | 6:H:84:MET:HA    | 2.11         | 0.51        |
| 2:P:816:DG:C2'   | 2:P:817:MRG:O5'  | 2.59         | 0.50        |
| 3:A:331:LYS:CB   | 3:A:421:PRO:HG2  | 2.26         | 0.50        |
| 4:B:178:ILE:CG2  | 4:B:179:VAL:N    | 2.73         | 0.50        |
| 4:B:393:ILE:CG1  | 4:B:394:GLN:N    | 2.74         | 0.50        |
| 5:L:124:GLN:HG2  | 5:L:129:GLY:O    | 2.10         | 0.50        |
| 5:L:150:ILE:N    | 5:L:153:SER:O    | 2.43         | 0.50        |
| 6:H:129:PRO:HB3  | 6:H:155:TYR:HB3  | 1.94         | 0.50        |
| 1:T:706:DA:C6    | 1:T:707:DG:C6    | 2.99         | 0.50        |
| 3:A:303:LEU:HD11 | 3:A:307:ARG:HD2  | 1.92         | 0.50        |
| 3:A:545:ASN:O    | 3:A:546:GLU:C    | 2.49         | 0.50        |



|                  | ti a             | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:223:LYS:NZ   | 6:H:55:TRP:CH2   | 2.79         | 0.50        |
| 1:T:714:DG:H2"   | 1:T:715:DA:OP2   | 2.10         | 0.50        |
| 1:T:715:DA:C2    | 1:T:716:DA:C5    | 2.99         | 0.50        |
| 6:H:40:ARG:HB2   | 6:H:50:LEU:CD1   | 2.42         | 0.50        |
| 3:A:303:LEU:O    | 3:A:307:ARG:HG3  | 2.11         | 0.50        |
| 3:A:443:ASP:OD1  | 3:A:478:GLU:OE1  | 2.29         | 0.50        |
| 3:A:262:GLY:HA2  | 3:A:265:ASN:HD22 | 1.76         | 0.50        |
| 3:A:416:PHE:CE1  | 3:A:417:VAL:O    | 2.63         | 0.50        |
| 3:A:486:LEU:HD21 | 3:A:495:ILE:HD11 | 1.92         | 0.50        |
| 3:A:507:GLN:O    | 3:A:509:GLN:HG3  | 2.12         | 0.50        |
| 4:B:198:HIS:O    | 4:B:199:ARG:C    | 2.49         | 0.50        |
| 6:H:102:ILE:HG12 | 6:H:108:SER:HB2  | 1.93         | 0.50        |
| 3:A:61:PHE:N     | 3:A:61:PHE:CD2   | 2.78         | 0.50        |
| 3:A:247:PRO:O    | 3:A:252:TRP:HH2  | 1.94         | 0.50        |
| 3:A:296:THR:HG22 | 3:A:297:GLU:H    | 1.77         | 0.50        |
| 3:A:403:THR:HG23 | 3:A:404:GLU:N    | 2.26         | 0.50        |
| 3:A:405:TYR:CD1  | 3:A:406:TRP:N    | 2.78         | 0.50        |
| 4:B:200:THR:HG22 | 4:B:201:LYS:N    | 2.26         | 0.50        |
| 6:H:21:THR:HG23  | 6:H:81:PHE:CE2   | 2.47         | 0.50        |
| 1:T:709:DC:H2"   | 1:T:710:DG:C5'   | 2.42         | 0.50        |
| 3:A:115:TYR:O    | 3:A:117:SER:N    | 2.44         | 0.50        |
| 4:B:2:ILE:HD12   | 4:B:2:ILE:C      | 2.31         | 0.50        |
| 4:B:12:LEU:HD11  | 4:B:127:TYR:CE2  | 2.46         | 0.50        |
| 4:B:360:ALA:HB1  | 4:B:367:GLN:HE21 | 1.77         | 0.50        |
| 3:A:139:THR:OG1  | 3:A:140:PRO:HD2  | 2.12         | 0.50        |
| 3:A:504:GLY:O    | 3:A:505:ILE:C    | 2.49         | 0.50        |
| 4:B:325:LEU:HD12 | 4:B:343:GLN:HG2  | 1.92         | 0.50        |
| 3:A:143:ARG:HG3  | 3:A:143:ARG:NH1  | 2.19         | 0.49        |
| 4:B:309:ILE:N    | 4:B:309:ILE:HD13 | 2.27         | 0.49        |
| 6:H:2:ILE:HG12   | 6:H:26:GLY:HA3   | 1.93         | 0.49        |
| 1:T:709:DC:H2"   | 1:T:710:DG:H5'   | 1.94         | 0.49        |
| 4:B:254:VAL:HB   | 4:B:289:LEU:HA   | 1.95         | 0.49        |
| 4:B:257:ILE:HB   | 4:B:283:LEU:HD21 | 1.93         | 0.49        |
| 2:P:817:MRG:H2'  | 2:P:818:DC:C6    | 2.47         | 0.49        |
| 3:A:328:GLU:HG3  | 3:A:390:LYS:HB2  | 1.94         | 0.49        |
| 3:A:425:LEU:HD13 | 3:A:509:GLN:OE1  | 2.12         | 0.49        |
| 3:A:465:LYS:HD2  | 3:A:467:VAL:HG13 | 1.94         | 0.49        |
| 6:H:122:SER:HB3  | 6:H:156:PHE:CZ   | 2.47         | 0.49        |
| 3:A:60:VAL:O     | 3:A:60:VAL:HG13  | 2.12         | 0.49        |
| 3:A:227:PHE:HB2  | 3:A:234:LEU:HB2  | 1.93         | 0.49        |
| 3:A:416:PHE:HD1  | 3:A:417:VAL:N    | 2.09         | 0.49        |



|                  |                  | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:325:LEU:HD22 | 4:B:385:LYS:HG2  | 1.93         | 0.49        |
| 3:A:106:VAL:HB   | 3:A:227:PHE:CE1  | 2.33         | 0.49        |
| 3:A:121:ASP:OD1  | 3:A:123:ASP:N    | 2.45         | 0.49        |
| 3:A:353:LYS:HD2  | 3:A:353:LYS:O    | 2.12         | 0.49        |
| 4:B:244:ILE:HD13 | 4:B:244:ILE:N    | 2.03         | 0.49        |
| 1:T:713:DC:C2'   | 1:T:714:DG:O5'   | 2.61         | 0.49        |
| 4:B:46:LYS:CD    | 4:B:116:PHE:HB3  | 2.42         | 0.49        |
| 3:A:283:LEU:N    | 3:A:283:LEU:HD23 | 2.28         | 0.49        |
| 3:A:523:GLU:O    | 3:A:526:ILE:HG22 | 2.12         | 0.49        |
| 4:B:221:HIS:HA   | 4:B:229:TRP:CD1  | 2.48         | 0.49        |
| 4:B:394:GLN:O    | 4:B:395:LYS:C    | 2.49         | 0.49        |
| 6:H:12:VAL:HG12  | 6:H:13:GLN:O     | 2.11         | 0.49        |
| 3:A:338:THR:CG2  | 3:A:339:TYR:N    | 2.75         | 0.49        |
| 3:A:407:GLN:HG3  | 4:B:393:ILE:HA   | 1.94         | 0.49        |
| 3:A:478:GLU:HG2  | 3:A:499:SER:HB3  | 1.95         | 0.49        |
| 3:A:485:ALA:O    | 3:A:489:SER:HB2  | 2.13         | 0.49        |
| 3:A:501:TYR:CE1  | 3:A:505:ILE:CD1  | 2.92         | 0.49        |
| 4:B:113:ASP:O    | 4:B:114:ALA:C    | 2.50         | 0.49        |
| 4:B:344:GLU:HA   | 4:B:344:GLU:OE2  | 2.13         | 0.49        |
| 5:L:61:ARG:HG2   | 5:L:61:ARG:NH1   | 2.27         | 0.49        |
| 5:L:89:GLN:HA    | 5:L:97:THR:O     | 2.12         | 0.49        |
| 5:L:117:ILE:CD1  | 5:L:194:CYS:HB2  | 2.42         | 0.49        |
| 3:A:221:HIS:N    | 3:A:221:HIS:CD2  | 2.80         | 0.49        |
| 3:A:329:ILE:HG12 | 3:A:391:LEU:CD2  | 2.41         | 0.49        |
| 4:B:260:LEU:HD11 | 4:B:264:LEU:HD11 | 1.95         | 0.49        |
| 1:T:713:DC:H2"   | 1:T:714:DG:C5'   | 2.43         | 0.48        |
| 3:A:232:TYR:N    | 3:A:232:TYR:CD1  | 2.81         | 0.48        |
| 3:A:257:ILE:CG2  | 3:A:283:LEU:HD21 | 2.40         | 0.48        |
| 3:A:517:LEU:HD13 | 3:A:521:ILE:HG13 | 1.93         | 0.48        |
| 4:B:286:THR:OG1  | 4:B:286:THR:O    | 2.30         | 0.48        |
| 4:B:87:PHE:HD2   | 4:B:88:TRP:HB3   | 1.77         | 0.48        |
| 5:L:146:VAL:HA   | 5:L:195:GLU:O    | 2.12         | 0.48        |
| 6:H:162:VAL:HA   | 6:H:206:ASN:O    | 2.13         | 0.48        |
| 2:P:820:DC:C2'   | 2:P:821:DC:O5'   | 2.61         | 0.48        |
| 3:A:501:TYR:HD1  | 3:A:501:TYR:O    | 1.95         | 0.48        |
| 4:B:282:LEU:N    | 4:B:282:LEU:HD23 | 2.27         | 0.48        |
| 4:B:403:THR:O    | 4:B:406:TRP:N    | 2.40         | 0.48        |
| 1:T:705:DT:H2"   | 1:T:706:DA:O5'   | 2.14         | 0.48        |
| 3:A:261:VAL:HA   | 3:A:264:LEU:HD12 | 1.96         | 0.48        |
| 3:A:329:ILE:HG13 | 3:A:391:LEU:HD22 | 1.94         | 0.48        |
| 4:B:406:TRP:O    | 4:B:407:GLN:NE2  | 2.47         | 0.48        |



|                  |                  | Interatomic             | Clash       |
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| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 3:A:225:PRO:HA   | 3:A:226:PRO:C    | 2.33                    | 0.48        |
| 4:B:47:ILE:HD12  | 4:B:47:ILE:HA    | 1.65                    | 0.48        |
| 6:H:39:ILE:HG23  | 6:H:48:GLU:O     | 2.13                    | 0.48        |
| 6:H:65:LEU:O     | 6:H:67:SER:N     | 2.46                    | 0.48        |
| 3:A:342:TYR:HD2  | 3:A:344:GLU:O    | 1.96                    | 0.48        |
| 5:L:190:ASN:O    | 5:L:210:ASN:HA   | 2.13                    | 0.48        |
| 3:A:50:ILE:HG23  | 3:A:145:GLN:HB3  | 1.96                    | 0.48        |
| 3:A:339:TYR:CZ   | 3:A:352:GLY:HA3  | 2.49                    | 0.48        |
| 3:A:533:LEU:N    | 3:A:533:LEU:CD1  | 2.77                    | 0.48        |
| 4:B:262:GLY:O    | 4:B:263:LYS:C    | 2.52                    | 0.48        |
| 6:H:34:ILE:H     | 6:H:34:ILE:CD1   | 2.25                    | 0.48        |
| 3:A:253:THR:HA   | 3:A:292:VAL:HA   | 1.96                    | 0.48        |
| 4:B:125:ARG:HD3  | 4:B:147:ASN:HA   | 1.95                    | 0.48        |
| 4:B:131:THR:CG2  | 4:B:132:ILE:N    | 2.76                    | 0.48        |
| 3:A:143:ARG:HH11 | 3:A:143:ARG:CG   | 2.21                    | 0.48        |
| 3:A:491:LEU:HD23 | 3:A:529:GLU:OE1  | 2.13                    | 0.48        |
| 4:B:165:THR:HG23 | 4:B:166:LYS:N    | 2.29                    | 0.48        |
| 4:B:423:VAL:HG12 | 4:B:425:LEU:H    | 1.78                    | 0.48        |
| 5:L:151:ASP:O    | 5:L:153:SER:N    | 2.38                    | 0.48        |
| 3:A:112:GLY:O    | 3:A:215:THR:HG23 | 2.14                    | 0.47        |
| 3:A:331:LYS:HD3  | 3:A:332:GLN:H    | 1.79                    | 0.47        |
| 4:B:96:HIS:HE1   | 4:B:380:ILE:O    | 1.96                    | 0.47        |
| 4:B:193:LEU:N    | 4:B:193:LEU:HD23 | 2.28                    | 0.47        |
| 3:A:493:VAL:C    | 3:A:494:ASN:HD22 | 2.17                    | 0.47        |
| 4:B:113:ASP:O    | 4:B:116:PHE:N    | 2.43                    | 0.47        |
| 4:B:223:LYS:HE3  | 6:H:58:ASP:HB3   | 1.96                    | 0.47        |
| 4:B:113:ASP:C    | 4:B:115:TYR:N    | 2.66                    | 0.47        |
| 4:B:254:VAL:HB   | 4:B:289:LEU:O    | 2.14                    | 0.47        |
| 5:L:83:ILE:HG21  | 5:L:106:ILE:CG1  | 2.42                    | 0.47        |
| 4:B:156:SER:O    | 4:B:158:ALA:N    | 2.48                    | 0.47        |
| 4:B:306:ASN:CA   | 4:B:309:ILE:HG12 | 2.43                    | 0.47        |
| 5:L:35:TRP:CE3   | 5:L:88:CYS:HB3   | 2.50                    | 0.47        |
| 5:L:105:GLU:OE2  | 5:L:173:TYR:OH   | 2.32                    | 0.47        |
| 3:A:344:GLU:HB3  | 3:A:345:PRO:CD   | 2.43                    | 0.47        |
| 3:A:511:ASP:OD2  | 3:A:511:ASP:O    | 2.31                    | 0.47        |
| 4:B:210:LEU:HD12 | 4:B:210:LEU:HA   | 1.59                    | 0.47        |
| 4:B:244:ILE:HD11 | 4:B:271:TYR:CE2  | 2.50                    | 0.47        |
| 4:B:302:GLU:HA   | 4:B:305:GLU:CB   | 2.44                    | 0.47        |
| 6:H:53:ILE:HG23  | 6:H:53:ILE:O     | 2.15                    | 0.47        |
| 1:T:715:DA:N3    | 1:T:716:DA:C5    | 2.82                    | 0.47        |
| 3:A:128:THR:OG1  | 3:A:146:TYR:HB2  | 2.15                    | 0.47        |



|                  | loub page        | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:169:GLU:HB3  | 3:A:170:PRO:HD3  | 1.97         | 0.47        |
| 3:A:265:ASN:HA   | 3:A:268:SER:OG   | 2.14         | 0.47        |
| 3:A:439:THR:CG2  | 4:B:289:LEU:H    | 2.09         | 0.47        |
| 3:A:473:THR:CG2  | 3:A:474:ASN:N    | 2.77         | 0.47        |
| 3:A:478:GLU:OE1  | 3:A:498:ASP:CG   | 2.53         | 0.47        |
| 4:B:244:ILE:HD11 | 4:B:271:TYR:CZ   | 2.50         | 0.47        |
| 4:B:291:GLU:HG2  | 4:B:293:ILE:CD1  | 2.45         | 0.47        |
| 4:B:320:ASP:N    | 4:B:343:GLN:OE1  | 2.40         | 0.47        |
| 4:B:332:GLN:NE2  | 4:B:426:TRP:O    | 2.48         | 0.47        |
| 5:L:167:ASP:OD2  | 5:L:167:ASP:C    | 2.53         | 0.47        |
| 6:H:32:SER:O     | 6:H:55:TRP:CE2   | 2.68         | 0.47        |
| 6:H:134:LEU:HB2  | 6:H:149:GLY:CA   | 2.45         | 0.47        |
| 6:H:155:TYR:N    | 6:H:155:TYR:CD2  | 2.83         | 0.47        |
| 3:A:87:PHE:N     | 3:A:87:PHE:CD2   | 2.83         | 0.47        |
| 3:A:442:VAL:HG12 | 3:A:481:ALA:HB1  | 1.95         | 0.47        |
| 4:B:57:ASN:ND2   | 4:B:58:THR:N     | 2.62         | 0.47        |
| 4:B:166:LYS:O    | 4:B:168:LEU:N    | 2.48         | 0.47        |
| 4:B:329:ILE:HA   | 4:B:338:THR:O    | 2.15         | 0.47        |
| 4:B:12:LEU:H     | 4:B:12:LEU:CD1   | 1.99         | 0.47        |
| 4:B:13:LYS:HE2   | 4:B:85:GLN:HB3   | 1.96         | 0.47        |
| 4:B:207:GLN:O    | 4:B:210:LEU:N    | 2.48         | 0.47        |
| 5:L:151:ASP:C    | 5:L:153:SER:H    | 2.15         | 0.47        |
| 3:A:27:THR:O     | 3:A:30:LYS:N     | 2.45         | 0.47        |
| 4:B:101:LYS:HG3  | 4:B:102:LYS:HG3  | 1.97         | 0.47        |
| 5:L:131:SER:HA   | 5:L:179:LEU:O    | 2.15         | 0.47        |
| 5:L:132:VAL:HG12 | 5:L:148:TRP:HH2  | 1.80         | 0.47        |
| 3:A:253:THR:O    | 3:A:254:VAL:C    | 2.53         | 0.46        |
| 3:A:498:ASP:OD1  | 3:A:498:ASP:N    | 2.47         | 0.46        |
| 4:B:56:TYR:O     | 4:B:143:ARG:NH2  | 2.47         | 0.46        |
| 3:A:153:TRP:CZ3  | 3:A:155:GLY:HA3  | 2.50         | 0.46        |
| 3:A:181:TYR:CD2  | 4:B:138:GLU:HG3  | 2.50         | 0.46        |
| 3:A:430:GLU:HG2  | 3:A:531:VAL:O    | 2.15         | 0.46        |
| 3:A:536:VAL:HG13 | 3:A:542:ILE:HG13 | 1.98         | 0.46        |
| 4:B:420:PRO:HB3  | 4:B:421:PRO:HD2  | 1.96         | 0.46        |
| 6:H:174:HIS:O    | 6:H:189:SER:HA   | 2.15         | 0.46        |
| 3:A:27:THR:C     | 3:A:29:GLU:N     | 2.66         | 0.46        |
| 3:A:115:TYR:CE2  | 3:A:156:SER:HB3  | 2.50         | 0.46        |
| 3:A:389:PHE:HB3  | 3:A:391:LEU:HD21 | 1.98         | 0.46        |
| 3:A:475:GLN:HB3  | 3:A:501:TYR:HE2  | 1.78         | 0.46        |
| 4:B:47:ILE:CD1   | 4:B:146:TYR:HA   | 2.43         | 0.46        |
| 3:A:90:VAL:HG12  | 4:B:140:PRO:HB3  | 1.97         | 0.46        |



|                  | ti a             | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 3:A:260:LEU:HD23 | 3:A:279:LEU:HD12 | 1.96         | 0.46        |
| 4:B:229:TRP:HA   | 4:B:232:TYR:CZ   | 2.49         | 0.46        |
| 1:T:716:DA:H1'   | 1:T:717:DC:H5'   | 1.97         | 0.46        |
| 3:A:116:PHE:N    | 3:A:116:PHE:CD1  | 2.83         | 0.46        |
| 3:A:306:ASN:O    | 3:A:307:ARG:C    | 2.54         | 0.46        |
| 3:A:460:ASN:ND2  | 4:B:288:ALA:HB2  | 2.25         | 0.46        |
| 4:B:69:THR:HG22  | 4:B:69:THR:O     | 2.16         | 0.46        |
| 4:B:166:LYS:O    | 4:B:167:ILE:C    | 2.54         | 0.46        |
| 4:B:360:ALA:CB   | 4:B:367:GLN:HE21 | 2.29         | 0.46        |
| 5:L:150:ILE:HG22 | 5:L:192:TYR:CD2  | 2.50         | 0.46        |
| 4:B:225:PRO:HB2  | 4:B:226:PRO:CD   | 2.35         | 0.46        |
| 5:L:63:SER:O     | 5:L:73:LEU:HD12  | 2.16         | 0.46        |
| 5:L:105:GLU:HB3  | 5:L:106:ILE:H    | 1.62         | 0.46        |
| 3:A:140:PRO:O    | 3:A:141:GLY:O    | 2.33         | 0.46        |
| 3:A:459:THR:HG21 | 3:A:463:ARG:HB3  | 1.91         | 0.46        |
| 4:B:85:GLN:C     | 4:B:87:PHE:N     | 2.66         | 0.46        |
| 4:B:202:ILE:O    | 4:B:205:LEU:N    | 2.48         | 0.46        |
| 5:L:15:LEU:H     | 5:L:15:LEU:CD1   | 2.19         | 0.46        |
| 5:L:176:SER:HB2  | 6:H:176:PHE:CD1  | 2.51         | 0.46        |
| 6:H:152:VAL:HB   | 6:H:187:LEU:HD12 | 1.98         | 0.46        |
| 1:T:706:DA:C6    | 1:T:707:DG:O6    | 2.69         | 0.46        |
| 2:P:815:DG:C6    | 2:P:816:DG:C6    | 3.04         | 0.46        |
| 3:A:86:ASP:OD2   | 3:A:86:ASP:N     | 2.48         | 0.46        |
| 3:A:90:VAL:CG1   | 4:B:141:GLY:N    | 2.75         | 0.46        |
| 4:B:279:LEU:HD12 | 4:B:279:LEU:N    | 2.31         | 0.46        |
| 3:A:494:ASN:HB3  | 4:B:289:LEU:CD1  | 2.45         | 0.46        |
| 4:B:111:VAL:O    | 4:B:111:VAL:CG2  | 2.59         | 0.46        |
| 4:B:414:TRP:CD1  | 4:B:414:TRP:C    | 2.89         | 0.46        |
| 6:H:18:PHE:CD2   | 6:H:87:VAL:HG11  | 2.50         | 0.46        |
| 6:H:208:ALA:HB2  | 6:H:215:LYS:HD2  | 1.98         | 0.46        |
| 3:A:296:THR:O    | 3:A:300:GLU:HB2  | 2.15         | 0.46        |
| 3:A:317:VAL:HG13 | 3:A:349:LEU:HD23 | 1.97         | 0.46        |
| 4:B:280:SER:O    | 4:B:283:LEU:HD12 | 2.16         | 0.46        |
| 4:B:55:PRO:HG2   | 4:B:56:TYR:CE1   | 2.51         | 0.45        |
| 4:B:343:GLN:HG3  | 4:B:349:LEU:HD11 | 1.98         | 0.45        |
| 5:L:148:TRP:CE3  | 5:L:179:LEU:HD22 | 2.50         | 0.45        |
| 2:P:805:DG:C6    | 2:P:806:DT:C4    | 3.05         | 0.45        |
| 3:A:132:ILE:O    | 3:A:132:ILE:HG12 | 2.17         | 0.45        |
| 3:A:223:LYS:C    | 3:A:225:PRO:HD2  | 2.36         | 0.45        |
| 3:A:484:LEU:C    | 3:A:486:LEU:N    | 2.70         | 0.45        |
| 4:B:115:TYR:OH   | 4:B:157:PRO:HB3  | 2.16         | 0.45        |



|                  | A h O            | Interatomic  | Clash       |
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| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 5:L:188:ARG:O    | 5:L:189:HIS:CG   | 2.70         | 0.45        |
| 2:P:805:DG:H2"   | 2:P:806:DT:OP2   | 2.17         | 0.45        |
| 3:A:180:ILE:HA   | 3:A:188:TYR:O    | 2.16         | 0.45        |
| 4:B:307:ARG:HG3  | 4:B:308:GLU:N    | 2.30         | 0.45        |
| 4:B:372:VAL:HG13 | 4:B:389:PHE:CE2  | 2.51         | 0.45        |
| 3:A:125:ARG:HB3  | 3:A:145:GLN:HG3  | 1.98         | 0.45        |
| 3:A:420:PRO:HB3  | 3:A:421:PRO:HA   | 1.98         | 0.45        |
| 3:A:473:THR:CG2  | 3:A:474:ASN:H    | 2.28         | 0.45        |
| 4:B:23:GLN:HG2   | 4:B:133:PRO:HG3  | 1.99         | 0.45        |
| 4:B:296:THR:HG22 | 4:B:297:GLU:N    | 2.31         | 0.45        |
| 6:H:65:LEU:O     | 6:H:66:LYS:C     | 2.54         | 0.45        |
| 5:L:125:LEU:CD2  | 5:L:130:ALA:HB2  | 2.46         | 0.45        |
| 1:T:706:DA:H2'   | 1:T:707:DG:H8    | 1.78         | 0.45        |
| 3:A:23:GLN:HE22  | 3:A:60:VAL:H     | 1.64         | 0.45        |
| 4:B:252:TRP:HB2  | 4:B:257:ILE:HD11 | 1.99         | 0.45        |
| 3:A:41:MET:HE1   | 3:A:73:LYS:HD3   | 1.99         | 0.45        |
| 3:A:379:SER:O    | 3:A:381:VAL:N    | 2.49         | 0.45        |
| 3:A:531:VAL:HG12 | 3:A:532:TYR:N    | 2.32         | 0.45        |
| 5:L:179:LEU:HD23 | 5:L:181:LEU:HD11 | 1.98         | 0.45        |
| 3:A:175:ASN:HB3  | 3:A:178:ILE:HD12 | 1.98         | 0.45        |
| 3:A:354:TYR:HD2  | 3:A:354:TYR:HA   | 1.50         | 0.45        |
| 3:A:416:PHE:HE1  | 3:A:417:VAL:O    | 2.00         | 0.45        |
| 5:L:77:ASN:HD22  | 5:L:77:ASN:H     | 1.64         | 0.45        |
| 6:H:164:TRP:CH2  | 6:H:205:CYS:HB2  | 2.51         | 0.45        |
| 3:A:222:GLN:O    | 3:A:224:GLU:HG3  | 2.17         | 0.45        |
| 3:A:326:ILE:O    | 3:A:341:ILE:HA   | 2.16         | 0.45        |
| 3:A:447:ASN:HB3  | 3:A:450:THR:OG1  | 2.17         | 0.45        |
| 4:B:87:PHE:HD2   | 4:B:88:TRP:N     | 2.13         | 0.45        |
| 4:B:116:PHE:HA   | 4:B:148:VAL:HG21 | 1.99         | 0.45        |
| 4:B:369:THR:O    | 4:B:373:GLN:HG3  | 2.17         | 0.45        |
| 4:B:424:LYS:HD2  | 4:B:424:LYS:HA   | 1.86         | 0.45        |
| 3:A:132:ILE:CG2  | 3:A:142:ILE:HB   | 2.44         | 0.45        |
| 3:A:246:LEU:HD12 | 3:A:307:ARG:HE   | 1.82         | 0.45        |
| 4:B:23:GLN:NE2   | 4:B:60:VAL:O     | 2.44         | 0.45        |
| 3:A:454:LYS:HB2  | 3:A:552:VAL:HG13 | 1.98         | 0.44        |
| 3:A:539:HIS:N    | 3:A:539:HIS:CD2  | 2.83         | 0.44        |
| 6:H:163:THR:O    | 6:H:206:ASN:HB2  | 2.18         | 0.44        |
| 3:A:327:ALA:HB3  | 3:A:389:PHE:CD1  | 2.53         | 0.44        |
| 3:A:369:THR:HG22 | 3:A:370:GLU:N    | 2.31         | 0.44        |
| 3:A:397:THR:CG2  | 3:A:424:LYS:HA   | 2.44         | 0.44        |
| 3:A:410:TRP:CD2  | 4:B:363:ASN:OD1  | 2.70         | 0.44        |



|                  | 1                | Interatomic             | Clash       |
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| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 3:A:455:ALA:HA   | 3:A:552:VAL:HG11 | 1.98                    | 0.44        |
| 4:B:193:LEU:HD13 | 4:B:197:GLN:OE1  | 2.17                    | 0.44        |
| 4:B:200:THR:O    | 4:B:202:ILE:N    | 2.50                    | 0.44        |
| 4:B:291:GLU:O    | 4:B:293:ILE:HD13 | 2.16                    | 0.44        |
| 4:B:320:ASP:O    | 4:B:343:GLN:NE2  | 2.40                    | 0.44        |
| 5:L:66:GLY:HA3   | 5:L:71:TYR:CG    | 2.51                    | 0.44        |
| 6:H:89:THR:HA    | 6:H:121:VAL:HB   | 1.99                    | 0.44        |
| 3:A:498:ASP:OD2  | 3:A:538:ALA:HB2  | 2.17                    | 0.44        |
| 4:B:44:GLU:OE1   | 4:B:46:LYS:NZ    | 2.33                    | 0.44        |
| 5:L:121:SER:O    | 5:L:122:SER:C    | 2.55                    | 0.44        |
| 5:L:118:PHE:HA   | 5:L:119:PRO:HD3  | 1.77                    | 0.44        |
| 5:L:136:LEU:HD12 | 5:L:136:LEU:N    | 2.33                    | 0.44        |
| 6:H:129:PRO:HB2  | 6:H:152:VAL:HG12 | 1.98                    | 0.44        |
| 3:A:94:ILE:HG13  | 3:A:95:PRO:O     | 2.17                    | 0.44        |
| 3:A:116:PHE:N    | 3:A:116:PHE:HD1  | 2.15                    | 0.44        |
| 3:A:257:ILE:HG21 | 3:A:283:LEU:CD2  | 2.42                    | 0.44        |
| 3:A:372:VAL:HG13 | 3:A:389:PHE:CZ   | 2.53                    | 0.44        |
| 3:A:486:LEU:HD21 | 3:A:495:ILE:CD1  | 2.48                    | 0.44        |
| 3:A:509:GLN:N    | 3:A:510:PRO:CD   | 2.80                    | 0.44        |
| 3:A:532:TYR:C    | 3:A:533:LEU:HD12 | 2.37                    | 0.44        |
| 4:B:327:ALA:HA   | 4:B:340:GLN:O    | 2.17                    | 0.44        |
| 4:B:366:LYS:O    | 4:B:370:GLU:HG3  | 2.17                    | 0.44        |
| 5:L:18:ARG:HA    | 5:L:76:SER:O     | 2.17                    | 0.44        |
| 5:L:77:ASN:N     | 5:L:77:ASN:ND2   | 2.66                    | 0.44        |
| 4:B:58:THR:CG2   | 4:B:59:PRO:CD    | 2.95                    | 0.44        |
| 4:B:369:THR:HG22 | 4:B:398:TRP:HZ3  | 1.80                    | 0.44        |
| 5:L:189:HIS:O    | 5:L:211:ARG:NE   | 2.50                    | 0.44        |
| 1:T:714:DG:OP1   | 3:A:285:GLY:N    | 2.42                    | 0.44        |
| 2:P:812:DT:C5    | 2:P:813:DT:H73   | 2.53                    | 0.44        |
| 3:A:373:GLN:HE22 | 4:B:397:THR:HG23 | 1.81                    | 0.44        |
| 3:A:385:LYS:HZ2  | 3:A:385:LYS:CB   | 2.31                    | 0.44        |
| 4:B:314:VAL:CG1  | 4:B:315:HIS:H    | 2.29                    | 0.44        |
| 4:B:330:GLN:HG2  | 4:B:338:THR:OG1  | 2.17                    | 0.44        |
| 4:B:401:TRP:O    | 4:B:402:TRP:C    | 2.53                    | 0.44        |
| 5:L:186:TYR:C    | 5:L:188:ARG:H    | 2.21                    | 0.44        |
| 2:P:814:DC:H2"   | 2:P:815:DG:C8    | 2.53                    | 0.44        |
| 3:A:195:ILE:HG22 | 3:A:195:ILE:O    | 2.18                    | 0.44        |
| 3:A:269:GLN:HA   | 3:A:351:THR:O    | 2.18                    | 0.44        |
| 3:A:354:TYR:CE1  | 3:A:374:LYS:CB   | 2.90                    | 0.44        |
| 3:A:365:VAL:O    | 3:A:366:LYS:C    | 2.56                    | 0.44        |
| 3:A:442:VAL:HG22 | 3:A:495:ILE:HG22 | 1.99                    | 0.44        |



|                  | ti a             | Interatomic  | Clash       |
|------------------|------------------|--------------|-------------|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |
| 4:B:2:ILE:HG23   | 4:B:3:SER:N      | 2.32         | 0.44        |
| 4:B:47:ILE:CG2   | 4:B:144:TYR:HD1  | 2.31         | 0.44        |
| 4:B:56:TYR:O     | 4:B:57:ASN:HB2   | 2.17         | 0.44        |
| 4:B:103:LYS:HD3  | 4:B:192:ASP:OD1  | 2.18         | 0.44        |
| 4:B:295:LEU:HD23 | 4:B:299:ALA:CB   | 2.47         | 0.44        |
| 5:L:144:ILE:HG13 | 5:L:198:HIS:ND1  | 2.32         | 0.44        |
| 3:A:442:VAL:HG23 | 3:A:496:VAL:O    | 2.18         | 0.43        |
| 4:B:135:ILE:HD12 | 4:B:135:ILE:O    | 2.18         | 0.43        |
| 4:B:214:LEU:HD12 | 4:B:214:LEU:N    | 2.33         | 0.43        |
| 4:B:225:PRO:CB   | 4:B:226:PRO:CD   | 2.96         | 0.43        |
| 5:L:58:VAL:HG13  | 5:L:59:PRO:HD2   | 2.00         | 0.43        |
| 3:A:460:ASN:HD22 | 4:B:288:ALA:CB   | 2.28         | 0.43        |
| 3:A:500:GLN:NE2  | 3:A:500:GLN:N    | 2.53         | 0.43        |
| 6:H:53:ILE:HD13  | 6:H:73:LYS:HB3   | 2.00         | 0.43        |
| 4:B:363:ASN:HD22 | 4:B:363:ASN:C    | 2.21         | 0.43        |
| 5:L:4:MET:SD     | 5:L:25:ALA:HA    | 2.58         | 0.43        |
| 5:L:90:GLN:NE2   | 5:L:93:LYS:H     | 2.15         | 0.43        |
| 3:A:138:GLU:O    | 3:A:139:THR:O    | 2.36         | 0.43        |
| 3:A:339:TYR:CD2  | 3:A:375:ILE:HD11 | 2.53         | 0.43        |
| 4:B:106:VAL:HG13 | 4:B:234:LEU:CB   | 2.46         | 0.43        |
| 4:B:115:TYR:CD1  | 4:B:156:SER:HB3  | 2.53         | 0.43        |
| 4:B:403:THR:O    | 4:B:404:GLU:C    | 2.56         | 0.43        |
| 6:H:126:THR:HA   | 6:H:156:PHE:O    | 2.18         | 0.43        |
| 3:A:296:THR:O    | 3:A:300:GLU:N    | 2.51         | 0.43        |
| 3:A:438:GLU:CD   | 3:A:463:ARG:HH21 | 2.22         | 0.43        |
| 3:A:459:THR:HG22 | 3:A:463:ARG:N    | 2.33         | 0.43        |
| 4:B:72:ARG:HG3   | 4:B:73:LYS:O     | 2.19         | 0.43        |
| 3:A:180:ILE:HG23 | 3:A:189:VAL:HG22 | 2.00         | 0.43        |
| 3:A:367:GLN:O    | 3:A:368:LEU:C    | 2.55         | 0.43        |
| 3:A:398:TRP:O    | 3:A:401:TRP:N    | 2.52         | 0.43        |
| 4:B:24:TRP:O     | 4:B:25:PRO:C     | 2.56         | 0.43        |
| 4:B:148:VAL:O    | 4:B:149:LEU:C    | 2.56         | 0.43        |
| 4:B:357:MET:HG3  | 4:B:370:GLU:OE1  | 2.18         | 0.43        |
| 2:P:819:DG:H2"   | 2:P:820:DC:C5'   | 2.47         | 0.43        |
| 3:A:401:TRP:CZ2  | 3:A:405:TYR:CD2  | 3.06         | 0.43        |
| 3:A:457:TYR:HA   | 3:A:548:VAL:HG11 | 1.99         | 0.43        |
| 4:B:2:ILE:HG23   | 4:B:3:SER:H      | 1.84         | 0.43        |
| 4:B:207:GLN:O    | 4:B:208:HIS:C    | 2.57         | 0.43        |
| 4:B:221:HIS:HB3  | 4:B:229:TRP:CE2  | 2.53         | 0.43        |
| 1:T:709:DC:H2"   | 1:T:710:DG:O5'   | 2.18         | 0.43        |
| 3:A:63:ILE:HG13  | 3:A:64:LYS:N     | 2.34         | 0.43        |



|                  |                 | Interatomic  | Clash       |
|------------------|-----------------|--------------|-------------|
| Atom-1           | Atom-2          | distance (Å) | overlap (Å) |
| 3:A:137:ASN:OD1  | 3:A:137:ASN:O   | 2.36         | 0.43        |
| 5:L:82:ASP:O     | 5:L:84:ALA:N    | 2.52         | 0.43        |
| 3:A:303:LEU:HD12 | 3:A:307:ARG:HG3 | 2.01         | 0.43        |
| 4:B:146:TYR:CG   | 4:B:150:PRO:HB3 | 2.54         | 0.43        |
| 4:B:246:LEU:HD12 | 4:B:307:ARG:HA  | 2.00         | 0.43        |
| 5:L:21:ILE:O     | 5:L:72:SER:HA   | 2.18         | 0.43        |
| 5:L:34:ASN:HB2   | 5:L:89:GLN:HE21 | 1.80         | 0.43        |
| 6:H:84:MET:HG2   | 6:H:87:VAL:HG12 | 2.00         | 0.43        |
| 1:T:705:DT:H2"   | 1:T:706:DA:H8   | 1.84         | 0.43        |
| 2:P:808:DC:H2"   | 2:P:809:DC:O5'  | 2.19         | 0.43        |
| 4:B:101:LYS:O    | 4:B:236:PRO:CB  | 2.67         | 0.43        |
| 4:B:156:SER:N    | 4:B:157:PRO:HD2 | 2.34         | 0.43        |
| 5:L:83:ILE:HG23  | 5:L:105:GLU:O   | 2.18         | 0.43        |
| 3:A:484:LEU:O    | 3:A:485:ALA:C   | 2.57         | 0.42        |
| 4:B:144:TYR:N    | 4:B:144:TYR:HD2 | 2.16         | 0.42        |
| 4:B:175:ASN:HD21 | 4:B:201:LYS:CE  | 2.32         | 0.42        |
| 4:B:266:TRP:CZ3  | 4:B:422:LEU:HB3 | 2.53         | 0.42        |
| 4:B:350:LYS:HE2  | 4:B:378:GLU:OE1 | 2.18         | 0.42        |
| 6:H:148:LEU:HD13 | 6:H:220:ILE:CG2 | 2.43         | 0.42        |
| 1:T:715:DA:H2"   | 1:T:716:DA:OP2  | 2.19         | 0.42        |
| 3:A:188:TYR:CD1  | 3:A:188:TYR:C   | 2.91         | 0.42        |
| 3:A:260:LEU:O    | 3:A:261:VAL:C   | 2.57         | 0.42        |
| 3:A:498:ASP:CB   | 3:A:538:ALA:HB2 | 2.49         | 0.42        |
| 4:B:210:LEU:C    | 4:B:212:TRP:N   | 2.72         | 0.42        |
| 4:B:270:ILE:HB   | 4:B:271:TYR:CD2 | 2.54         | 0.42        |
| 4:B:296:THR:HG22 | 4:B:298:GLU:N   | 2.15         | 0.42        |
| 4:B:425:LEU:C    | 4:B:427:TYR:N   | 2.73         | 0.42        |
| 6:H:99:GLN:OE1   | 6:H:99:GLN:O    | 2.37         | 0.42        |
| 3:A:344:GLU:OE1  | 3:A:344:GLU:HA  | 2.18         | 0.42        |
| 4:B:181:TYR:HB3  | 4:B:188:TYR:HB2 | 2.01         | 0.42        |
| 5:L:195:GLU:HG3  | 5:L:206:VAL:CG2 | 2.41         | 0.42        |
| 6:H:55:TRP:CE3   | 6:H:55:TRP:N    | 2.88         | 0.42        |
| 6:H:69:LEU:CD2   | 6:H:84:MET:HE2  | 2.49         | 0.42        |
| 6:H:156:PHE:HA   | 6:H:157:PRO:HA  | 1.74         | 0.42        |
| 3:A:367:GLN:HA   | 3:A:370:GLU:CG  | 2.50         | 0.42        |
| 4:B:37:ILE:HG13  | 4:B:37:ILE:O    | 2.19         | 0.42        |
| 4:B:47:ILE:HG23  | 4:B:144:TYR:CD1 | 2.53         | 0.42        |
| 4:B:260:LEU:O    | 4:B:260:LEU:CD1 | 2.67         | 0.42        |
| 5:L:170:ASP:C    | 5:L:170:ASP:OD1 | 2.57         | 0.42        |
| 3:A:3:SER:HB3    | 3:A:5:ILE:CG1   | 2.48         | 0.42        |
| 3:A:241:VAL:HG13 | 3:A:241:VAL:O   | 2.19         | 0.42        |



|                  | A i a            | Interatomic  | Clash       |  |
|------------------|------------------|--------------|-------------|--|
| Atom-1           | Atom-2           | distance (Å) | overlap (Å) |  |
| 3:A:463:ARG:CG   | 3:A:464:GLN:N    | 2.82         | 0.42        |  |
| 4:B:329:ILE:O    | 4:B:392:PRO:HG3  | 2.18         | 0.42        |  |
| 5:L:179:LEU:CD2  | 5:L:181:LEU:HD11 | 2.50         | 0.42        |  |
| 2:P:815:DG:C6    | 2:P:816:DG:O6    | 2.72         | 0.42        |  |
| 3:A:46:LYS:HD3   | 3:A:46:LYS:N     | 2.34         | 0.42        |  |
| 3:A:85:GLN:O     | 3:A:154:LYS:NZ   | 2.51         | 0.42        |  |
| 4:B:8:VAL:HA     | 4:B:9:PRO:HD3    | 1.78         | 0.42        |  |
| 6:H:9:PRO:O      | 6:H:11:ILE:N     | 2.46         | 0.42        |  |
| 6:H:122:SER:HB3  | 6:H:156:PHE:HZ   | 1.84         | 0.42        |  |
| 6:H:128:PRO:HA   | 6:H:209:HIS:CD2  | 2.54         | 0.42        |  |
| 2:P:816:DG:H2"   | 2:P:817:MRG:O5'  | 2.20         | 0.42        |  |
| 3:A:18:GLY:H     | 3:A:56:TYR:HE2   | 1.66         | 0.42        |  |
| 3:A:221:HIS:CD2  | 3:A:221:HIS:H    | 2.38         | 0.42        |  |
| 3:A:410:TRP:HB3  | 4:B:365:VAL:HG23 | 2.00         | 0.42        |  |
| 4:B:97:PRO:O     | 4:B:98:ALA:C     | 2.56         | 0.42        |  |
| 4:B:124:PHE:O    | 4:B:124:PHE:CD1  | 2.72         | 0.42        |  |
| 6:H:145:MET:SD   | 6:H:194:PRO:HG3  | 2.60         | 0.42        |  |
| 3:A:115:TYR:C    | 3:A:117:SER:N    | 2.71         | 0.42        |  |
| 3:A:363:ASN:OD1  | 3:A:365:VAL:HG23 | 2.20         | 0.42        |  |
| 3:A:439:THR:OG1  | 3:A:441:TYR:HE1  | 2.03         | 0.42        |  |
| 3:A:494:ASN:N    | 3:A:494:ASN:HD22 | 2.16         | 0.42        |  |
| 4:B:9:PRO:HA     | 4:B:121:ASP:OD2  | 2.20         | 0.42        |  |
| 4:B:88:TRP:CG    | 4:B:154:LYS:HB3  | 2.53         | 0.42        |  |
| 4:B:96:HIS:HA    | 4:B:97:PRO:HD3   | 1.74         | 0.42        |  |
| 5:L:38:GLN:NE2   | 6:H:41:GLN:NE2   | 2.58         | 0.42        |  |
| 3:A:417:VAL:O    | 3:A:417:VAL:CG1  | 2.67         | 0.42        |  |
| 3:A:444:GLY:HA2  | 3:A:552:VAL:HG11 | 2.02         | 0.42        |  |
| 3:A:494:ASN:HB3  | 4:B:289:LEU:HD11 | 2.01         | 0.42        |  |
| 3:A:517:LEU:O    | 3:A:521:ILE:HG13 | 2.20         | 0.42        |  |
| 4:B:75:VAL:CG1   | 4:B:77:PHE:CE2   | 3.03         | 0.42        |  |
| 4:B:156:SER:C    | 4:B:158:ALA:N    | 2.73         | 0.42        |  |
| 4:B:266:TRP:CE3  | 4:B:423:VAL:HG23 | 2.55         | 0.42        |  |
| 5:L:58:VAL:HA    | 5:L:59:PRO:HD3   | 1.92         | 0.42        |  |
| 5:L:142:LYS:H    | 5:L:142:LYS:HG2  | 1.45         | 0.42        |  |
| 6:H:102:ILE:HG12 | 6:H:108:SER:CB   | 2.49         | 0.42        |  |
| 1:T:718:DA:C2    | 2:P:811:DG:C2    | 3.08         | 0.42        |  |
| 3:A:194:GLU:C    | 3:A:196:GLY:H    | 2.23         | 0.42        |  |
| 3:A:235:HIS:HB2  | 3:A:238:LYS:O    | 2.19         | 0.42        |  |
| 3:A:273:GLY:O    | 3:A:274:ILE:HD13 | 2.20         | 0.42        |  |
| 3:A:439:THR:HA   | 3:A:494:ASN:HB2  | 2.02         | 0.42        |  |
| 4:B:202:ILE:O    | 4:B:204:GLU:N    | 2.53         | 0.42        |  |



| Interatomic Clash |                  |              |             |  |
|-------------------|------------------|--------------|-------------|--|
| Atom-1            | Atom-2           | distance (Å) | overlap (Å) |  |
| 4:B:305:GLU:OE1   | 4:B:309:ILE:HD11 | 2.19         | 0.42        |  |
| 4:B:314:VAL:CG1   | 4:B:315:HIS:N    | 2.83         | 0.42        |  |
| 4:B:407:GLN:CA    | 4:B:407:GLN:HE21 | 2.32         | 0.42        |  |
| 5:L:105:GLU:O     | 5:L:106:ILE:HG13 | 2.20         | 0.42        |  |
| 6:H:61:TYR:OH     | 6:H:71:VAL:N     | 2.53         | 0.42        |  |
| 6:H:155:TYR:CE1   | 6:H:160:VAL:HG13 | 2.55         | 0.42        |  |
| 3:A:215:THR:C     | 3:A:217:PRO:HD3  | 2.39         | 0.41        |  |
| 3:A:334:GLN:HG2   | 3:A:512:LYS:NZ   | 2.35         | 0.41        |  |
| 4:B:87:PHE:CE2    | 4:B:155:GLY:HA2  | 2.53         | 0.41        |  |
| 4:B:132:ILE:HA    | 4:B:133:PRO:HD3  | 1.77         | 0.41        |  |
| 4:B:146:TYR:CD2   | 4:B:150:PRO:HB3  | 2.54         | 0.41        |  |
| 5:L:26:SER:O      | 5:L:27:GLN:HB3   | 2.20         | 0.41        |  |
| 5:L:83:ILE:H      | 5:L:83:ILE:HG12  | 1.71         | 0.41        |  |
| 5:L:115:VAL:HG12  | 5:L:116:SER:N    | 2.34         | 0.41        |  |
| 3:A:222:GLN:O     | 3:A:223:LYS:C    | 2.58         | 0.41        |  |
| 3:A:222:GLN:C     | 3:A:223:LYS:HG3  | 2.40         | 0.41        |  |
| 3:A:363:ASN:O     | 3:A:367:GLN:HG3  | 2.20         | 0.41        |  |
| 3:A:439:THR:HG21  | 4:B:289:LEU:HG   | 2.02         | 0.41        |  |
| 4:B:271:TYR:CD2   | 4:B:271:TYR:N    | 2.88         | 0.41        |  |
| 4:B:325:LEU:HB3   | 4:B:387:PRO:HA   | 2.02         | 0.41        |  |
| 4:B:360:ALA:HB1   | 4:B:367:GLN:HG2  | 2.02         | 0.41        |  |
| 5:L:34:ASN:HD22   | 5:L:89:GLN:HE22  | 1.66         | 0.41        |  |
| 6:H:10:GLY:HA2    | 6:H:118:SER:O    | 2.20         | 0.41        |  |
| 3:A:242:GLN:HA    | 3:A:243:PRO:HD2  | 1.78         | 0.41        |  |
| 3:A:441:TYR:CD2   | 3:A:544:GLY:C    | 2.94         | 0.41        |  |
| 3:A:507:GLN:C     | 3:A:509:GLN:H    | 2.22         | 0.41        |  |
| 3:A:516:GLU:O     | 3:A:517:LEU:C    | 2.59         | 0.41        |  |
| 4:B:194:GLU:OE2   | 4:B:195:ILE:HG22 | 2.20         | 0.41        |  |
| 4:B:389:PHE:HB3   | 4:B:391:LEU:CD2  | 2.50         | 0.41        |  |
| 6:H:56:ASP:O      | 6:H:57:ASP:HB2   | 2.21         | 0.41        |  |
| 6:H:150:CYS:HB2   | 6:H:164:TRP:CH2  | 2.55         | 0.41        |  |
| 6:H:150:CYS:HB2   | 6:H:164:TRP:CZ2  | 2.56         | 0.41        |  |
| 3:A:124:PHE:CD1   | 3:A:127:TYR:HD2  | 2.38         | 0.41        |  |
| 3:A:143:ARG:NH1   | 3:A:143:ARG:CG   | 2.82         | 0.41        |  |
| 3:A:516:GLU:HA    | 3:A:519:ASN:HB2  | 2.03         | 0.41        |  |
| 4:B:200:THR:O     | 4:B:201:LYS:C    | 2.58         | 0.41        |  |
| 4:B:283:LEU:HA    | 4:B:287:LYS:HE2  | 2.03         | 0.41        |  |
| 6:H:19:ARG:HH11   | 6:H:83:ASN:HD21  | 1.68         | 0.41        |  |
| 6:H:24:PHE:CE1    | 6:H:78:ASN:HB3   | 2.56         | 0.41        |  |
| 6:H:34:ILE:HD12   | 6:H:34:ILE:N     | 2.32         | 0.41        |  |
| 3:A:105:SER:HB2   | 3:A:198:HIS:ND1  | 2.35         | 0.41        |  |



|                  | A de la construction de la const | Interatomic  | Clash       |
|------------------|--|--------------|-------------|
| Atom-1           | Atom-2   | distance (Å) | overlap (Å) |
| 3:A:229:TRP:CE2  | 3:A:230:MET:HG2  | 2.56         | 0.41        |
| 3:A:276:VAL:O    | 3:A:276:VAL:HG12   | 2.20         | 0.41        |
| 4:B:106:VAL:HA   | 4:B:189:VAL:O  | 2.21         | 0.41        |
| 4:B:325:LEU:HD12 | 4:B:325:LEU:HA   | 1.85         | 0.41        |
| 4:B:391:LEU:HA   | 4:B:392:PRO:HD2  | 1.97         | 0.41        |
| 5:L:27:GLN:O     | 5:L:29:ILE:HG23  | 2.21         | 0.41        |
| 5:L:77:ASN:H     | 5:L:77:ASN:ND2   | 2.18         | 0.41        |
| 6:H:24:PHE:CD1   | 6:H:78:ASN:HB3   | 2.55         | 0.41        |
| 6:H:59:ASN:N     | 6:H:59:ASN:ND2   | 2.69         | 0.41        |
| 3:A:3:SER:HA     | 3:A:4:PRO:HD3  | 1.70         | 0.41        |
| 3:A:261:VAL:HG23 | 3:A:276:VAL:HG11   | 2.03         | 0.41        |
| 3:A:296:THR:HG22 | 3:A:297:GLU:N  | 2.34         | 0.41        |
| 3:A:442:VAL:CG2  | 3:A:495:ILE:CG2  | 2.98         | 0.41        |
| 6:H:54:TRP:HB3   | 6:H:55:TRP:CZ3   | 2.56         | 0.41        |
| 3:A:5:ILE:HD13   | 3:A:167:ILE:HD11   | 2.03         | 0.41        |
| 3:A:38:CYS:O     | 3:A:39:THR:C   | 2.59         | 0.41        |
| 3:A:171:PHE:O    | 3:A:175:ASN:ND2  | 2.42         | 0.41        |
| 3:A:368:LEU:O    | 3:A:369:THR:C  | 2.58         | 0.41        |
| 3:A:410:TRP:CE2  | 4:B:363:ASN:OD1  | 2.73         | 0.41        |
| 4:B:112:GLY:C    | 4:B:151:GLN:HE21   | 2.24         | 0.41        |
| 4:B:304:ALA:HA   | 4:B:307:ARG:HG2  | 2.02         | 0.41        |
| 4:B:319:TYR:CZ   | 4:B:321:PRO:HA   | 2.55         | 0.41        |
| 4:B:372:VAL:HG13 | 4:B:389:PHE:CD2  | 2.56         | 0.41        |
| 3:A:385:LYS:HB2  | 3:A:385:LYS:NZ   | 2.36         | 0.41        |
| 4:B:295:LEU:HD23 | 4:B:299:ALA:HB3  | 2.02         | 0.41        |
| 5:L:120:PRO:HG2  | 5:L:130:ALA:HB1  | 2.03         | 0.41        |
| 6:H:37:THR:OG1   | 6:H:100:SER:HB2  | 2.19         | 0.41        |
| 6:H:220:ILE:HD12 | 6:H:220:ILE:HG23   | 1.89         | 0.41        |
| 1:T:707:DG:C2'   | 1:T:708:DG:C5'   | 2.99         | 0.41        |
| 2:P:817:MRG:S24  | 3:A:283:LEU:HD13   | 2.60         | 0.41        |
| 3:A:31:ILE:C     | 3:A:33:ALA:N   | 2.73         | 0.41        |
| 3:A:302:GLU:O    | 3:A:303:LEU:C  | 2.58         | 0.41        |
| 3:A:317:VAL:CG1  | 3:A:349:LEU:HD23   | 2.51         | 0.41        |
| 3:A:472:THR:CG2  | 3:A:477:THR:HG22   | 2.51         | 0.41        |
| 4:B:54:ASN:ND2   | 4:B:126:LYS:HB2  | 2.36         | 0.41        |
| 4:B:142:ILE:HG22 | 4:B:144:TYR:CE2  | 2.55         | 0.41        |
| 4:B:183:TYR:CD2  | 4:B:380:ILE:HD13   | 2.55         | 0.41        |
| 4:B:330:GLN:NE2  | 4:B:340:GLN:NE2  | 2.59         | 0.41        |
| 5:L:115:VAL:CG1  | 5:L:116:SER:N  | 2.84         | 0.41        |
| 5:L:151:ASP:CA   | 5:L:191:SER:HB3  | 2.48         | 0.41        |
| 3:A:171:PHE:CZ   | 3:A:205:LEU:HD12   | 2.55         | 0.41        |



| A 4 1            | A + 0            | Interatomic             | Clash       |
|------------------|------------------|-------------------------|-------------|
| Atom-1           | Atom-2           | distance $(\text{\AA})$ | overlap (Å) |
| 3:A:220:LYS:HB2  | 3:A:220:LYS:HE3  | 1.76                    | 0.41        |
| 4:B:91:GLN:HG3   | 4:B:92:LEU:HG    | 2.03                    | 0.41        |
| 4:B:156:SER:O    | 4:B:157:PRO:C    | 2.58                    | 0.41        |
| 5:L:50:TYR:O     | 5:L:52:SER:N     | 2.53                    | 0.41        |
| 5:L:55:HIS:CD2   | 5:L:56:SER:N     | 2.89                    | 0.41        |
| 6:H:39:ILE:CG2   | 6:H:40:ARG:N     | 2.84                    | 0.41        |
| 3:A:220:LYS:HE2  | 3:A:222:GLN:HB3  | 2.02                    | 0.40        |
| 3:A:385:LYS:HG2  | 3:A:386:THR:N    | 2.36                    | 0.40        |
| 3:A:393:ILE:HG23 | 3:A:393:ILE:O    | 2.21                    | 0.40        |
| 4:B:47:ILE:HD11  | 4:B:146:TYR:CD1  | 2.56                    | 0.40        |
| 6:H:155:TYR:HD2  | 6:H:155:TYR:H    | 1.67                    | 0.40        |
| 3:A:167:ILE:O    | 3:A:170:PRO:HD2  | 2.21                    | 0.40        |
| 3:A:246:LEU:HD12 | 3:A:307:ARG:NE   | 2.36                    | 0.40        |
| 3:A:412:PRO:O    | 3:A:413:GLU:C    | 2.59                    | 0.40        |
| 3:A:503:LEU:HD12 | 3:A:503:LEU:O    | 2.21                    | 0.40        |
| 4:B:301:LEU:O    | 4:B:305:GLU:HB2  | 2.21                    | 0.40        |
| 4:B:28:GLU:O     | 4:B:29:GLU:C     | 2.59                    | 0.40        |
| 4:B:118:VAL:H    | 4:B:148:VAL:HG23 | 1.86                    | 0.40        |
| 4:B:153:TRP:O    | 4:B:155:GLY:N    | 2.54                    | 0.40        |
| 5:L:140:TYR:CE2  | 5:L:141:PRO:HG3  | 2.56                    | 0.40        |
| 3:A:171:PHE:CE2  | 3:A:205:LEU:HD12 | 2.57                    | 0.40        |
| 3:A:194:GLU:C    | 3:A:196:GLY:N    | 2.75                    | 0.40        |
| 3:A:459:THR:CG2  | 3:A:463:ARG:CB   | 2.91                    | 0.40        |
| 4:B:47:ILE:CG2   | 4:B:144:TYR:CD1  | 3.04                    | 0.40        |
| 4:B:54:ASN:HA    | 4:B:55:PRO:HD2   | 1.94                    | 0.40        |
| 4:B:225:PRO:HG2  | 5:L:92:SER:CA    | 2.48                    | 0.40        |
| 4:B:266:TRP:CE3  | 4:B:423:VAL:CG2  | 3.04                    | 0.40        |
| 5:L:83:ILE:HG21  | 5:L:106:ILE:CD1  | 2.51                    | 0.40        |
| 3:A:278:GLN:H    | 3:A:278:GLN:HG2  | 1.48                    | 0.40        |
| 4:B:195:ILE:CG2  | 4:B:196:GLY:H    | 2.34                    | 0.40        |

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

| Atom-1        | Atom-2               | Interatomic<br>distance (Å) | Clash<br>overlap (Å) |
|---------------|----------------------|-----------------------------|----------------------|
| 4:B:2:ILE:CD1 | 4:B:2:ILE:CD1[6_565] | 1.62                        | 0.58                 |



### 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 | Per | centiles | $\mathbf{s}$ |
|-----|-------|-----------------|------------|-----------|----------|-----|----------|--------------|
| 3   | А     | 556/558~(100%)  | 424 (76%)  | 102 (18%) | 30 (5%)  | 2   | 12       |              |
| 4   | В     | 427/430~(99%)   | 317 (74%)  | 77 (18%)  | 33~(8%)  |     | 1 5      |              |
| 5   | L     | 209/211~(99%)   | 165 (79%)  | 32 (15%)  | 12 (6%)  | 1   | 10       |              |
| 6   | Н     | 223/225~(99%)   | 191 (86%)  | 21 (9%)   | 11 (5%)  | 2   | 14       |              |
| All | All   | 1415/1424~(99%) | 1097 (78%) | 232 (16%) | 86 (6%)  |     | 1 9      |              |

All (86) Ramachandran outliers are listed below:

| Mol | Chain | $\mathbf{Res}$ | Type |
|-----|-------|----------------|------|
| 3   | А     | 137            | ASN  |
| 3   | А     | 139            | THR  |
| 3   | А     | 249            | LYS  |
| 3   | А     | 254            | VAL  |
| 3   | А     | 273            | GLY  |
| 3   | А     | 393            | ILE  |
| 3   | А     | 485            | ALA  |
| 4   | В     | 2              | ILE  |
| 4   | В     | 87             | PHE  |
| 4   | В     | 225            | PRO  |
| 4   | В     | 247            | PRO  |
| 4   | В     | 286            | THR  |
| 4   | В     | 315            | HIS  |
| 4   | В     | 404            | GLU  |
| 5   | L     | 51             | THR  |
| 5   | L     | 76             | SER  |
| 6   | Н     | 32             | SER  |
| 6   | Н     | 105            | VAL  |
| 6   | Н     | 141            | GLN  |
| 6   | Н     | 143            | ASN  |
| 3   | А     | 22             | LYS  |
| 3   | А     | 116            | PHE  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | А     | 195 | ILE  |
| 3   | А     | 278 | GLN  |
| 3   | А     | 287 | LYS  |
| 3   | А     | 490 | GLY  |
| 3   | А     | 543 | GLY  |
| 3   | А     | 544 | GLY  |
| 4   | В     | 114 | ALA  |
| 4   | В     | 116 | PHE  |
| 4   | В     | 154 | LYS  |
| 4   | В     | 270 | ILE  |
| 4   | В     | 300 | GLU  |
| 4   | В     | 314 | VAL  |
| 4   | В     | 332 | GLN  |
| 4   | В     | 361 | HIS  |
| 4   | В     | 424 | LYS  |
| 5   | L     | 83  | ILE  |
| 6   | Н     | 34  | ILE  |
| 6   | Н     | 66  | LYS  |
| 3   | А     | 243 | PRO  |
| 3   | А     | 321 | PRO  |
| 3   | А     | 345 | PRO  |
| 3   | А     | 505 | ILE  |
| 4   | В     | 355 | ALA  |
| 4   | В     | 421 | PRO  |
| 4   | В     | 425 | LEU  |
| 5   | L     | 28  | ASP  |
| 5   | L     | 61  | ARG  |
| 5   | L     | 171 | SER  |
| 5   | L     | 199 | LYS  |
| 3   | Α     | 53  | GLU  |
| 3   | А     | 141 | GLY  |
| 3   | A     | 302 | GLU  |
| 3   | А     | 484 | LEU  |
| 3   | A     | 547 | GLN  |
| 3   | А     | 549 | ASP  |
| 4   | В     | 201 | LYS  |
| 4   | В     | 203 | GLU  |
| 4   | В     | 227 | PHE  |
| 4   | В     | 238 | LYS  |
| 5   | L     | 152 | GLY  |
| 6   | Н     | 126 | THR  |
| 3   | А     | 133 | PRO  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | А     | 466 | VAL  |
| 4   | В     | 44  | GLU  |
| 4   | В     | 200 | THR  |
| 4   | В     | 211 | ARG  |
| 4   | В     | 212 | TRP  |
| 4   | В     | 217 | PRO  |
| 4   | В     | 290 | THR  |
| 4   | В     | 292 | VAL  |
| 4   | В     | 427 | TYR  |
| 5   | L     | 82  | ASP  |
| 6   | Н     | 210 | PRO  |
| 3   | А     | 380 | ILE  |
| 4   | В     | 324 | ASP  |
| 5   | L     | 25  | ALA  |
| 6   | Н     | 9   | PRO  |
| 6   | Н     | 10  | GLY  |
| 5   | L     | 68  | GLY  |
| 6   | Н     | 17  | PRO  |
| 4   | В     | 167 | ILE  |
| 3   | A     | 261 | VAL  |
| 3   | A     | 272 | PRO  |
| 5   | L     | 99  | GLY  |

#### 5.3.2 Protein sidechains (i)

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  | Perc | entiles |
|-----|-------|-----------------|------------|-----------|------|---------|
| 3   | А     | 485/498~(97%)   | 414 (85%)  | 71 (15%)  | 3    | 13      |
| 4   | В     | 388/392~(99%)   | 324 (84%)  | 64 (16%)  | 2    | 10      |
| 5   | L     | 190/190~(100%)  | 168~(88%)  | 22 (12%)  | 5    | 22      |
| 6   | Н     | 196/196~(100%)  | 169~(86%)  | 27 (14%)  | 3    | 16      |
| All | All   | 1259/1276~(99%) | 1075 (85%) | 184 (15%) | 3    | 13      |

All (184) residues with a non-rotameric sidechain are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | А     | 22  | LYS  |
| 3   | А     | 24  | TRP  |
| 3   | А     | 55  | PRO  |
| 3   | А     | 61  | PHE  |
| 3   | А     | 67  | ASP  |
| 3   | А     | 80  | LEU  |
| 3   | А     | 83  | ARG  |
| 3   | А     | 85  | GLN  |
| 3   | А     | 86  | ASP  |
| 3   | А     | 94  | ILE  |
| 3   | А     | 105 | SER  |
| 3   | А     | 132 | ILE  |
| 3   | А     | 145 | GLN  |
| 3   | A     | 162 | SER  |
| 3   | А     | 175 | ASN  |
| 3   | A     | 177 | ASP  |
| 3   | А     | 180 | ILE  |
| 3   | А     | 186 | ASP  |
| 3   | А     | 188 | TYR  |
| 3   | А     | 205 | LEU  |
| 3   | А     | 215 | THR  |
| 3   | А     | 219 | LYS  |
| 3   | A     | 220 | LYS  |
| 3   | А     | 221 | HIS  |
| 3   | А     | 223 | LYS  |
| 3   | А     | 232 | TYR  |
| 3   | A     | 240 | THR  |
| 3   | A     | 245 | VAL  |
| 3   | А     | 246 | LEU  |
| 3   | А     | 250 | ASP  |
| 3   | A     | 268 | SER  |
| 3   | А     | 278 | GLN  |
| 3   | A     | 279 | LEU  |
| 3   | А     | 283 | LEU  |
| 3   | A     | 286 | THR  |
| 3   | A     | 290 | THR  |
| 3   | A     | 300 | GLU  |
| 3   | A     | 325 | LEU  |
| 3   | A     | 344 | GLU  |
| 3   | A     | 353 | LYS  |
| 3   | А     | 354 | TYR  |
| 3   | A     | 365 | VAL  |
| 3   | А     | 369 | THR  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | А     | 373 | GLN  |
| 3   | А     | 374 | LYS  |
| 3   | А     | 397 | THR  |
| 3   | А     | 405 | TYR  |
| 3   | А     | 407 | GLN  |
| 3   | А     | 409 | THR  |
| 3   | А     | 415 | GLU  |
| 3   | А     | 416 | PHE  |
| 3   | А     | 419 | THR  |
| 3   | А     | 425 | LEU  |
| 3   | А     | 442 | VAL  |
| 3   | А     | 451 | LYS  |
| 3   | А     | 464 | GLN  |
| 3   | А     | 465 | LYS  |
| 3   | А     | 468 | PRO  |
| 3   | А     | 469 | LEU  |
| 3   | А     | 472 | THR  |
| 3   | А     | 478 | GLU  |
| 3   | А     | 488 | ASP  |
| 3   | А     | 497 | THR  |
| 3   | А     | 500 | GLN  |
| 3   | А     | 501 | TYR  |
| 3   | А     | 511 | ASP  |
| 3   | А     | 519 | ASN  |
| 3   | А     | 525 | LEU  |
| 3   | А     | 545 | ASN  |
| 3   | А     | 547 | GLN  |
| 3   | А     | 548 | VAL  |
| 4   | В     | 5   | ILE  |
| 4   | В     | 12  | LEU  |
| 4   | В     | 27  | THR  |
| 4   | B     | 35  | VAL  |
| 4   | В     | 37  | ILE  |
| 4   | В     | 38  | CYS  |
| 4   | В     | 42  | GLU  |
| 4   | В     | 47  | ILE  |
| 4   | В     | 91  | GLN  |
| 4   | В     | 92  | LEU  |
| 4   | В     | 105 | SER  |
| 4   | В     | 109 | LEU  |
| 4   | В     | 113 | ASP  |
| 4   | В     | 143 | ARG  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | В     | 144 | TYR  |
| 4   | В     | 162 | SER  |
| 4   | В     | 163 | SER  |
| 4   | В     | 169 | GLU  |
| 4   | В     | 189 | VAL  |
| 4   | В     | 191 | SER  |
| 4   | В     | 193 | LEU  |
| 4   | В     | 197 | GLN  |
| 4   | В     | 199 | ARG  |
| 4   | В     | 206 | ARG  |
| 4   | В     | 212 | TRP  |
| 4   | В     | 216 | THR  |
| 4   | В     | 218 | ASP  |
| 4   | В     | 221 | HIS  |
| 4   | В     | 225 | PRO  |
| 4   | В     | 233 | GLU  |
| 4   | В     | 238 | LYS  |
| 4   | В     | 244 | ILE  |
| 4   | В     | 250 | ASP  |
| 4   | В     | 253 | THR  |
| 4   | В     | 271 | TYR  |
| 4   | В     | 276 | VAL  |
| 4   | В     | 277 | ARG  |
| 4   | В     | 282 | LEU  |
| 4   | В     | 284 | ARG  |
| 4   | В     | 286 | THR  |
| 4   | В     | 293 | ILE  |
| 4   | В     | 295 | LEU  |
| 4   | В     | 305 | GLU  |
| 4   | В     | 315 | HIS  |
| 4   | В     | 318 | TYR  |
| 4   | В     | 324 | ASP  |
| 4   | В     | 330 | GLN  |
| 4   | B     | 348 | ASN  |
| 4   | В     | 349 | LEU  |
| 4   | В     | 351 | THR  |
| 4   | В     | 353 | LYS  |
| 4   | В     | 357 | MET  |
| 4   | В     | 358 | ARG  |
| 4   | В     | 363 | ASN  |
| 4   | В     | 385 | LYS  |
| 4   | В     | 386 | THR  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | В     | 401 | TRP  |
| 4   | В     | 403 | THR  |
| 4   | В     | 407 | GLN  |
| 4   | В     | 409 | THR  |
| 4   | В     | 418 | ASN  |
| 4   | В     | 419 | THR  |
| 4   | В     | 424 | LYS  |
| 4   | В     | 427 | TYR  |
| 5   | L     | 7   | THR  |
| 5   | L     | 8   | THR  |
| 5   | L     | 10  | SER  |
| 5   | L     | 11  | LEU  |
| 5   | L     | 33  | LEU  |
| 5   | L     | 39  | LYS  |
| 5   | L     | 48  | ILE  |
| 5   | L     | 69  | THR  |
| 5   | L     | 77  | ASN  |
| 5   | L     | 89  | GLN  |
| 5   | L     | 97  | THR  |
| 5   | L     | 117 | ILE  |
| 5   | L     | 142 | LYS  |
| 5   | L     | 143 | ASP  |
| 5   | L     | 144 | ILE  |
| 5   | L     | 170 | ASP  |
| 5   | L     | 171 | SER  |
| 5   | L     | 173 | TYR  |
| 5   | L     | 190 | ASN  |
| 5   | L     | 197 | THR  |
| 5   | L     | 203 | SER  |
| 5   | L     | 211 | ARG  |
| 6   | Н     | 1   | GLN  |
| 6   | Н     | 4   | LEU  |
| 6   | Н     | 7   | SER  |
| 6   | Н     | 9   | PRO  |
| 6   | Н     | 23  | THR  |
| 6   | Н     | 29  | LEU  |
| 6   | Н     | 32  | SER  |
| 6   | Н     | 55  | TRP  |
| 6   | Н     | 72  | SER  |
| 6   | Н     | 88  | GLU  |
| 6   | Н     | 107 | ASP  |
| 6   | Н     | 111 | ASP  |



| Mol | Chain | $\mathbf{Res}$ | Type |
|-----|-------|----------------|------|
| 6   | Н     | 117            | THR  |
| 6   | Н     | 120            | THR  |
| 6   | Н     | 129            | PRO  |
| 6   | Н     | 155            | TYR  |
| 6   | Н     | 157            | PRO  |
| 6   | Н     | 160            | VAL  |
| 6   | Н     | 171            | SER  |
| 6   | Н     | 175            | THR  |
| 6   | Н     | 181            | GLN  |
| 6   | Н     | 187            | LEU  |
| 6   | Н     | 189            | SER  |
| 6   | Н     | 192            | THR  |
| 6   | Н     | 204            | THR  |
| 6   | Н     | 215            | LYS  |
| 6   | Н     | 218            | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | А     | 23  | GLN  |
| 3   | А     | 161 | GLN  |
| 3   | А     | 207 | GLN  |
| 3   | А     | 221 | HIS  |
| 3   | А     | 235 | HIS  |
| 3   | А     | 265 | ASN  |
| 3   | А     | 306 | ASN  |
| 3   | А     | 447 | ASN  |
| 3   | А     | 471 | ASN  |
| 3   | А     | 480 | GLN  |
| 3   | А     | 494 | ASN  |
| 3   | А     | 500 | GLN  |
| 3   | А     | 520 | GLN  |
| 3   | А     | 539 | HIS  |
| 4   | В     | 57  | ASN  |
| 4   | В     | 137 | ASN  |
| 4   | В     | 151 | GLN  |
| 4   | В     | 175 | ASN  |
| 4   | В     | 182 | GLN  |
| 4   | В     | 235 | HIS  |
| 4   | В     | 242 | GLN  |
| 4   | В     | 330 | GLN  |
| 4   | В     | 340 | GLN  |



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | В     | 363 | ASN  |
| 4   | В     | 394 | GLN  |
| 4   | В     | 418 | ASN  |
| 5   | L     | 38  | GLN  |
| 5   | L     | 77  | ASN  |
| 5   | L     | 89  | GLN  |
| 5   | L     | 90  | GLN  |
| 5   | L     | 137 | ASN  |
| 5   | L     | 138 | ASN  |
| 5   | L     | 166 | GLN  |
| 5   | L     | 190 | ASN  |
| 5   | L     | 210 | ASN  |
| 6   | Н     | 59  | ASN  |
| 6   | Н     | 62  | ASN  |
| 6   | Н     | 141 | GLN  |
| 6   | Н     | 174 | HIS  |
| 6   | Н     | 181 | GLN  |
| 6   | Н     | 206 | ASN  |
| 6   | Н     | 209 | HIS  |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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).

| Mal   | Type | Chain | Deg Link |        | Bo       | ond leng | ths     | E        | ond ang           | gles     |
|-------|------|-------|----------|--------|----------|----------|---------|----------|-------------------|----------|
| IVIOI | туре | Chain | nes      | S LINK | Counts   | RMSZ     | # Z >2  | Counts   | RMSZ              | # Z >2   |
| 2     | ATM  | Р     | 822      | 2,1    | 16,23,24 | 2.00     | 5 (31%) | 17,32,35 | 3.20              | 4 (23%)  |
| 2     | MRG  | Р     | 817      | 2,3,1  | 22,28,29 | 2.63     | 8 (36%) | 23,39,42 | <mark>3.29</mark> | 10 (43%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



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

| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 2   | ATM  | Р     | 822 | 2,1   | -       | 2/7/24/25 | 0/2/2/2 |
| 2   | MRG  | Р     | 817 | 2,3,1 | -       | 2/8/26/27 | 0/3/3/3 |

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | Р     | 817 | MRG  | C2-N2   | 7.12  | 1.45        | 1.34     |
| 2   | Р     | 817 | MRG  | C6-N1   | 5.48  | 1.42        | 1.33     |
| 2   | Р     | 817 | MRG  | C8-N7   | -4.92 | 1.25        | 1.34     |
| 2   | Р     | 822 | ATM  | N4'-N3' | 4.87  | 1.36        | 1.23     |
| 2   | Р     | 822 | ATM  | C1'-N1  | -3.72 | 1.38        | 1.49     |
| 2   | Р     | 817 | MRG  | C21-N2  | -3.21 | 1.39        | 1.45     |
| 2   | Р     | 817 | MRG  | C5-C4   | -2.78 | 1.33        | 1.40     |
| 2   | Р     | 822 | ATM  | C5A-C5  | 2.72  | 1.56        | 1.51     |
| 2   | Р     | 817 | MRG  | C4-N3   | -2.62 | 1.31        | 1.35     |
| 2   | Р     | 817 | MRG  | C2-N3   | -2.56 | 1.27        | 1.34     |
| 2   | Р     | 822 | ATM  | C4-N3   | 2.22  | 1.36        | 1.33     |
| 2   | Р     | 822 | ATM  | C6-C5   | 2.06  | 1.45        | 1.40     |
| 2   | Р     | 817 | MRG  | C2-N1   | 2.03  | 1.40        | 1.34     |

All (13) bond length outliers are listed below:

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-------------|-------|------------------|---------------|
| 2   | Р     | 822 | ATM  | C4-N3-C2    | 10.98 | 124.41           | 115.14        |
| 2   | Р     | 817 | MRG  | C5-C6-N1    | -9.57 | 110.34           | 123.43        |
| 2   | Р     | 817 | MRG  | C22-C23-S24 | 7.18  | 136.04           | 112.96        |
| 2   | Р     | 817 | MRG  | C23-C22-C21 | -4.89 | 96.94            | 112.65        |
| 2   | Р     | 822 | ATM  | C3'-C2'-C1' | 4.64  | 108.22           | 103.25        |
| 2   | Р     | 817 | MRG  | C6-N1-C2    | 4.24  | 122.77           | 115.18        |
| 2   | Р     | 817 | MRG  | C2-N3-C4    | -3.96 | 110.78           | 115.28        |
| 2   | Р     | 822 | ATM  | C5A-C5-C4   | 3.93  | 128.41           | 121.37        |
| 2   | Р     | 817 | MRG  | C6-C5-C4    | -3.31 | 117.64           | 120.80        |
| 2   | Р     | 817 | MRG  | C2'-C1'-N9  | 2.58  | 120.22           | 114.27        |
| 2   | Р     | 817 | MRG  | C2'-C3'-C4' | -2.49 | 97.58            | 102.76        |
| 2   | Р     | 822 | ATM  | O4'-C4'-C5' | 2.41  | 117.30           | 109.37        |
| 2   | Р     | 817 | MRG  | O4'-C4'-C3' | 2.17  | 110.73           | 105.67        |
| 2   | Р     | 817 | MRG  | C3'-C2'-C1' | 2.16  | 107.96           | 102.54        |

There are no chirality outliers.



| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | Р     | 822 | ATM  | C4'-C3'-N3'-N4' |
| 2   | Р     | 822 | ATM  | C3'-N3'-N4'-N5' |
| 2   | Р     | 817 | MRG  | C21-C22-C23-S24 |
| 2   | Р     | 817 | MRG  | C3'-C4'-C5'-O5' |

All (4) torsion outliers are listed below:

There are no ring outliers.

1 monomer is involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | Р     | 817 | MRG  | 9       | 0            |

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.7 Other polymers (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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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        | $\langle RSRZ \rangle$ | #RSRZ>2       | $OWAB(Å^2)$      | Q < 0.9 |
|-----|-------|-----------------|------------------------|---------------|------------------|---------|
| 1   | Т     | 21/27~(77%)     | 0.14                   | 0 100 100     | 64, 84, 98, 107  | 0       |
| 2   | Р     | 18/21~(85%)     | 0.01                   | 0 100 100     | 75, 83, 100, 103 | 0       |
| 3   | А     | 556/558~(99%)   | -0.13                  | 11 (1%) 65 44 | 44, 91, 110, 110 | 1 (0%)  |
| 4   | В     | 428/430~(99%)   | -0.14                  | 5 (1%) 79 61  | 35, 80, 110, 110 | 2 (0%)  |
| 5   | L     | 211/211 (100%)  | -0.11                  | 0 100 100     | 56, 88, 110, 110 | 0       |
| 6   | Н     | 225/225~(100%)  | -0.24                  | 4 (1%) 68 47  | 51, 78, 105, 110 | 0       |
| All | All   | 1459/1472~(99%) | -0.14                  | 20 (1%) 75 56 | 35, 85, 110, 110 | 3~(0%)  |

All (20) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 6   | Н     | 141 | GLN  | 5.1  |
| 3   | А     | 67  | ASP  | 4.3  |
| 4   | В     | 315 | HIS  | 3.7  |
| 3   | А     | 448 | ARG  | 3.6  |
| 3   | А     | 64  | LYS  | 3.6  |
| 6   | Н     | 138 | SER  | 3.3  |
| 4   | В     | 90  | VAL  | 3.1  |
| 3   | А     | 223 | LYS  | 2.6  |
| 3   | А     | 258 | CYS  | 2.6  |
| 6   | Н     | 142 | THR  | 2.5  |
| 6   | Н     | 222 | PRO  | 2.5  |
| 3   | А     | 66  | LYS  | 2.4  |
| 4   | В     | 426 | TRP  | 2.4  |
| 3   | А     | 283 | LEU  | 2.3  |
| 3   | А     | 286 | THR  | 2.3  |
| 4   | В     | 312 | GLU  | 2.3  |
| 3   | А     | 2   | ILE  | 2.2  |
| 3   | А     | 297 | GLU  | 2.2  |
| 3   | А     | 71  | TRP  | 2.1  |



| Mol | Chain | $\operatorname{Res}$ | Type | RSRZ |
|-----|-------|----------------------|------|------|
| 4   | В     | 274                  | ILE  | 2.0  |

### 6.2 Non-standard residues in protein, DNA, RNA chains (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,  $95^{th}$  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  | $\mathbf{B}	ext{-factors}(\mathrm{\AA}^2)$ | Q<0.9 |
|-----|------|-------|-----|-------|------|------|--|-------|
| 2   | MRG  | Р     | 817 | 26/27 | 0.87 | 0.20 | 92,92,92,92                                | 0     |
| 2   | ATM  | Р     | 822 | 22/23 | 0.92 | 0.20 | 62,68,87,87                                | 0     |

### 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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  | $\mathbf{B}	ext{-factors}(\mathrm{\AA}^2)$ | Q<0.9 |
|-----|------|-------|------|-------|------|------|--|-------|
| 7   | MG   | А     | 1001 | 1/1   | 0.98 | 0.61 | 62,62,62,62                                | 0     |

### 6.5 Other polymers (i)

There are no such residues in this entry.

